13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Integrated Nonlinear Multi-scale Material Modelling of Composite Materials Using Digimat

Laurent ADAM*

*MSC Software Belgium S.A. (e-Xstream engineering)

ABSTRACT

The simulation of composites has to master several characteristics of these materials (anisotropic behavior following the local microstructure, nonlinear behaviors and various failure mechanisms, effects of residual stresses, strain rate and temperature dependences, etc) in order to deliver predictive results. Multi-scale methods relying on continuum models which enable to account for the material microstructure and constituents properties are becoming standards across the industry. Amongst these methods, mean-field and full-field homogenization methods are used for years in order to predict the nonlinear stiffness and strength of heterogeneous materials like composites. Such methods are commonly used to perform material engineering, virtual testing and also ICME. In order to be used in the industry, such methods have not only to reach a sufficient level of TRL but also be efficient, available in smooth and easy to use workflows, and cover various application cases, from simple stress analysis over the investigation of crash performance of composite part. The current presentation will show latest advances in combining mean and full-field homogenization methods in order to predict composite stiffness and strength. Different linking and coupling methods will also be shown in order to propagate material behaviors in between the different scales as well as from the process to the structural simulation. These different coupling methods allows to balance CPU time with the richness of the generated results. Material variabilities can also be studied numerically by using such simulation chain so that, for example, allowable (A/B basis) can be computed. The supporting technologies are developed in Digimat and will be exposed during the presentation. Representative applications will also be illustrated.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Robust Water Flooding Reservoir Management Based on Surrogate Models

SILVANA AFONSO*, Jefferson Wellano**, Ramiro Willmersdorf***

*Federal University of Pernambuco, **Federal University of Pernambuco, ***Federal University of Pernambuco

ABSTRACT

A big challenge in water flooding reservoir optimization is the reservoir spatial variability and the uncertainties at geological parameters. An approach to reduce the uncertainties impact on the solutions is named robust optimization. In this work it will be built an automatic tool for optimal robust management based on a diferent optimization formulation. This is in contrast with most of works reported in literature in which robust optimization is based on uniobjective problem formulation, combining in a unique weight function the expected function and standard deviation of the net present value (NPV). Here, robust optimization will be conduct from a given set of realizations. The NPV is calculated for each realization considering pre-defined rate controls. A small subset of realizations is select aiming time processing reduction for the statistics calculations. Two approaches of selecting a representative subset of realizations are done, one ranks the realizations according to the performance of each realization in terms of NPV (Net Present Value), the other is based on clustering the uncertain field, e.g. in terms of permeability field, using a K-means procedure. In order to reduce simulation costs due to several function calls required in the optimization process, data fitting based surrogate models are applied in the Sequential Approximated Optimization strategy. The optimization results based on the realizations subset is then applied to all existing realizations. It was found that the net present value evaluated at the robust optimization solution is almost independent of economical parameters such as produced oil costs, injected and produced water costs. This means that uncertainties found on NPV calculations are due geological parameters. Finally, the technical applicability of the proposed tool will be checked against a benchmark example reported in literature.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Reliability-based Maintenance Optimization Planning of Logistic Corridor Bridges by Using Time-variant Reliability Analysis and Kriging Metamodeling

Younes AOUES*, Arnaud KNIPPEL**, Eduardo SOUZA DE CURSI***

*Normandie Univ, INSA Rouen Normandie, LMN, 76000 Rouen, France, **Normandie Univ, INSA Rouen Normandie, LMI, 76000 Rouen, France, ***Normandie Univ, INSA Rouen Normandie, LMN, 76000 Rouen, France

ABSTRACT

Logistic corridors fluidity depends on the reliability of infrastructure transportations. Highway bridges are considered the most critical and vital links in any transportation network, where a full or partial failure of these infrastructures leads to decrease the operational efficiency of the network and can provoke serious economic impacts. These infrastructures undergo various degradation (decay, aging, corrosion, fatigue) due to the weather conditions, natural disaster, the increase in traffic of the last decades. In the current economic context, the prolongation of infrastructure lifetime is based on the maintenance and rehabilitation operations. However, the scheduling management of several infrastructures throughout the life cycle involves the search of the best compromise between conflicting objectives and requirements. This study presents an efficient approach integrating uncertainty in the decision making of the maintenance planning optimization. The optimal planning of the maintenance and inspection actions is the best solution that minimizes the total expected total cost of an infrastructure network while fulfilling reliability and functionality requirements over the lifetime. The total expected cost is composed from the maintenance costs and the failure cost due to failure consequences. This approach is based on quantitative evaluation of the structural performance in term of reliability and risk, where the reliability-based maintenance optimization approach aims to provide the optimal and robust solution of the maintenance plan, that are less sensitive for the various uncertainties affecting the system. Predictive degradation models have already been used to predict maintenance operations. However, a purely deterministic approach limits the quality of the provided solution. Thus, the rational approach is to use the probability theory to predict the future condition. Time-variant reliability analysis can be used for predicting the performance of infrastructure components, systems and networks. The time variant reliability analysis allows to capture the time-dependence of the probability of failure and the uncertainty of the deterioration process. However, for realistic situation, the time-variant reliability analysis is very time consuming because it requires several evaluations of the mechanical model describing the structural behavior. Thus, Kriging metamodeling aims to overcome this issue, where the mechanical model is replaced by a simple analytical function that is easy to evaluate. This paper presents an original approach of the reliability-based maintenance optimization in conjunction with time-variant reliability analysis and kriging metamodels for programming maintenance actions. The proposed approach is used to find the optimal maintenance planning of bridges in order to increase the fluidity of the logistic corridors of the Normandy region.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Establishment of Bounds for the Statistical Moments of the Crack Size Using the Fast Bounds Crack Method According to the Collipriest Model

CLAUDIO ROBERTO AVILA DA SILVA JÚNIOR*, LUCAS GIMENIS DE MOURA**

*PPGEM/UTFPR-CURITIBA, **PPGEM/UTFPR-CURITIBA

ABSTRACT

The existence of cracks in a realistic approach of structures and mechanical components is admitted. Their presence is generally associated with the phenomenon of fatigue. There are several mathematical models that describe the propagation of cracks. In general, crack propagation models are classified by the type of loading, which can be a loading with constant amplitudeof stress (CAS) or variable amplitude ofstress (VAS). For many engineering applications, up to a certain point, it is not necessary to have great accuracy in predictions about the behavior ofthe evolution of a crack, but a reliable prediction, within certain limits, of such behavior. This work presents theoretical results consistingin obtaining lower and upper bounds that "envelop" the first and second orderstatistical moment estimators of the crack size function based on the Fast Bounds Crack method. These bounds are polynomials defined in the variable “number of cycles” that consider the uncertainties of the parameters that describe the crack propagation models. The performance of the bounds for the statistical moments of the crack size is evaluated through the relative deviation between the bounds and the approximate numerical solutions of the initial value problems (IVP) that describe the crack evolution laws.For this work, the Collipriest modelwill be used. Quantification of these uncertainties will be done with aid of the Monte Carlo method. In general, the definition of the function "factor of correction of the stress intensity factor " makes it impossible to obtain the explicit determination of the function “crack size”. Thus, the IVP solution describing the Collipriest model can be obtained through the use of numerical methods, such as the explicit fourth-order Runge-Kutta method (RK4). The use of a computational environment makes it possible to evaluate the computational time of the proposed methodology and the deviations of the bounds from the approximate solutions, confirming the efficiency of the method.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Density-based Topology Optimization of Coated Structures Subject to Dynamic Loading

Niels Aage*, Malte Wollert Torp**, Frank Edberg Olsen***

*Technical University of Denmark, **Technical University of Denmark, ***Technical University of Denmark

ABSTRACT

Topology optimization and additive manufacturing forms a near perfect match, in which the design freedom from the material distribution methods complement the geometric freedom provided by 3D printing and vica versa. Therefore, many obvious directions for further extensions and research exists, with one of them being the design of optimized coating and infill patterns for light weight constructions as shown in e.g. [1,2]. The basic idea of the coating approach is to use the projected gradient of the density field to identify the coating region and to overlay this with the background density field to obtain a single-design field representation of interior, void and coating domains. The infill approach, on the other hand, consists of adding a local volume constraint to the interior domain through a second design variable field. The second design is filtered to ensure a prescribed level of design freedom and the locality is circumvented by a p-norm statement. Thus, one extra design field and one extra constraint is all that is needed compared to the standard minimum compliance problem. The novelty of the presented work consists of extending the above methodologies to cover dynamic loading and adding the possibility to have two distinct materials in the coating region; for example one with highly damping material properties (and a high cost) and one with standard material properties (and a low cost). Firstly, the dynamics are introduced as harmonic loading in the low frequency range. This, amongst others, means that full material utilization is no longer optimal for all problems. To alleviate this we introduce modifications to the interpolation functions and derive bounds on material property-ratios that ensures crisp material interfaces. Secondly, introducing the extra material in the coated region requires the addition of yet a design field as well as the development of new material interpolation functions. We show that this can be obtained by a total of ten filters/projections operations on a total of three globally defined design fields. The application of the proposed design methodology is demonstrated on a number of numerical examples in which different forms of dynamic compliance measures are minimized. [1] Clausen, A., Aage, N., & Sigmund, O. (2015). Topology optimization of coated structures and material interface problems. CMAME, 290, 524–541. [2] Wu, J., Aage, N., Westermann, U., & Sigmund, O. (2017). Infill Optimization for Additive Manufacturing –Approaching Bone-like Porous Structures. IEEE Trans. Vis. Comput. Graph 24(2), 1127–1140.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Planar 3D: A Scalable, Hybrid Parallel Simulator for Multiple Hydraulic Fractures

Safdar Abbas*, Aman Verma**, Anthony Peirce***

*Schlumberger, **Schlumberger, ***University of British Columbia

ABSTRACT

Planar 3D models have been developed as an alternative to both simplistic pseudo 3D models and full 3D models to better predict fracture propagation in a vertical plane with different vertical layer properties. One of these planar 3D models has been enhanced recently with the possibility to simulate the propagation of multiple simultaneous fractures. The referenced model is distinguished from other planar 3D approaches by the more accurate treatment of the fracture front crossing the layered interfaces by incorporating a multilayer elasticity equation (spectral-based displacement discontinuity), fluid flow (2D finite difference method with zero flux boundary conditions), leakoff, and fracture propagation (a consistent volume of fluid formulation accounting for rock toughness and different fracture propagation regimes) in one fully coupled robust and efficient scheme. The proppant transport model also accounts for proppant packing and bridging. In this enhancement of the planar 3D approach, the fracture communication and impact of the fractures on each other's growth are modeled through a wellbore communication algorithm and the stress shadow effect. The enhanced fidelity and capabilities of the simulator would normally incur a significant computational expense. However parallel programming paradigms are leveraged to drastically reduce the simulation runtime. This enables engineers to explore the vast decision space in reasonable time for optimal completion design. Note that domain decomposition in the context of DDM is very challenging without Fast Multipole Methods. Hence a multi-level, hybrid parallel framework is designed to provide greater throughput from an efficient single fracture simulator. Each fracture can be simulated using multiple CPU cores and GPU on a single node. This is implemented using vectorization (AVX), shared memory parallelization (TBB, OpenMP) and offloading to GPU (CUDA). This single fracture simulator is encapsulated in an MPI based wrapper which enables the entire simulation to run on multiple, distributed nodes. This hybrid parallel simulator is shown to exhibit good performance scaling with the number of fractures. It has been commercially deployed in the public cloud (Microsoft, Google) for several years now. The robustness and scalability of the model are demonstrated by application to field cases.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Moment-Guided Isogeometric Analysis for the Boltzmann Equation

Michael Abdelmalik*, Thomas Hughes**

*ICES University of Texas at Austin; Eindhoven University of Technology, **ICES University of Texas at Austin

ABSTRACT

Kinetic theory of fluids is concerned with a generalized phase-space description of molecular flow. In kinetic theory, the description of fluid dynamics is based on the Boltzmann equation that governs a one-molecule phase-space distribution which depends on velocity, space and time variables. Of particular significance is the account provided by the Boltzmann equation for fluid dynamics that do not conform to continuum models. The equation is of fundamental importance in a range of high-tech applications, such as semiconductor photolithography devices. However, the velocity-space-time phase-space description of the flow renders a high dimensional problem setting. Moreover, the domain of the velocity variable is unbounded. The computational cost of resolving such high dimensional problems with unbounded domains using traditional numerical methods is prohibitive. In this presentation we consider a novel numerical approximation technique for the Boltzmann equation, in which the velocity discretization is based on a global moment-system approximation [1] and a local isogeometric-based refinement. The moment method infers an approximate distribution function that is consistent with macroscopic observables. Generally, moment-based approximations provide a sharper estimate of the tails than of the main-mass of the distribution; see [2] for more details. We use the statistical information provided by the moment-based approximation to guide a localized refinement strategy based on isogeometric analysis. The b-spline bases associated with isogeometric analysis provides an ideal candidate to enrich the moment-system approximation locally for the generally noteworthy accuracy per-degree-of-freedom of isogeometric discretizations. Further efficiency opportunities are provided by efficient integration rules that can be devised for integrating such b-spline bases [3]. We establish that the proposed velocity discretization preserves the fundamental properties of the Boltzmann equation, namely entropy dissipation and conservation of mass, momentum and energy. Furthermore, we show that the proposed velocity discretization facilitates the use of traditional numerical methods, such as finite-elements, to discretize the space and time variables. Finally, we will conclude this presentation with some numerical results to illustrate the approximation properties of the proposed method. [1] Abdelmalik, M.R.A. and van Brummelen, E.H. Moment closure approximations of the Boltzmann equation based on ?-divergences. J. Stat. Phys., Vol. 164, pp. 77–104, (2016). [2] Brinks, R. On the convergence of derivatives of B-splines to derivatives of the Gaussian function Comput & Appl Math 27 (2008), pp. 79–92. [3] Calabro F., Sangalli G. and Tani, M. Fast formation of isogeometric Galerkin matrices by weighted quadrature. Comput. Methods in Appl. Mech. Eng., Vol. 316, pp. 606-622, (2017).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Origin-Destination Matrix Estimation with Incomplete Signal Dataset for Microscopic Traffic Simulation

Kazuki Abe*, Hideki Fujii**, Shinobu Yoshimura***

*The University of Tokyo, **The University of Tokyo, ***The University of Tokyo

ABSTRACT

Nowadays, multi-agent-based microscopic traffic simulators are useful for making decisions for solving traffic-related problems, e.g. traffic jams, evacuation planning, etc. Traffic demand is a sort of essential input data to use such simulators, which is described in the form of Origin-Destination (OD) matrix. Since the matrix cannot be observed directly, indirect estimation methods are indispensable. One of them is using link traffic volume, which is obtained by fixed-point observation. We have been proposing this type of OD estimation method using the traffic simulator, which estimates the input data for that simulator itself [1]. The proposed OD estimation method mainly consists of the following two processes: (1) a process of calculating estimated link traffic volume from the assumed OD matrix, and (2) a process of updating OD matrix with some constraints. In the process (1), a microscopic traffic simulator ADVENTURE_Mates [2] developed by the authors is used. In the process (2), a new OD matrix is obtained by solving a quadratic programming problem. In this process, the norm of residual between the simulated link traffic volume and observed one is minimized with the constraints of non-negative traffic volume in OD matrix satisfied. Until that norm satisfies a convergence criterion, the OD matrix is updated repeatedly. When microscopic traffic simulators are employed in the process (1), due to their precise resolution and route search algorithm, estimated results are easily affected from the congestion around intersections in the simulation. It sometimes causes unrealistic results. For instance, long waiting queues can be formed in a few links even if most of other links are vacant. To avoid this problem, we add a new feasible constraint to each link by comparing its traffic demand and the traffic capacity calculated from the light durations. Additionally, even if all of the signal datasets in the real world are not accessible, our proposed method provides the complemented ones simultaneously. Since the results of this completion and the OD estimation depend on each other, these methods are used alternately to solve the whole OD estimation problem. References: [1] K. Abe, H. Fujii and S. Yoshimura. Inverse Analysis of Origin-Destination Matrix for Microscopic Traffic Simulator. Computer Modeling in Engineering and Science. Vol. 113, No. 1, pp. 68-85, 2017. [2] H. Fujii, H. Uchida and S. Yoshimura. Agent-based Simulation Framework for Mixed Traffic of Cars, Pedestrians and Trams. Transportation Research Part C: Emerging Technologies, Vol. 85, pp. 234-248, 2017.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Adaptive Space-Time Discontinuous Galerkin Method for Unsteady Elliptic and Parabolic PDEs with First-Order Hyperbolic System Approach

Reza Abedi*, Alireza Mazaheri**, Robert Haber***

*University of Tennessee Space Institute, **NASA Langley Research Center, ***University of Illinois at Urbana-Champaign

ABSTRACT

We present a pseudo-time approach to relax elliptic and parabolic PDEs to hyperbolic equations. When an elliptic PDE is solved, the pseudo-time plays the role of physical time for a hyperbolic equation. However, for parabolic equation pseudo-time is added to the physical time and for each physical time advance the problem is solved in pseudo-time until it reaches steady state in pseudo-time. The relaxation times, target solutions for the hyperbolized discontinuous Galerkin method, and other aspects of the pseudo-time formulation are carefully chosen to optimize the convergence of the hyperbolized system to its steady state limit at each pseudo-time step [1]. In [1], this hyperbolic system is solved in pseudo-time using an implicit time marching scheme. Our main contribution will be to demonstrate, for the first time, an adaptive space-time discontinuous Galerkin for first-order system of hyperbolic equations. For this purpose, the spatial discretization is extruded in physical time to form implicit spacetime finite elements. We will also verify the order of accuracy of the solution and solution gradients for time-dependent problems. More specifically, we will demonstrate that the spatial order of accuracy of both solution and solution gradients is (k+1) for Pk polynomial. When an elliptic problem is hyperbolized by the pseudo-time approach, the resulting system can also be solved with other spacetime discontinuous Galerkin formulations such as [2]. Therein, adaptivity in spacetime [3] can expedite the convergence of solution in pseudo-time. Thus, quality, order of accuracy, and efficiency of the proposed approach will be compared with those presented in [2] and [3].
References: [1] Alireza Mazaheri and Hiroaki Nishikawa. Efficient high-order discontinuous Galerkin schemes with first-order hyperbolic advection-diffusion system approach. Journal of Computational Physics, 321:729-54, 2016. [2] R. Abedi, B. Petracovici, and R.B. Haber, “A spacetime discontinuous Galerkin method for linearized elastodynamics with element–wise momentum balance”, Computer Methods in Applied Mechanics and Engineering, 195:3247 – 3273, 2006. [3] R. Abedi, R. B. Haber, S. Thite, and J. Erickson. An h-adaptive spacetime discontinuous Galerkin method for linearized elastodynamics. European Journal of Computational Mechanics, 15(6):619-42, 2006.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Towards an Optimal Parameter Free Stabilisation for Systems of Nonlinear Conservation Laws: An Application of Neural Networks

Remi Abgrall*, Maria Han Veiga**, Karim Obrial***

*University of Zurich, **University of Zurich, ***University of Zurich

ABSTRACT

We are interested in a parameter free limiter for hyperbolic conservation laws. We want to identify cells which are in need of limiting by just using the local structure of the solution as the eye of a good engineer would optimally do. If successfull, we would put nonlinear stabilization only where really needed. Neural networks gained new popularity recently due to the computational tractability of back-propagation algorithm, used for the learning of weights and biases in a deep neural network, see [1] for example. Furthermore, it has been empirically shown to generate robust models for classification in many areas of application and theoretically, to generate universal classifiers and function approximators. Preliminary applications in the hyperbolic setting can also be found in [2]. In this work, we train a neural network using labelled data run on several CFD simulations, and the use this to flag the trouble cells. In detail, we show how to construct a training dataset, perform feature selection and how to integrate this model with different CFD codes. We show the performance of this trouble cell indicator for three numerical methods, the Residual Distribution and Discontinuous Galerkin methods (denoting the necessary changes to the inference model), for scalar and systems in one and two dimensions. We also apply the same philosophy on a standard second order scheme where the dissipation ranges from the Lax-Wendroff ones to the pure upwind one, extending the work of Kurganov et al. [3]. It is our belief that these ideas can be applied to other problems which depend on certain local properties of the numerical solution, such as scheme stabilisation through addition of artificial viscosity or scheme blending, ultimately contributing towards CFD codes which are robust to different initial conditions and that require less parameter tuning to produce readily usable results. References: [1] Alex Krizhevsky, Ilya Sutskever, and Geoffrey E. Hinton. Imagenet classification with deep convolutional neural networks. In Proceedings of the 25th International Conference on Neural Information Processing Systems - Volume 1, NIPS'12, pages 1097–1105, USA, 2012. Curran Associates Inc. [2]D. Ray and J. Hesthaven. An artificial neural network as trouble-cell indicator. Journal of Computational Physics, 2017. submitted. [3]Alexander Kurganov and Yu Liu. New adaptive artificial viscosity method for hyperbolic systems of conservation laws. J. Comput. Phys., 231(24):8114–8132, 2012.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Structural Behavior of Composite Thin Walled Structures-An Experimental and Numerical Overview

Haim Abramovich*

*Aerospace Engineering, Technion, I.I.T., Israel

ABSTRACT

Laminated composite thin walled structures or sandwich based structures are today one of the most effective ways of reducing weight and increasing performance of aircraft and space launchers. To be able to realize this target, it is necessary to develop the appropriate reliable tools, which are complemented and validated by a sound experimental data base to correctly and safely predict the behavior of a laminated composite stringer-stiffened shells in the " deep" postbuckling region and its collapse load, which is characterized by the probable following failure modes : separation between the skin and the stringers, delaminations, crack propagations and matrix failure, as well as to get better insight and understanding of the phenomena associated with its behavior under repeated buckling, particularly in the range of "deep" postbuckling loading. During its normal service life, a fuselage, which is composed of many curved laminated composite stringer-stiffened panels, may experience no more than a few hundreds of buckling postbuckling cycles. In parallel, to safely enable an economical use of sandwich type shells ?? a reliable launcher structure, the knock-down factor associated with the behavior of thin walled shells has to be investigated and understood. Since 2000, the author had been part of 4 extensive campaigns sponsored by the EU to investigate the above topics. It started with the POSICOSS (Improved POstbuckling SImulation for Design of Fibre COmposite Stiffened Fuselage Structures) program, followed by the COCOMAT (Improved MATerial Exploitation at Safe Design of COmposite Airframe Structures by Accurate Simulation of COllapse) and DAEDALOS (Dynamics in Aircraft Engineering Design and Analysis for Light Optimized Structures, and finalized with the DESICOS (New Robust DESign Guideline for Imperfection Sensitive COmposite Launcher Structures). Typical results from those programs will be highlighted, presenting effective ways of experimental and numerical investigations of stringer stiffened curved panels and sandwich shells and cones under compressive loading, with a focus on their buckling and postbuckling behavior. Emphasize will be made on various inherent characteristics of those structures, at buckling and beyond, like: skin-stringer separation, repeated buckling in the presence of prescribed delaminations, and deep postbuckling behavior. The effective width method adopted for laminated composite stringer stiffened panels, to calculate the collapse loads of the plates, will also be outlined and typical results will be presented.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Benchmark Numerical Solutions for Flows of Complex Fluids Governed by the Rolie-Poly Constitutive Model

Jade Abuga*, Dr. Tirivanhu Chinyoka**

*University of Cape Town, **University of Cape Town

ABSTRACT

Polymer melts are a group of fluids that are classified as complex fluids. The understanding of the flow and properties of such fluids is essential due to their great importance in industrial sectors such as those involving plastic and food processing. It is thus of fundamental importance to understand the flow and physical properties of these fluids via appropriate scientific modelling techniques. It is only recently that the different forms of constitutive equations have been developed to describe molten polymers with the most adept mathematical models being the tube-based models which are derived from the Doi-Edwards tube-based model [2] . Examples of such models include the pom-pom [3] and the Rolie-Poly [1] constitutive equations. This work presents a validation for the developed solver for viscoelastic fluid flow computations, with particular focus on the flow of fluids governed by the Rolie-Poly constitutive equation. The solver is based on the finite volume method and is built on the open source software, OpenFoam platform. The two well-known benchmark problems used for this validation for the new numerical method are the lid-driven cavity flow and the 4:1 planar contraction flow. Additionally, we implement and investigate the efficiency of numerical stabilization techniques, with particular reference to the Discrete Elastic Viscous Stress Splitting (DEVSS) and the log- Conformation stabilization techniques. Comparison is done between our numerical results, obtained using each of the two stabilization techniques, against data from existing literature. The numerical results obtained for the contraction flow using the log-conformation reformulation approach are in good agreement with the existing literature for a wider range of Deborah numbers. For the lid-driven cavity flow, good agreement is observed for low Deborah numbers using either of the two stabilization techniques. References 1. Alexei E. Likhtman and Richard S. Graham. Simple constitutive equation for linear polymer melts derived from molecular theory: Rolie-poly equation. Journal of Non-Newtonian Fluid Mechanics, 114:1–12, 2003. 2. M. Doi and S. F. Edwards. The theory of Polymer dynamics. Oxford University Press, New York, 1986. 3. T. C. B. McLeish and R. G. Larson. Molecular constitutive equations for a class of branched polymers: The pom-pom polymer. Journal of Rheology, 42(1):81, 1998.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

3D Method and Codes for Fluid Structure Interaction Problems in Euler Variables

Mustafa Abuziarov*

*reseach instituteof mechanics Nizhny novgorod satet university

ABSTRACT

3D method and codes for fluid structure interaction problems in Euler variables M.H. Abuziarov Research institute for mechanics of Nizhnii Novgorod state university, Russia. abouziar@mech.unn.ru The 3D codes based on the explicit numerical method for modeling shock wave and fluid structure interaction problems in Euler variables are presented. The method is based on the modified Godunov scheme of increased accuracy, uniform for solving equations of fluid dynamics and elastic-plastic flows [1]. The increase of the scheme accuracy is achieved by using 3D spatial time dependent solution of the discontinuity problem (3D space time dependent Riemann's solver). The same solution is used to calculate the interaction at the fluid-solid surface (Fluid Structure Interaction problem). These codes do not require complex 3D mesh generators, only the surfaces of the calculating objects as the STL files created by CAD systems, which greatly simplifies the preparing the task and makes it convenient to use directly by the designer at the design stage. To set the initial geometry and follow the deformation of the calculating domains in the process of interaction it is enough to take into account the interacting surfaces constituted by a set of triangles. Fixed Cartesian grid and local mobile grids associated with each triangle of the surface are used. The flow parameters are interpolated from the Cartesian grid to the local grids and vice versa. The results of the test solutions and applications related to the generation and extension of the detonation and shock waves, loading the constructions are presented. This work was supported by the RFBR grants (15-48-02333 R_povolzhe_a, 16-08-00458 a, 14-08-00197 a). References [1] Abouziarov M., Aiso H., Takahashi T. An application of conservative scheme to structure problems. Series from research institute of mathematics of Kyoto university. Mathematical analysis in fluid and gas dynamics. 2004, N2 1353 , pp. 192-201

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Efficient Computation of N-component Cahn-Hilliard Systems

Ruyam Acar*

*Okan University

ABSTRACT

We propose an algorithmic approach for efficient computation of N-component Cahn-Hilliard systems with constant surface tension. When pairwise surface tensions are homogeneous, diffusion term in the Cahn-Hilliard equation becomes isotropic and the energy term involves the summation of free energy contributions from each phase. Since diffusion is isotropic we suggest that instead of tracking the evolution of N phase variables it is sufficient to use a single parameter. Accordingly, we divide the value range of the phase parameter into N parts to represent N different components. In this way, for example values between 0 and 0.1 will correspond to phase one, values in range [0.1,0.2] will correspond to phase two and so on. Furthermore, in the energy term, we need to calculate the energy contribution only from the components in the diffusion range since components outside this range do not affect the current phase evolution. (Free energy values of these components also vanish in the N-component formulation. [1]) We can find the components that will contribute to the current energy with a simple neighborhood search in the local diffusion area based on the interface thickness. Once we find the relevant components, we can calculate the energy contribution from each component using the corresponding energy function defined in the given phase value range. In this way, we compute an N-component Cahn-Hilliard system by the evolution of a single parameter and using adaptive free energy calculations. Using one phase parameter also ensures mass conservation. We use a fast, stable, spectral method [2] based on a semi-implicit discretization for the numerical solution. Using a one-component solution provides a more efficient computation compared to the multigrid solution proposed for N-component systems in [1]. Furthermore, it allows flexibility in designing different physical properties for different components. [1] Lee, H.G., Choi, J-W and Kim, J., A practically uncoditionally gradient stable scheme for the N-component Cahn-Hilliard system, Physica A 391, 2012, 1009–1019. [2] Badalassi , V., Ceniceros , H., and Banerjee , S. 2003. Computation of multiphase systems with phase field models. Phys. D. 190, 371–397.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Computer Simulation Model of Bone Osteoporosis and Drug Treatment for In-silico Experiment and Observation

Taiji Adachi*, Yuki Miya**, Yoshitaka Kameo***, Tomoki Nakashima****

*Kyoto University, **Kyoto University, ***Kyoto University, ****Tokyo Medical and Dental University

ABSTRACT

Osteoporosis, loss of bone mass and functional structure, increases a risk of bone fractures caused by unbalance between osteoclastic resorption and osteoblastic formation. At the cellular level, complex couplings between mechanical and biochemical factors locally regulate cellular remodeling activities. To understand the mechanism of bone metabolism and remodeling in osteoporosis, in this study, we develop mathematical models incorporating biochemical regulatory factors combined with a mechano-adaptation model. In addition to this, drugs for osteoporosis treatment are modeled based on the diffusion-reaction type equations, some of which are mechanically regulated. Based on the model, we will discuss the applicability to predict effects of the drugs treatment for osteoporosis through in-silico experiment and observation. By introducing singling molecules identified in bone metabolism, cellular activities in bone were modeled. Osteoclastogenesis, for example, is promoted by the binding of RANKL to its receptor RANK, whereas OPG acts as a decoy receptor. Semaphorin 3A (Sema 3A) exerts a protective effect on bone by suppressing osteoclastic bone resorption and increases osteoblastic bone formation. For these biochemical signaling molecules, production, degradation, diffusion, and binding terms are modeled to predict spatiotemporal evolution of their molecular concentrations. Addition to this, the expression of these biochemical factors was coupled with mechanical factors on the trabecular surface and numerically solved in cancellous bone discretized into voxel finite elements. In silico experiments and observations were conducted for a mouse distal femur model that was built based on the X-ray micro-CT image data. Cancellous bone region was uniaxially compressed and the trabecular remodeling and cellular activities were observed. By comparing with in vivo experimental data, we validated the proposed model as an in-silico tool for perturbation experiments as well as for time-course observations in 3D. In addition, we discuss the effect of drugs for osteoporosis on the cellular activities and the resulting bone microstructure. This work was supported in part by the AMED-CREST (Mechanobiology), Japan.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Multiscale Shell Finite Element for Modeling the Out-of-plane Response of Masonry Walls

Daniela Addessi*, Paolo Di Re**, Elio Sacco***

*Sapienza University of Rome, Rome, Italy, **Sapienza University of Rome, Rome, Italy, ***University of Napples Federico II, Naples, Italy

ABSTRACT

The numerical simulation of nonlinear response of masonry structures is still an important and challenging task, as the stress/strain evolution in the material strongly depends on the progression of damage and micro-cracks in bricks and mortar as well as on the debonding phenomena at the brick/mortar interfaces, that influence the structural collapse. Masonry walls and vaults can experience different failure mechanisms, among which those out-of-plane are the most frequent. Multiscale finite element (FE) modeling [1,2] is a widely adopted and efficient procedure for the analysis of masonry structures, as it permits a detailed description of the nonlinear phenomena with a reasonable computational demand. This approach evaluates the response of a Unit Cell (UC), assumed as reference volume at the microscopic scale, and derives the response of the equivalent homogeneous medium at the macroscopic scale. Among the several proposals, shell-like models [3] have been widely developed based on proper homogenization procedures to link the responses at the micro and macro levels. This work proposes a thick shell FE based on a two-scale homogenization procedure to reproduce the out-of-plane response of masonry walls characterized by periodic textures. The constitutive relationship of the masonry assemblage is obtained through the homogenization process of three-dimensional UCs at the microscale, whose microscopic displacements are assumed as the sum of an assigned part, depending on the shell strains, and an unknown perturbation, due to the masonry heterogeneous nature. The bricks are considered as elastic, while a damage-friction model is used to reproduce the mortar response. The proposed FE model is implemented in a standard FE code and is used to perform numerical applications on masonry walls subjected to out-of-plane loading conditions. [1] Massart T.J., Peerlings R.H.J., and Geers M.G.D., "An enhanced multi-scale approach for masonry wall computations with localization of damage", Int J Numer Meth Eng, 69, 1022-1059 (2007). [2] Addessi D. and Sacco E., "A multi-scale enriched model for the analysis of masonry panel ", Int J of Solids Struct, 49, 865-880 (2012). [3] Petracca M., Pel L., Oller S., Camata G., and Spacone E., & amp;quot;Multiscale computational first order homogenization of thick shells for the analysis of out-of-plane loaded masonry walls ", Comput Method Appl M, 315, 273-301 (2017).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Data-driven Modeling & Uncertainty Quantification for Molecular Dynamics Simulations Using a Hierarchical Bayesian Framework

Yaser Afshar*, Shaowu Pan**, Karthik Duraisamy***

*University of Michigan, **University of Michigan, ***University of Michigan

ABSTRACT

The goal of the present work is to obtain a better understanding of Li+ -ion transport and solvation in various electrolytes via molecular dynamics (MD) computations. The reliability of the simulations, however, critically depends on the accuracy of the interaction potential models. The functional form of the interaction potential is inferred from heterogeneous data, and the uncertainty in predictions is propagated to the outputs of the MD simulation. The derivation of potentials can be considered as a single or multi-objective optimization problem, where the calibration data is obtained from different types of experiments and quantum mechanical calculations. Hierarchical Bayesian uncertainty quantification is utilized for this purpose with a highly scalable framework based on the Transitional Markov chain Monte Carlo sampling for populating the posterior probability distribution of the MD force-field. A machine-learned surrogate model is proposed to reduce the computational cost associated with a large number of MD model runs.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Efficient Crack Propagation Simulations Using Well Conditioned Extended/Generalized Finite Elements and a Deflated Conjugate Gradient Solver

Konstantinos Agathos*, Eleni Chatzi**, Stéphane P. A. Bordas***

*ETH Zurich, **ETH Zurich, ***University of Luxembourg

ABSTRACT

The incorporation of solution specific features in finite element approximations through partition of unity enrichment is known to significantly improve the approximation properties of the method, however it also introduces some numerical and implementation problems. Two important such problems are conditioning issues arising from linear dependencies between the enrichment functions and the finite element basis as well as blending problems between the standard and enriched part of the approximation. Since the early development of the extended/generalized finite element method (XFEM/GFEM) [1,2] several techniques have been proposed to handle the above issues, most of which require significant modifications to the original method thus increasing complexity and rendering application to existing codes problematic. In the present work two XFEM/GFEM variants are employed which significantly improve the conditioning of the resulting system matrices, while requiring only slight modifications to the original method. The discretization schemes are then combined to a deflated conjugate gradient (DCG) solver [3] and applied to 3D crack propagation problems where it is shown that a significant reduction in the computational time associated with solution of the linear systems can be achieved. Furthermore, since the schemes employed allow the application of geometrical enrichment, i.e. the use of singular enrichment functions in a fixed area around the crack front, a smoother variation of the stress intensity factors (SIFs) along the crack front is achieved, resulting in smoother crack paths. [1] Moës N, Dolbow J, Belytschko T. A finite element method for crack growth without remeshing. International Journal for Numerical Methods in Engineering 1999; 46(1): 131–150. [2] Strouboulis, T, Babuška, I, Copps, K. The design and analysis of the generalized finite element method. Computer methods in applied mechanics and engineering 2000; 181(1): 43-69. [3] Saad Y, Yeung M, Erhel J, Guyomarc 'h F. A deflated version of the conjugate gradient algorithm. SIAM Journal on Scientific Computing 2000; 21(5): 1909-1926.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Materials Informatics and Big Data: Realization of 4th Paradigm of Science in Materials Science

Ankit Agrawal*, Alok Choudhary**

*Northwestern University, **Northwestern University

ABSTRACT

Abstract In this age of “big data”, large-scale experimental and simulation data is increasingly becoming available in all fields of science, and materials science is no exception to it. Our ability to collect and store this data has greatly surpassed our capability to analyze it, underscoring the emergence of the fourth paradigm of science, which is data-driven discovery. The need to use of advanced data science approaches in materials science is also recognized by the Materials Genome Initiative (MGI), further promoting the emerging field of materials informatics. In this talk, I would present some of our recent works employing state-of-the-art data analytics approaches such as deep learning for exploring processing-structure-property-performance (PSPP) linkages in materials, both in terms of forward models (e.g. predicting property for a given material) and inverse models (e.g. discovering materials that possess a desired property). In particular, I will focus on some examples of microstructure informatics such as learning data-driven multi scale localization/homogenization linkages, identifying prior deformation from discrete dislocation dynamics images, and microstructure optimization of a magnetostrictive Fe-Ga alloy. I will also demonstrate some materials informatics tools we have developed that deploy machine learning models to predict materials properties. Such data-driven analytics can significantly accelerate prediction of material properties, which in turn can accelerate the optimization process and thus help realize the dream of rational materials design. The increasingly availability of materials databases along with groundbreaking advances in data science approaches offers lot of promise to successfully realize the goals of MGI, and aid in the discovery, design, and deployment of next-generation materials. Keywords Materials informatics, big data, deep learning, PSPP relationships, prediction, optimization Acknowledgment We gratefully acknowledge support from NIST Award 70NANB14H012, AFOSR Award FA9550-12-1-0458, DARPA Award N66001-15-C-4036, NSF BigData Spoke Award IIS-1636909, and Northwestern Data Science Initiative. References A. Agrawal and A. Choudhary, “Perspective: Materials informatics and big data: Realization of the ‘fourth paradigm’ of science in materials science,” APL Materials, vol. 4, no. 053208, pp. 1–10, 2016.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Lipids Catalyze Mitochondrial Fission via Geometric Instability

Ashutosh Agrawal*, Ehsan Irajizad**, Rajesh Ramachandran***

*University of Houston, **University of Houston, ***Case Western Reserve University School of Medicine

ABSTRACT

Balanced mitochondrial fission is essential for apoptosis and its disruption is linked to lung cancer, cardiac dysfunction and neurogenerative disorders. Pioneering experimental studies have provided molecular insights into mitochondrial fission. The fission pathway is characterized by three key steps: i) the initial constriction carried out by actin polymerization and actomyosin contraction, ii) the intermediate constriction executed by Drp1 (dynamin-related protein 1), and iii) the final fission carried out by dynamin. While the fission proteins play an inarguably critical role, a growing body of evidence reveals that conical lipids, regulate mitochondrial morphology and fission. But how conical lipids contribute to fission remains an open question. Here, we computationally model tubular mitochondria to reveal a new buckling instability-based mechanism for achieving a stable geometry conducive for fission. Employing membrane physics and differential geometry, the study reveals that buckling instabilities, triggered synergistically by cylindrical curvatures from proteins and spherical curvatures from conical lipids, help achieve superconstrictions for fission. We validate the role of conical lipids by an in vitro study in which membrane tubules with reduced concentration of conical lipids (PE) fail to undergo necking despite the presence of Drp1 proteins.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Comparative Study of Contact Problem Solution Based on Different Isogeometric Contact Formulations

Vishal Agrawal*, Sachin Singh Gautam**

*IIT Guwahati, India, **IIT Guwahati, India

ABSTRACT

Since the introduction of isogeometric analysis technique, it has been applied to a wide-range of contact problems due to its ability to exactly represent the complex shape of geometries and inherited tailorable continuity. It is observed that for the application of NURBS-based isogeometric analysis of different contact problems either the Gauss-Point-to-Surface (GPTS) [1] or the mortar based contact formulations [2] are most popularly employed for the treatment of contact constraints. However, it is known that the GPTS-based isogeometric analysis leads to excessive stiff and non-physical oscillations of the contact forces [2]. Hence, a post-processing scheme, which is developed within the spirit of mortar method in [3] and computes the regularized contact forces at the control points, is utilized with GPTS formulation and is denoted by GPTS(E). To the best of our knowledge, a comparative study between these formulations is not available and is the scope of present work. In this contribution, numerical behaviour, robustness, and accuracy of these two approaches are compared using the standard Hertz contact problem. For the enforcement of contact constraints penalty method is employed. It is found that mortar based contact formulation delivers slightly accurate results at a coarse mesh resolution in comparison to GPTS(E)-based formulation. As the mesh resolution is increased the former formulation approaches faster towards the exact solution than the latter one. Moreover, the distribution of contact pressure improves considerably in case of the mortar formulation with the order-elevation, whereas it remains unchanged for the GPTS(E)-based approach. It is shown that to achieve the numerical results similar to the former algorithm the contact boundary has to be discretized with a finer mesh resolution and a lower value of penalty parameter in the latter approach. But, as a result, the computational cost increases substantially. It is concluded that mortar based contact formulation delivers robust and superior quality result when compared with the GPTS(E)-based formulation. References [1] Fischer K. A., Wriggers P. Frictionless 2D contact formulations for finite deformations based on the mortar method. Comput. Mech., 36:226–244, 2005. [2] De Lorenzis L., Temizer I., Wriggers P., Zavarise G. A large deformation frictional contact formulation using NURBS-based isogeometric analysis. Int. J. Numer. Methods. Eng., 87:1278-1300, 2011. [3] Sauer R. A. Local finite element enrichment strategies for 2D contact computations and a corresponding post-processing scheme. Comput. Mech., 52:301-319, 2013.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Wave Propagation in Geological Reservoirs with the Generalized Finite Difference Method

Adriano José Aguiar Marçal*, Deane Roehl**

*Institute Tecgraf at PUC-Rio, **Civil and Environmental Engineering Department at PUC-Rio

ABSTRACT

The Generalized Finite Difference (GFD) is a kind of mesh free method. Therefore, like the classical Finite Difference Method (FD), it is not restricted to a regular grid. In the GFD, we numerically solve the partial differential equations by a second-order approximation of the derivatives using a Taylor 's series expansion for two or more variables. Hence, with the GFD, as with the Finite Element Method, we are capable of representing complex geological scenarios with more flexibility, keeping the computational efficiency of the classical Finite Difference Method. In most meshfree methods the assembly of the global system is very computationally intensive. In the classic FD method, since the mesh is structured, the approximation of the derivatives is calculated directly. On the other hand, the GFD requires the inversion of a local matrix at each point. Such matrix is small, symmetric and easy to solve numerically. However, to carry out an accurate discretization of complex geometries, we need thousands and even millions of points. Sometimes it is necessary to build a new point cloud. To mitigate the computational issues discussed above, we propose an analytical calculation of each local matrix. Following this procedure, we replace the numerical computation of inverse matrices by operations of product and sum of vectors, which are more efficient operations. We apply this methodology to model the propagation of seismic and electromagnetic waves in two-dimensional models using GFD. Such problems are common in geophysical simulations and of great interest to the oil and mining industry. Currently, these problems demand large investments in computer systems due to the complexity of geological scenarios.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

GPU-accelerated Structural Topology Optimization for Frequency Response Problems with Parameter Uncertainty

Miguel Aguilo*, Joshua Robbins**, James Warner***, Thomas Voth****, Brett Clark*****

*Sandia National Laboratories, **Sandia National Laboratories, ***NASA Langley Research Center, ****Sandia National Laboratories, *****Sandia National Laboratories

ABSTRACT

The intersection of additive processes and design optimization has introduced revolutionary capabilities for design, product development, and manufacturing. ``Complexity is free '' has been a common mantra with additive manufacturing processes. However, anyone involved in the qualification or certification of additive processes or materials will acknowledge that complexity is currently not free due to the prevailing lack of understanding of advanced manufacturing processes. One approach to address the highly variable nature of additive processes is to improve process determinism. An alternate, complementary approach is to account for these inherent uncertainties early in the design process by providing designers with uncertainty aware computational design tools that generate solutions that insure performance requirements are met and margins are quantified. This work presents a graphics processing unit (GPU) accelerated structural topology optimization solver for frequency response problems under uncertainty. Uncertainty aware optimization problems are computationally complex due to the substantial number of model evaluations that are necessary to accurately quantify and propagate uncertainties due to design imperfections. This computational complexity is magnified if a high-fidelity, physics-based numerical model is used during synthesis optimization. This work combines a GPU-accelerated structural dynamic finite element solver and the stochastic reduced order model (SROM) method to design a structural component that matches a prescribed frequency response. Results will highlight how the GPU-accelerated structural dynamic finite element solver and SROM method effectively 1) alleviate the prohibitive computational cost associated with uncertainty aware structural topology optimization for frequency response problems; and 2) quantify and propagate the inherent uncertainties due to design imperfections.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Computation of the Energy Release Rate Using a Complex Stiffness Derivative Approach

Andres Aguirre Mesa*, Daniel Ramirez Tamayo**, Manuel J. Garcia Ruiz***, Harry Millwater****

*Universidad EAFIT, **University of Texas at San Antonio, ***University of Texas at San Antonio, ****University of Texas at San Antonio

ABSTRACT

A variation of the virtual crack extension method, based on the stiffness derivative approach, is proposed using Complex Taylor Series Expansion (CTSE). The stiffness derivative approach for computing the Energy Release Rate of a cracked system is derived from the total potential energy of a finite element solution, and requires the computation a stiffness derivate, i.e, a first order sensitivity of the stiffness matrix with respect to the crack tip area perturbation. Several variations of this classical approach have been proposed for the computation of the stiffness derivative, including finite difference approximations and analytical solutions. The alternative presented here uses CTSE to compute the stiffness derivative. This is obtained as the imaginary part of a complex version of the stiffness matrix, which is created by adding a small imaginary perturbation to a set of nodal coordinates in the crack tip area. The method was implemented in a user-defined element subroutine of the commercial finite element software Abaqus, and it is particularly useful for the computation of the ERR of multiple cracked specimens. Preliminary results show that the ERR obtained by the Complex Stiffness Derivative approach has the same accuracy and superior efficiency with respect to J-integral results. Parks, D. M. (1974). A stiffness derivative finite element technique for determination of crack tip stress intensity factors. International Journal of Fracture, 10(4), 487-502. Hellen, T. K. (1975). On the method of virtual crack extensions. International Journal for numerical methods in engineering, 9(1), 187-207. Lin, S. C., & amp;amp;amp; Abel, J. F. (1988). Variational approach for a new direct-integration form of the virtual crack extension method. International Journal of Fracture, 38(3), 217-235.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Glycosaminoglycans in Aortic Dissection: A Model-Based Study Using Damage-based Smoothed Particle Hydrodynamics

Hossein Ahmadzadeh*, Manuel Rausch**, Jay Humphrey***

*Yale University, **University of Texas at Austin, ***Yale University

ABSTRACT

Aggregates of glycosaminoglycans (GAGs) localized within the medial layer of large arteries can sequester interstitial water and induce swelling of the intra-lamellar space. It is increasingly believed that this accumulation of GAGs, and the associated increase in the intramural mechanical stress field, can potentially trigger the damage and dissection that is often seen in thoracic aortic aneurysms. In this study, we present computational simulations using our previous smoothed particle hydrodynamics (SPH) model of soft tissues(1) that examine potential roles of pooled GAGs within the medial layer in initiating and propagating an intra-lamellar delamination. Mimicking the histological observations of the descending thoracic aorta of mouse models, the model aortic wall consists of an inner medial layer (composed of ~6-7 elastic laminae with associated smooth muscle cells and collagen fibers) and an outer collagen-rich adventitial layer. In order to elucidate the homeostatic in vivo state, the model aorta is initially axially stretched (60%) and subsequently pressurized intra-luminally (~12 kPa). The pooled GAGs are modeled by introducing a Gibbs-Donnan swelling pressure, which contributes to the stress field especially near the predefined GAG "particles". Our SPH model allows us to determine the evolution of the damage in discrete particles surrounding the GAGs. Specifically, in response to the swelling stress field induced by the GAGs, the maximum principal stretch of the neighboring particles is calculated and compared to a threshold value associated with the onset of the failure. The model shows that the swelling of intra-lamellar particles causes delamination between the elastic laminae, consistent with experimental observations. In addition, the damage experienced by the particles in the vicinity of the GAGs facilitates the propagation of the delamination in the circumferential direction. These results, combined with our sensitivity study on the input parameters of the model such as the luminal pressure and the size of the GAG pool, suggest that localized swelling can alter the mechanics in ways that eventually can cause catastrophic damage within the aortic wall. 1. Rausch, M.K., Karniadakis, G.E. & Humphrey, J.D. Biomech Model Mechanobiol (2017) 16: 249.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Three-dimensional Simulation of Spreading Dynamics of a Droplet on Substrate Using Multi-phase-field Model

Shintaro Aihara*, Tomohiro Takaki**, Naoki Takada***

*Kyoto Institute of Technology, **Kyoto Institute of Technology, ***National Institute of Advanced Industrial Science and Technology

ABSTRACT

Phase-field method has attracted much attention as a model for simulating not only material microstructures but also multiphase flow, because it can easily express a complicated morphological change by introducing a diffuse interface. In the multiphase flow area, the phase-field method has been extensively used in a two-phase flow problem. Recently, we have developed a multi-phase-field model which can express a dynamics of multiphase flow with three or more phases by introducing multiple phase-field variables [S. Aihara, T. Takaki, N. Takada, submitting]. In the study, we performed two-dimensional simulations to obtain an equilibrium droplet shape on solid substrate and to see droplet floating dynamics through a liquid-liquid interface. As a result of those simulations, we have confirmed that the simulation results agree well with theoretical ones. In this study, we extend the two-dimensional multi-phase-field model to the three-dimensional model. In addition, we enable a GPU (graphics processing unit) computation of the model to accelerate the three-dimensional simulation. Using the developed method, we simulate a wetting spread phenomenon of a three-dimensional droplet on a flat solid surface. We validate the developed three-dimensional multi-phase-field model by comparing the simulation results to the experimental ones [T.D. Blake, J.Colloid interface Sci., 299 (2006), 1].

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

ICME for Automotive Composites – A Perspective

Venkat Aitharaju*, Satvir Aashat**, William Rodgers***

*General Motors, **ETA, Inc., ***General Motors

ABSTRACT

Predictability of composite materials has been one of the bottlenecks hindering their large scale implementation in the industry. Several challenges exist in simulating the manufacturing and structural performance of these materials. The material properties of composites are a function of the manufacturing process used, and the performance predictability must include this aspect in great detail. Integrated Computational Materials Engineering (ICME) is an approach used to design the products, the materials that comprise them, and the associated material processing methods by linking material models at various length scales. ICME embraces a combined strategy of bottom-up and top-down modeling and simulation. Recently, there has been significant research in the area of ICME of automotive composite materials both in academia and at the national research labs. Some progress and success stories have been reported, but several unresolved issues, continue to prohibit the usage of these modeling developments in commercial industrial simulations. In the past, General Motors (GM) has successfully used composite materials for light-weighting of closures and non-critical structural composites in low volume applications. Additionally, GM is interested in evaluating carbon fiber composites in structural applications for potentially high volume vehicles. During service, these structural components are subject to complex long term loading conditions as well as potential crash events. Since the technology to validate the composite material designs in a virtual environment is not satisfactorily developed, GM has partnered with leading composite material simulation software companies, academia, and composite material molding companies (ESI, USC, Altair, CSP) through a Department of Energy funded project to develop state of the art probabilistic ICME tools to develop the required knowledge base and eliminate the current gaps. In this paper, a high level overview of the challenges and the progress realized in this project will be presented.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Study on Finite Element Model Selection in Sequential State Estimation Based on the Ensemble Kalman Filter

Takeshi Akita*

*Chiba Institute of Technology

ABSTRACT

Numerical simulations based on the finite element (FE) models play an important role in various engineering fields. The key to building effective FE models is to identify various uncertainties in the systems, such as uncertain structural parameters. These uncertainties are often time-variant, in such cases, a sequential parameter estimation technique, where structural uncertainties are simultaneously identified at each measurement time step, is effective. The Kalman filter is widely used for sequential parameter estimation, however, the conventional Kalman filter is mainly applied for low-order and linear systems. Recently, the ensemble Kalman filter (EnKF) have been proposed for high-order and nonlinear systems [1]. The EnKF is based on a Monte-Carlo calculation and can be easily incorporated into nonlinear finite element analysis codes. The author has applied the EnKF to sequential parameter estimations of FE models, and has presented a self-tuning scheme for noise settings in the EnKF [2]. The self-tuning is performed by maximizing the likelihood function of the innovation sequence in the EnKF. In the previous research, the self-tuning is limited to the same FE models. In this research, we extend the scheme for FE model selection problems. We quantify the effectiveness of a FE model by evaluating its likelihood function of the innovation sequence in the EnKF, which gives us a basic criteria for the FE model selection. A simple example is given to validate the presented scheme. [1] G. Evensen, Sequential Data Assimilation with a Nonlinear Quasi-Geostrophic Model Using Monte Carlo Methods to Forecast Error Statistics, Journal of Geophysical Research, 1994, pp. 10143-10162. [2] T. Akita, R. Takaki, N. Kogiso, An Adaptive Estimation of Nonlinear Structural Deformations by Using the Ensemble Kalman Filter, Aerospace Technology Japan, Vol. 14 (2016), No. ists30.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Computational Strategy for Solving Large Generalized Eigenvalue Problems in Fluid-structure Interactions

Quentin Akkaoui*, Evangéline Capiez-Lernout**, Christian Soize***, Roger Ohayon****

*Laboratoire Modélisation et Simulation Multi Echelle (MSME), **Laboratoire Modélisation et Simulation Multi Echelle (MSME), ***Laboratoire Modélisation et Simulation Multi Echelle (MSME), ****Conservatoire National des Arts et Métiers (CNAM)

ABSTRACT

For constructing reduced-order models of large-scale fluid-structure systems, computations of generalized eigenvalue problems are required [1]. For linear, and a fortiori for nonlinear dynamical systems, reduced-order models are essential for reducing the computational costs of the simulation in terms of CPU time and memory use. The algorithms and mathematical libraries involved for solving such generalized eigenvalue problems have demonstrated their efficiency and are suitable for analyzing large-scale models using parallel computers and massively parallel computers such as LAPACK. However, when dealing with a large-scale fluid-structure system, a stop of the calculation due to an out of memory can be encountered on mid-power and moderate-memory computers. For instance, this case occured when trying to compute the generalized eigenvalue problems for a fluid-structure computational model with 2 million degrees of freedom on a workstation with 264GB of RAM and 12 processors. For circumventing this problem, the present work is devoted to revisiting the algorithms in order to be able to compute these generalized eigenvalue problems on a mid-power computer. The methods proposed [2] are algorithms based on double projection and subspace iteration methods [3], which efficiently allow for reducing the computational cost of these calculations and above all for avoiding the stop of the calculation due to an out of memory. In such context, after briefly recalling the existing algorithms used for solving the three generalized eigenvalue problems related to the displacement of the elastic structure, the pressure in the acoustic fluid, and the free-surface elevation of the fluid, a new adapted computational strategy [2] is described for reducing the numerical cost of each generalized eigenvalue problem. Finally, a detailed quantification of the computer resources required for computing the reduced-order projection basis with both classical and new method is presented, validating the efficiency of the proposed strategy. [1] R. Ohayon, C. Soize, Nonlinear model reduction for computational vibration analysis of structures with weak geometrical nonlinearity coupled with linear acoustic liquids in the presence of linear sloshing and capillarity, Computers & Fluids 141 (2016) 82-89 [2] Q. Akkaoui, E. Capiez-Lernout, C. Soize, R. Ohayon, Solving generalized eigenvalue problems for large scale fluid-structure computational models with mid-power computers, Submitted to publication, October 2017. [3] K.-J. Bathe, The subspace iteration method–Revisited, Computers & Structures 126 (2013) 177–183.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Monolithic Time-Integration of Two-Fluid Flow with Correct Energy Behavior

Ido Akkerman*, Marco ten Eikelder**

*Delft University of Technology, **Delft University of Technology

ABSTRACT

Stable energy behavior for two-fluid simulation is not trivial, intact most practical time stepping approaches have a hidden instability, see [1] for a clear demonstration of the issue. A monolithic two-fluid formulation is presented that exhibits correct kinetic and potential energy evolution. This is achieved by solving the interface evolution with special care. Additional to the standard convection of the interface essential constraints on the interface evolution are enforced using global Lagrange multipliers. In order to allow the method to be monolithic a special level–set formulation is used [2]. In this level–set formulation the difficult non-linear Eikonal problem is translated to a simple linear projection problem. The formulation with Lagrange multipliers is solved with a Quasi-newton method. This method partially decouples the constraints from the rest of the problem. This results in a favorable matrix structure and the ability to solve the constraint to a strict tolerance without increasing the global iteration count. Divergence conforming NURBS spatial discretization is adopted. This avoids ambiguities with regard to mass conservation and volume conservation, which should be equivalent in the incompressible case. The energy properties of the proposed method are verified with the tried and tested dambreak problem. Examining the convergence of the energy evolution demonstrates the potential of the proposed formulation. The testcase involves low Reynolds-number flow. High Reynolds number flow would require the use of a stabilized formulation. A stabilized formulation with correct energy behaviour for a single fluid has been developed in parallel [3]. A stabilized formulation for two-fluids is work in progress. [1] I. Akkerman, Y. Bazilevs, D.J. Benson, and M.W. Farthing C.E.Kees. Free-Surface flow and fluid object interaction modeling with emphasis on ship hydrodynamics. Journal of Applied Mechanics, 79, 2012. [2] I. Akkerman. Monotone level-sets on arbitrary meshes without redistancing. Computers & Fluids, 146:74 – 85, 2017. [3] M.F.P. ten Eikelder and I. Akkerman. Correct energy evolution of stabilized formulations: The relation between VMS, SUPG and GLS via dynamic orthogonal small–scales and isogeometric analysis. I: The convective–diffusive context. Computer Methods in Applied Mechanics and Engineering, 331(Supplement C):259 – 280, 2018.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Local Boundary Conditions in Nonlocal Problems

Burak Aksoylu*, George Gazonas**

*U.S. Army Research Laboratory, **U.S. Army Research Laboratory

ABSTRACT

We present novel governing operators inspired by the theory of peridynamics (PD). They agree with the original PD operator in the bulk of the domain and simultaneously enforce local boundary conditions (BC). We present pure and mixed combinations of Neumann, Dirichlet, periodic, and antiperiodic BC. Our construction is systematic and easy to follow. We provide numerical experiments that validate our theoretical findings. The operators had been introduced in [1,2,3]. We extend the construction to more general inhomogeneous BC. We had proved that the nonlocal diffusion operator is a function of the classical operator. This observation opened a gateway to incorporate local BC to nonlocal problems on bounded domains. The main tool we use to define the novel governing operators is functional calculus, in which we replace the classical governing operator by a suitable function of it. We present how to apply functional calculus to general nonlocal problems in a methodical way. [1] B. Aksoylu and F. Celiker, Nonlocal problems with local Dirichlet and Neumann boundary conditions, Journal of Mechanics of Materials and Structures, 12(4) (2017), pp. 425-437. [2] B. Aksoylu, H.R. Beyer, and F. Celiker, Application and implementation of incorporating local boundary conditions into nonlocal problems, Numerical Functional Analysis and Optimization, 38(9) (2017), pp. 1077-1114. [3] B. Aksoylu, H.R. Beyer, and F. Celiker, Theoretical foundations of incorporating local boundary conditions into nonlocal problems, Reports on Mathematical Physics, 80(1) (2017), pp. 39-71.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Mechanics of Fluid Flow and Tissue Deformation inside a Solid Tumor

Meraj Alam*, Bibaswan Dey**, Raja Sekhar G. P.***

*Indian Institute of Technology, Kharagpur, India, 721302, **Indian Institute of Technology, Kharagpur, India, 721302, ***Indian Institute of Technology, Kharagpur, India, 721302

ABSTRACT

Introduction: Present work reports a mathematical modeling for the interstitial hydrodynamics and mechanical behavior of the solid phase inside a solid tumor. Mainly, there are two types of continuum models to describe the mechanics of soft biological tissue (i) theory of poroelasticity and theory of mixture. We use the concept of mixture theory to model the problem. In case of mixture theory, soft biological tissues are assumed to be a continuum binary mixture of solid and fluid phases. One can study the density variations within the components to evaluate the evolution of the stresses and mechanical interactions among the constituents. We assume tumor tissue as a visco-poroelastic deformable living biomaterial with cellular phase and extracellular matrix (ECM) constitutes the solid phase (also small volume of blood vessels) and physiological extracellular fluid is the fluid phase. The intravascular fluid or blood and the interstitial fluid form a single fluid phase. We write down the mass and momentum balance equations for both the phases. The momentum equations are coupled due to the relative interaction (or drag) force between the phases. Method: In this study we establish well-posedness (existence, uniqueness, and stability of solution) of the govern mathematical models (which is a system of partial differential equations) in the weak sense under following assumptions (i) motion of interstitial fluid flow and solid phase deformation are slow and (ii) nutrient proliferation rate is much faster than the tumor cell growth. To show the well-posedness we use semi-discrete Galerkin method. Further, we simulate some analytical results corresponding to the one-dimensional spherical symmetry model. We have adopted standard eigenfunction expansion method to solve the one-dimensional spherical symmetry model. Results: We have discussed the temporal variation of interstitial fluid pressure (IFP) and composite velocity and justified that corresponding to a long duration of perfusion; convection does not play a significant role because IFP and composite velocity become constant beyond a certain time level. Our results on unsteady hydrodynamics model would give an idea about the time required for the necrosis formation from the initial stage of perfusion. References: 1. Helen Byrne and Luigi Preziosi. Modelling solid tumour growth using the theory of mixtures. Mathematical Medicine and Biology, 20(4):341–366, 2003. 2. Bibaswan Dey and GP Raja Sekhar. Hydrodynamics and convection enhanced macromolecular fluid transport in soft biological tissues: Application to solid tumor. Journal of Theoretical Biology, 395:62–86, 2016.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Modeling, Simulations and Experiments of Cell Bulk and Cortex Mechanics

Sebastian Aland*, Elisabeth Fischer-Friedrich**

*HTW Dresden, **TU Dresden

ABSTRACT

Cell shape changes are vital for many physiological processes such as cell proliferation, cell migration and morphogenesis. They emerge from an orchestrated interplay of cellular force generation and cellular force response, both mainly dictated by the actin cytoskeleton. To understand cellular force response from a mechanistic point of view, we describe cells as incompressible viscoelastic bulk domains surrounded by an impermeable elastic surface (the cortex) under active tension. A comparison of simulated and experimental shapes of cells in a flow channel, permits extraction of cell mechanical parameters. As the cell cortex is found to be the dominant mechanical element, we investigate the cortical force response of cells which are clamped between two plates. We compare simulation results to cell-mechanical measurements to extract the Young's surface modulus and the surface Poisson ratio of the cortex. Our results corroborate the idea of the cortex as a thin, isotropic, incompressible material and provide a route to new medical diagnostics by cell mechanics.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Exploring Mechanical Properties of Amorphous Materials through Molecular Dynamics and Eshelby Inclusions Analysis

Tristan Albaret*, Francesca Boioli**, Anne Tanguy***, David Rodney****

*ILM-Physics Dept., Université Lyon 1, Villeurbanne, Auvergne-Rhône-Alpes , France., **ILM-Physics Dept., Université Lyon 1, Villeurbanne, Auvergne-Rhône-Alpes , France., ***LAMCOS, INSA de Lyon, Villeurbanne, Auvergne-Rhône-Alpes , France., ****ILM-Physics Dept., Université Lyon 1, Villeurbanne, Auvergne-Rhône-Alpes , France.

ABSTRACT

Understanding the mechanical properties of amorphous systems is tightly related with the identification and characterization of the elementary events that are at the origin of plasticity. Though these localized events involve rearrangements at the atomic scale, they can also be associated to mechanical heterogeneities in a continuous medium, also known as Eshelby inclusions. From molecular dynamics results we rebuild a representation in terms of Eshelby inclusions that is able to reproduce the stress-strain relations and give access, to some extent, to fine details such as the amplitude of the events, their size and their orientations. We used this mapping scheme to study the pressure dependence of plasticity in a model amorphous silicon bulk, or to inform mesoscopic models, for instance by detrermining activation volume through NEB calculations. I will also discuss more recent results on the Eshelby inclusion distributions as a function of the shear rate, in the first stages of plasticity. This should give an insight on the typical behaviour of the stress-strain relation in these regimes.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Cell-Based Topology Optimization Under the cgFEM Framework

José Albelda*, Mikel Barral**, Enrique Nadal***, Juan José Ródenas****

*Universitat Politècnica de València, **Universitat Politècnica de València, ***Universitat Politècnica de València, ****Universitat Politècnica de València

ABSTRACT

Today industries need to develop components meeting the needs of users each time faster. Therefore, companies need to generate optimal models for their components quickly. In this sense, various optimization processes are used in industry. The most usual of them is based on defining certain parameters characterizing the component and through a classical optimization process the combination of them that minimizes a certain objective function (weight, deflection, ...) is obtained. Another optimization technique, so called Topological Optimization (TO), has been used to optimize the geometry of various components. Unlike the previous one, the TO seeks the optimal distribution of a certain quantity of material maximizing the stiffness of the component. The results are much richer allowing important topological changes (appearance or collapse of holes) in a simple way. However, the optimization process entails a greater difficulty than other types of optimization, forcing the development of specific TO methods [1]. A problem of large structures so designed is that they need to be manufactured by additive manufacturing due to its complexity, which can be expensive. To alleviate this difficulty, this contribution proposes a method that, instead of obtaining the optimized structure of the whole component, subdivides the component into cells of manageable size and those cells are optimized by TO. All the software developed is integrated into the cgFEM environment [2], taking advantage of its computational performance. The process takes the following steps: i) a TO is carried out for the whole component with a certain parameter configuration so that it distributes the amount of material needed in each cell. ii) Using this information and the loads to which each cell is subjected to, a second TO process is launched at each cell defining the geometry of the same. iii) Finally, the global component is built by joining all cells together. In this way, additive manufacturing is only necessary for the construction of the cells and not for the entire component, thus being able to manufacture larger components. [1] O. Sigmund. A 99 line topology optimization code written in Matlab. Structural and Multidisciplinary Optimization. 21:120-127, 2001. [2] E. Nadal. Cartesian grid FEM (cgFEM): High performance h-adaptive FE analysis with e?cient error control: application to structural shape optimization. Ph.D. Thesis, Universitat Politècnica de València, 2014. AK The financial support to this work of Generalitat Valenciana (PROMETEO/2016/007) and the Spanish Ministerio de Economía, Industria y Competitividad (DPI2017-89816-R) is greatly acknowledged.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Combined Modeling and Experimental Study of the Structural Mechanobiology of Blood Clot Contraction and Deformation

Mark Alber*, Oleg Kim**, Samuel Britton***, Rustem Litvinov****, John Weisel*****

*University of California Riverside, **University of California Riverside, ***University of California Riverside, ****University of Pennsylvania, *****litvinov@mail.med.upenn.edu

ABSTRACT

Blood clot contraction plays an important role in prevention of bleeding and in thrombotic disorders. In this talk, we will unveil and quantify the structural mechanisms of clot contraction at the level of single platelets. A key elementary step of contraction is sequential extension–retraction of platelet filopodia attached to fibrin fibers. In contrast to other cell–matrix systems in which cells migrate along fibers, we will demonstrate that the "hand-over-hand" longitudinal pulling causes shortening and bending of platelet-attached fibers, resulting in formation of fiber kinks. When attached to multiple fibers, platelets were shown in [1] to densify the fibrin network by pulling on fibers transversely to their longitudinal axes. Single platelets and aggregates will be shown to use actomyosin contractile machinery and integrin-mediated adhesion to remodel the extracellular matrix, inducing compaction of fibrin into bundled agglomerates tightly associated with activated platelets. The revealed platelet-driven mechanisms of blood clot contraction demonstrate an important new biological application of cell motility principles. Recently developed multi-scale discrete worm-like chain model will be used to demonstrate that non-linear mechanical properties of compressed fibrin network can originate from structural re-arrangements of the entire fibrin network, as well as from alterations of individual fibers including fiber buckling, bending and reorientation. Model simulation results support novel hypothesized mechanism of stress propagation through the network and quantify how rearrangement and linkage of fibrin fibers effects network stiffening. The new model was also used to determine how contractile function of platelets, their distribution within the fibrin network and fibrin properties affect mechanical response of a blood clot to applied stresses in blood flow. Lastly, a novel multi-phase computational model will be described that simulates active interactions between platelets and fibrin, to study the impact of various physiologically relevant blood shear flow conditions on deformation and embolization of a partially obstructive clot with variable permeability [2]. Simulations provide new insights into mechanisms underlying clot stability and embolization that cannot be studied experimentally at this time. References 1. Oleg V. Kim, Rustem I. Litvinov, Mark S. Alber and John W. Weisel [2017], Quantitative Structural Mechanobiology of Platelet-Driven Blood Clot Contraction, Nature Communications 8: 1274. https://www.nature.com/articles/s41467-017-00885-x.pdf. 2. Shixin Xu, Zhiliang Xu, Oleg Kim, Rustem I. Litvinov, John W. Weisel and Mark Alber [2017], Model Predictions of Deformation, Embolization, and Permeability of Partially Obstructive Blood Clots under Variable Shear Flow, Journal of the Royal Society Interface 14: 20170441. http://rsif.royalsocietypublishing.org/content/14/136/20170441.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Topology Optimization of Periodic Elastoplastic Energy Dissipating Microstructures

Ryan Alberdi*, Kapil Khandelwal**

*University of Notre Dame, **University of Notre Dame

ABSTRACT

A framework for the design of periodic elastoplastic energy dissipating microstructures is developed using topology optimization. While the topology optimization of elastic microstructures has been carried out in numerous studies, microstructural design considering inelastic behavior is relatively untouched due to a number of reasons which are addressed in this study. An RVE-based homogenization approach is employed along with periodic boundary conditions, satisfying the Hill-Mandel principle. The plastic anisotropy which may be prevalent in materials fabricated through additive manufacturing processes is considered by modeling the constitutive behavior at the microscale with Hoffman plasticity. Discretization is done using enhanced assumed strain (EAS) elements to avoid locking from incompressible plastic flow under plane strain conditions and a Lagrange multiplier approach is used to enforce periodic boundary conditions in the discrete system. The design problem is formulated using a density-based design parameterization in conjunction with a SIMP-like material interpolation scheme. The total plastic work in the RVE is maximized and the path-dependent sensitivity analysis is carried out using an adjoint method. Attention is devoted to issues such as dependence on initial design, material and geometric symmetry and the enforcement of microstructural connectivity. A number of microstructural designs are obtained under different prescribed macroscopic strains.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Flat-top Partition of Unity Method for Unit Cell Problems

Clelia Albrecht*, Marc Alexander Schweitzer**

*Fraunhofer SCAI, **University of Bonn / Fraunhofer SCAI

ABSTRACT

In this presentation we are concerned with the application of the flat-top partition of unity method to unit cell problems which are solved in a representative volume element and subject to periodic boundary conditions. To use the full approximation power of the PUM, we use problem-dependent enrichment functions. We present techniques, implemented within the PUMA software framework, to construct these enrichment functions as well as to handle occurring stability problems of the resulting system matrices. To demonstrate the effectiveness of this approach, we discuss examples for unit cell problems like the solution of the Schrödinger equation for quantum mechanical calculations (collaboration with J. Pask and N. Sukumar) or the simulation of heterogeneous materials. For these examples, we examine their approximation properties as well as parallel performance.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Discrete Element Approach for Modeling the 3D Thermal-induced Damage

Ghassan Alhajj Hassan*, Solange Humblet**, Grégory Martic***, Emmanuel Bellenger****, Willy Leclerc*****, Meric Tandja******, Mohammed Guessasma*******, Christine Pelegris********, Marc Duquennoy*********, Maurice Gonon**********

*LTI, UPJV, Universty of Picardie Jules Verne, France, **SIRRIS, Gosselies, Belgium, ***BCRC (Belgian Ceramic Research Centre), Belgium, ****LTI, UPJV, Universty of Picardie Jules Verne, France, *****LTI, UPJV, Universty of Picardie Jules Verne, France, ******LTI, UPJV, Universty of Picardie Jules Verne, France, *******LTI, UPJV, Universty of Picardie Jules Verne, France, ********LTI, UPJV, Universty of Picardie Jules Verne, France, *********IEMN/DOAE, UVHC, University of Valenciennes, France, **********Faculty of Engineering, University of Mons, Belgium

ABSTRACT

This work is treated in the framework of CUBISM project funded by INTERREG V program. The purpose of the project is to develop a pressure and humidity SAW sensor, in order to follow the drying of refractory materials under high temperature and pressure conditions. More precisely, we aim to describe and predict the thermo-mechanical behavior of the piezoelectric SAW substrate under such conditions for a full set of geometrical configurations and materials. Besides, we expect to take into account the micro-cracks resulting from thermal expansion mismatch between the substrate and its environment. However, at the microscopic scale, the finite element method is less suitable to describe discontinuities induced by micro-cracks. For that reason, we propose to study the thermo-mechanical behavior using the discrete elements method (DEM). This choice is also motivated by the advantage of DEM to describe the crack propagation. This contribution presents significant improvement for DEM to model the 3D thermal-induced damage due to thermal expansion. Furthermore, this study allows to follow the damage level of the material during its lifetime. Thanks to the MULTICOR3D++ code developed in our laboratory, a hybrid particulate-lattice model [1], based on the equivalence between a granular system and a network of cohesive beam elements, is generated. Our contribution is to introduce the linear thermal expansion at the scale of the contact by modifying the initial free length of each link, using the model introduced in 2D by [2]. Heat transfer by conduction is taken into account, what requires contact areas which can be computed using two approaches. The first one consists in calibrating a coefficient describing the mean ratio between particle and contact areas. The second one is to associate a polyhedral element to each particle, using the concept of representative elements. Besides, we study the characteristics of materials in terms of the number of discrete elements, also the equivalent stress and strain of each particle are determined using a representative area. In addition, a model of damage resulting from thermal expansion was introduced. We consider that the fracture occurs when the hydrostatic stress for local tensile solicitations is greater than a given tensile strength limit. [1] H. Haddad. Modélisation du comportement thermomécanique de l’interface de contact par une approche couplée MED-MEF. PhD thesis, France, 2013. [2]W. Leclerc, H. Haddad, M. Guessasma. On a Discrete Element Method to simulate thermal-induced damage in 2D composite materials, In Computers & Structures, 2017, ISSN 0045-7949.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Nonlinear Oscillations of a Biomimetic Scale Elastica

Hessein Ali*, Hossein Ebrahimi**, Ranajay Ghosh***

*University of Central Florida, **University of Central Florida, ***University of Central Florida

ABSTRACT

Biomimetic scales are ubiquitous in nature and known to provide the organism several mechanical and multifunctional advantages. Such scales significantly change the curvature dependent properties of mechanical materials giving rise to complex nonlinearities that can be apparent even in small deformations due to scales engagement. Accordingly, mimicking such structures in materials has been of great interest to acquire high performance including stiffness gains and tunable elasticity. The essential source of these behaviors are difficult to model further than simple geometries due to the complexity arises from scales interaction. This work focuses on the dynamic behavior of such biomimetic systems. Furthering a deeper understanding of the origins of these nonlinearities for a scale-covered elastic can provide useful information towards controlling their deformation behavior in various twisting and bending modes. Such nonlinearities involve various aspect of scales interaction, geometrical sliding, interfacial friction and their combinations. In this study, we explore a special class of these materials, one which behave like nonlinear elastica. The vibrational characteristic and different nonlinearities will be discussed and suitable means of controlling them introduced.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Simulation of Blood Flow in Circle of Willis in Case of an Artery Stenosis

Aria Alimi*, Olaf Wünsch**

*University of Kassel, **University of Kassel

ABSTRACT

Numerical simulation of blood flow in deformable arteries in human body can be used to study the effect of phenomena that change normal blood flow behavior in the body. One of these phenomena is the arterial stenosis that can occur in brain arteries. The main reason of brain stenosis is not known, but certain habits and conditions like smoking or unhealthy diet can increase the risk of this disease. In this work, numerical calculations are performed to study the blood flow in the main arteries of Circle of Willis in case of an artery stenosis. Intracranial arterial stenosis is the narrowing of the arteries inside the brain. It could be caused by buildup of a plaque inside of the artery on the inner wall. Stenosis may occur in any artery in the circle of Willis but the arteries that most likely are affected by stenosis are internal carotid artery (ICA), the middle cerebral artery (MCA), the vertebral arteries and the basilar artery [2][3]. Over time, the plaque would harden and get larger. Hence, it reduces or completely blocks the blood flow and could lead to a stroke. Different size of plaques and multiple locations are studied, and the results are discussed. Finite-Volume method is used for the calculations of the 3D model of arteries by means of foam-extend-3.1. Different arteries are assigned with in-vivo blood pressure read from the medical experiments on patients. Fluid-structure interaction simulation is used to study a more realistic behavior of the arteries. Brain is assumed to have a homogeneous, linear elastic incompressible material [1]. Blood is modeled to be an incompressible Newtonian fluid. As the plaques are hardened tissues stuck to the wall of the arteries, the stenosis cases are modeled by narrowing the arteries on the location that plaque exists.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Analysis of Functionally Graded Mindlin Sector Microplates under Transverse Loading

F. Alinaghizadeh*, M. Shariati**, Jacob Fish***

*Columbia University/Ferdowsi University of Mashhad, **Ferdowsi University of Mashhad, ***Columbia University

ABSTRACT

In this work bending analysis of functionally graded sector microplates is studied. The modified couple stress theory with a single material length scale parameters is used to capture the size effect. The equilibrium equations are obtained based on the first-order shear deformation plate theory using principle of minimum total potential energy. Two types of Hooke 's law are considered in calculations. The material properties of the plates are considered to be graded through thickness direction according to a power-law distribution of the volume fraction of the constituents. The equilibrium equations of the microplates are a system of five forth-order partial differential equations. A polynomial based generalized differential quadrature method is employed to solve the equilibrium equations of the plates for different boundary conditions. The effects of power-law index, material length scale parameters and geometrical parameters on deflections of plates are investigated. It is observed that the effect of length scale parameter is to make the plate behavior stiffer. Furthermore, deflection values predicted by using the 3-D Hooke's law are less than those that are obtained by the Hooke's law.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Coupled Chemo-Mechanical Cell-Matrix Model to Predict Mechanical Feedback Between Cells and Extracellular Matrices

Farid Alisafaei*, Matthew Hall**, Mingming Wu***, vivek Shenoy****

*University of Pennsylvania, **University of Michigan, ***Cornell University, ****University of Pennsylvania

ABSTRACT

Introduction: Reciprocal mechanical interactions between cells and their surrounding extracellular matrices (ECMs) regulate various physiological and pathological processes such as cell motility, and tumor growth. Our recent study [1] reveals a mechanical cross-talk (feedback loop) between breast tumor cells and fibrous ECMs. Contractile cells pulling on their surrounding ECMs reorganize, align, and subsequently stiffen the fibrous collagen matrices in their immediate vicinity. In return, the matrix stiffening leads to greater cell force generation and cell stiffening. Here, we propose a novel nonlinear chemo-mechanical cell model, coupled with a fiber network-inspired continuum matrix model, to link the mechanics of the cell (stiffness and architecture) to its surrounding extracellular matrix. Materials and Methods: We engineer an array of type 1 collagen matrices with different microstructures modulated by altering; (i) collagen concentration, (ii) polymerization temperature, and (iii) cross-linking via preglycation with ribose. Using a parallel-plate oscillatory shear rheometer, we also measure the shear modulus of all nine collagen matrices. To study the interaction between cells and matrices, MDA-MB-231 breast cancer cells are embedded within the collagen matrices covalently bonded to fluorescent marker beads. Using a 3D particle tracking microscopy from the laboratory of M.W. and coworkers [1], the 3D displacements of ~10,000 beads are measured in the vicinity of each cell. Results and Discussion: As reported in [1], collagen matrices with larger pore sizes exhibit greater fiber alignment accompanied by an increased range of displacement propagation. Our experimental results also show that actin filaments are more aligned (along the cell's major axis) in stiffer matrices than in softer matrices indicating that cell body stiffness increases with matrix stiffness; cells actively respond to their stiffened surrounding by alignment of f-actin filament along the long axis of the cell. We propose a coupled cell-matrix model to qualitatively predict (i) displacement fields induced by pulling cells within their surrounding matrices, (ii) cell-generated forces, actin fiber alignment, and cell stiffening as functions of matrix stiffness, and (iii) strain-induced fiber alignment of fibrous matrices and its associated long-range displacement propagation.
References: [1] M.S. Hall, F. Alisafaei, E. Ban, X. Feng, C-Y Hui, V.B. Shenoy, M. Wu, Proc Natl Acad Sci USA, 113:14043-14048, 2016.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Study of Shear Band Broadening in Simulated Glasses

Darius Alix-Williams*, Michael Falk**

*Johns Hopkins University, **Johns Hopkins University

ABSTRACT

We investigate the broadening of shear bands in three distinct glassy materials systems – a two-dimensional binary Lennard-Jones system, a Cu64Zr36 EAM system and a Stillinger-Weber silicon system. For each material system, three glassy configurations are prepared via quenches from well-equilibrated liquids to low temperature at various rates. These configurations are subsequently deformed in simple shear to 1000% strain and, in all cases, shear bands form and broaden. The rate of shear band broadening is inconsistent with an assumption that the band grows at a rate proportional to the strain rate within the band. This implies that additional time scales are important in determining the rate of band broadening. We explore potential causes for the discrepancy between the assumed model and our simulation results with the objective of constraining the underlying constitutive response theory appropriate for amorphous solids subject to large deformations.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Numerical Implementation of Thermomechanical Problem Considering Heterogeneous Media Using Multiscale Procedures Combined with eXtended Finite Element Method

Nasser Alkmim*, Francisco Evangelista Junior**

*University of Brasilia, **University of Brasilia

ABSTRACT

In this work we present the description and a in-house implementation of a multi-scale procedure for modeling heterogeneous media considering linear and nonlinear material behavior. The model considers a weak coupling between temperature effects on the mechanical problem. All material nonlinearity that may result during analysis is solved only in the microscale problem, no constitutive equations are needed for the macroscale. The implemented approach relies on the XFEM (eXtended finite element method) with level-set functions to model material interfaces in the microscale of the material. The homogenized material properties at a quadrature points are obtained from the microscale analysis and used during construction of macroscale element stiffness matrices. The implemented solution -- \texttt{scikit-mechanics} -- was done using Python programming language which offers a highly legible syntax and benefits of object-oriented programming paradigm.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Modeling the E ffects of Microstructure on Localization in Polycrystalline Stainless Steel

Coleman Alleman*, James W. Foulk III**, Alejandro Mota***, Hojun Lim****, David Littlewood*****

*Sandia National Laboratories, **Sandia National Laboratories, ***Sandia National Laboratories, ****Sandia National Laboratories, *****Sandia National Laboratories

ABSTRACT

In a polycrystalline aggregate, the heterogeneous plastic deformation introduced by the local anisotropy of the microstructure plays a critical role in the localization of the deformation. To accurately resolve this incipient stage of failure, it is therefore necessary to incorporate microstructure with sufficient resolution, including accurate representations of interfaces such as grain boundaries. However, modeling the entire body at the required level of resolution is computationally prohibitive. In this study, the authors demonstrate the use of concurrent multiscale modeling to incorporate explicit, finely resolved microstructure in a critical region while resolving the smoother mechanical fi elds outside this region with a coarser discretization to limit computational cost. The Schwarz alternating method is a well-established technique for the solution of elliptic PDEs by means of domain decomposition. This concurrent multiscale method enables the flow of information between fine and coarse scales to achieve strong two-way coupling, which is critical in the accurate simulation of localization of plastic deformation leading to void or crack initiation in the incipient failure regime. The Schwarz method avoids the use of Lagrange multipliers or gradients that afflict other coupling methods, instead directly imposing the solution of each domain on the others in a way that guarantees convergence of the combined problem. This presentation will discuss the formulation of the Schwarz method and its implementation in the open-source Albany fi nite element platform developed at Sandia National Laboratories and demonstrate the use of the method as an e ffective approach for concurrent coupling in fi nite deformation solid mechanics. In particular, the Schwarz method is applied in this study to analyze the behavior of stainless steel tension specimens undergoing the localization of plastic deformation during the necking process. The gauge section of the specimen{where localization occurs{is resolved at a scale where the polycrystalline microstructure is discretized explicitly, and an anisotropic crystal elasto-viscoplasticity constitutive model is employed. The far field domain is coarsely discretized, and a simpli fied, isotropic elastoplastic constitutive relation is employed to capture the aggregate response of a polycrystalline region in a phenomenological manner. A suite of microstructural realizations are simulated to investigate the e ffects of microstructural variability on the necking process.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Multiscale and Non-conforming Interface Coupling for the Non Invasive Global-local Analysis of Heterogeneous Structures

Olivier Allix*, Maxence Wangermez**, Pierre-Alain Guidault***, Oana Ciobanu****, Christian Rey*****

*LMT Cachan, **LMT Cachan / Safran Tech, ***LMT Cachan, ****Safran Tech, *****Safran Tech

ABSTRACT

This contribution presents an interface coupling technique between a heterogeneous microscopic (local) model and a first order homogenised (global) model, representative of the macroscopic behaviour of a structure. It addresses the problematic of replacing a local part of the homogenised macroscopic model where the RVE (Representative Volume Element) is not fully representative of the microstructure or where the first order homogenization hypothesis are no longer respected. The key point of this multiscale based coupling technique is that we operate a scale separation on the interfaces between models. An interface fields scale separation is performed into macroscopic and microscopic contributions and ensure perfect interface equilibrium between models in a macroscopic sense: continuity of macro-displacements and equilibrium of macro-forces. Then, we add a priori conditions on the microscopic interface quantities that depends on the locations and external loading of the microscopic details. The first situation corresponds to the one where the microscopic detail is far from the edges and submitted to large wavelength loading. The coupling technique is performed such that the local solution corresponds to the one of the standard first order periodic homogenization. For this the global and local models are tied through interface mean displacements. The complementary microscopic part which are incompatible are used to impose a priori periodic condition between opposite faces on the local model. As such the technique leads to a complex and non-standard formulation which, in turn, can be easily recovered in a non-intrusive way and therefore applied in legacy codes. The validation of the method is done on a 2D and 3D steady mechanical academic problem under linear elasticity assumption with matching geometries on the interface between local and global meshes. The non conforming interface coupling techniques along with its non-intrusive are currently extended to high gradient area implying macroscopic stress concentration as cracks, edges and so on.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Coupled Multi-Scale Study of Lithium Ion Batteries to Evaluate Performance of Deformed Electrodes

Srikanth Allu*, Hsin Wang**, Srdjan Simunovic***, John Turner****

*Oak Ridge National Laboratory, **Oak Ridge National Laboratory, ***Oak Ridge National Laboratory, ****Oak Ridge National Laboratory

ABSTRACT

Mechanical abuse of Lithium Ion Batteries (LIB) has become an important research topic mainly because of the commercialization of electric vehicles and increasing possibility of accidents involving large number of Li-ion cells. Since internal short can lead to the thermal runaway, extreme importance is given safety design aspect of LIB packs. It is important to fully understand the value of mechanical abuse simulation. In general, a Li-ion cell can be put under one of the three conditions after mechanical abuse: 1) short circuit is induced and followed by thermal runaway, 2) short circuit is induced without thermal runaway and cell slowly discharges, and 3) no short circuit is induced and the cell can still function. Most studies have been focused on the simulation of mechanical damages in the first two cases in which failure of the battery components led to discharge, thermal runaway, fire and explosion. But there has been no report on how the cells will function under the last case. In many cases, the multiple layer structure of the LIBs made them very tolerant to mechanical abuse. In fact, studies showed a typical battery take more than 80% compression without short circuit. In this talk we will present a coupled multi-physics model of species transport, charge conservation and chemical kinetics developed for lithium-Ion batteries. The developed model is used to simulate the indentation damage and the consequences it has on electrochemical transport corresponding to capacity loss.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

The Strong Form Collocation Method for the Prediction of Polycrystalline Solidification with the Diffuse-interface Approach

Ashkan Almasi*, Jeong-Hoon Song**

*University of Colorado Boulder, **University of Colorado Boulder

ABSTRACT

Application of a diffuse-interface, or phase field, approach to modelling polycrystalline solidification has become a significant topic of interest in science and engineering research. Such modelling requires suitable computational methods to solve the relevant differential equations. In this study, we use the particle difference method (PDM) [1-2], a strong-form point collocation method, to model solidification of polycrystalline materials and perform a subsequent stress analysis. The PDM is a meshfree method based on Taylor polynomial expansion and the moving least square approach. One of its distinct features is that the PDM can directly discretize the strong form of governing partial differential equations. Consequently, the PDM neither performs domain integration nor constructs a mesh, thus saving computational time. After describing the formulation of the PDM and some techniques used in the subsequent analysis, this study takes advantage of these benefits of the PDM to predict the solidification process in two cases, one with 5 grains and the other with 36 grains, using grain growth kinetics [3]. Afterward, stress analysis is performed with the predicted polycrystalline morphology, yielding results for displacement, strain, stress, and Von Mises stress in the polycrystalline solid for various levels of discretization. Finally, these results are compared to results from the finite element method for verification, demonstrating that the PDM successfully predicts polycrystalline solidification and computes stress in the predicted morphology. References [1] Young-Cheol Yoon and Jeong-Hoon Song. Extended particle difference method for weak and strong discontinuity problems: part i. derivation of the extended particle derivative approximation for the representation of weak and strong discontinuities. Computational Mechanics, 53(6):1087–1103, 2014. [2] Young-Cheol Yoon and Jeong-Hoon Song. Extended particle difference method for moving boundary problems. Computational Mechanics, 54(3):723–743, 2014. [3] Danan Fan and L-Q Chen. Computer simulation of grain growth using a continuum field model. Acta Materialia, 45(2):611–622, 1997.

13th World Congress on Computational Mechanics (WCCM XIII) and 2nd Pan American Congress on Computational Mechanics (PANACM II), July 22-27, 2018, New York City, NY, USA

TOPOLOGY OPTIMIZATION OF PERIODIC PIEZOELECTRIC MATERIALS FOR ENERGY HARVESTING DEVICES

BRENO V. DE ALMEIDA*, RENATO PAVANELLO†

*School of Mechanical Engineering, University of Campinas
Cidade Universitria Zeferino Vaz - Barao Geraldo, 13083-970
Campinas, Sao Paulo, Brazil
brenodealmeida4@gmail.com

†School of Mechanical Engineering, University of Campinas
Cidade Universitria Zeferino Vaz - Barao Geraldo, 13083-970
Campinas, Sao Paulo, Brazil
pava@fem.unicamp.br

Key words: Piezoelectric, periodic, energy harvester

1 INTRODUCTION

There has been effort in the past decades to improve the performance of energy harvesting devices, in order to efficiently recharge or even independently power small electronic devices, thus decreasing the amount of batteries needed to power them, which can yield financial as well as environmental benefits. These devices work by converting ambient waste energy to useful electrical energy and there are three main phenomena which favor this process: electromagnetic, electrostatic and piezoelectric; of which the most advantageous, considering power density and ease of application, is piezoelectric [1].

In the context of topology optimization of piezoelectric energy harvesting devices, Zheng et. al. [2] optimized a beam-like piezoelectric harvester using a finite element (FE) mesh in three dimensions considering a static load and Noh and Yoon [3] extended this analysis using the SIMP model and studying the effect of using different penalization factors for the interpolation of the piezoelectric properties, for both static and dynamic excitations. Lin et. al. [4] optimized the harvester considering a range of base vibration frequencies, also in three dimensions but with only one element thickness per piezoelectric layer. Kiyono et. al. [5] considered a multilayered shell element.

Most of these piezoelectric topology optimization articles used the SIMP method for the optimization problem and, to the best of the authors' knowledge, only perform topology optimization of the piezoelectric layers modelled as plate [4], shell [5] or using a three-dimensional model with only one or two elements per layer in the thickness direction [2,3] and a FE analysis of the optimal topology for the thickness direction is seldom done. This

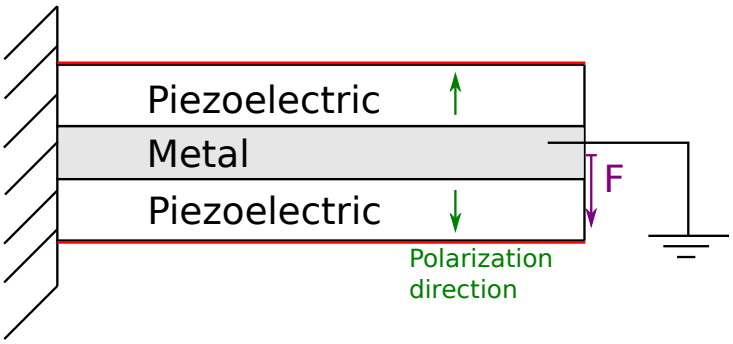


Figure 1: Two-dimensional model of the optimized bimorph harvester. The green arrows represent the piezoelectric polarization directions of the two layers. The red line is the initial position of the electrodes and the purple arrow indicates where the harmonic force is applied. The harvester is clamped in the left hand-side and the metal substrate is grounded. The harvester is optimized in open-circuit conditions.

may be due to difficulties in the production of complex piezoelectric structures, which in recent years has seen considerable improvements with advances in Additive Manufacturing (AM) techniques, and may enable the manufacturing of more sophisticated harvester designs, including the production of composite piezoelectric materials for energy harvesting [6,7].

Thus, in this extended abstract, a piezoelectric energy harvester is modeled as a bimorph two-dimensional beam under plain strain hypothesis [8]. The beam is composed of two piezoelectric layers of opposing polarities (series connection) and an intermediate metallic substrate, under open-circuit conditions, as shown in Fig. 1. It is subjected to a harmonic excitation in the free end. Its topology is optimized using the Bidirectional Evolutionary Structural Optimization (BESO) method [9]. An initial optimization process is done considering no periodicity constraint. Next, the concept of cells is used for the application of the periodicity constraint [10,11] and the results are compared to the initial one.

The FE model is shown in section 2 and the topology optimization procedure is shown in section 3. The objective function consists on minimizing the inverse ratio of the output electric energy by the input force work [2,3]. The BESO method is then used to optimize the topology of the piezoelectric material of the harvester, considering a harmonic load on the free end of the beam and a fixed topology for the metallic substrate. The sensitivities of a minimization problem are derived, and different penalization parameters are used for each of the piezoelectric material's stiffness [3] in order to find a better convergence. Section 4 shows the results of the topology optimization of the harvester considering no periodicity and periodicity, with 36 cells. A conclusion summarizing the results is presented in section 5.

2 MODEL FORMULATION

The piezoelectric energy harvesting device is modeled as a bimorph beam under plain-strain hypothesis, with series connection of the parallel piezoelectric layers and grounded on the substrate. Linear isoparametric four-node elements are considered for the FE analysis.

After simplifying the constitutive equations of piezoelectricity using plain-strain hypothesis from the linear Hamilton principle and knowing the linear stress-displacement and electric field-electric potential relations, the element piezoelectric and mass stiffness matrices can be obtained. After an assembly procedure, considering a harmonic excitation of amplitude F and excitation frequency ω and that the harvester is in open-circuit condition (no electric charges), the following linear equation is obtained [12,13]:

$$\left(\begin{bmatrix} \mathbf{K}_{uu} & \mathbf{K}_{\phi u}^T \\ \mathbf{K}_{\phi u} & -\mathbf{K}_{\phi\phi} \end{bmatrix} - \omega^2 \begin{bmatrix} \mathbf{M} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \right) \begin{Bmatrix} \boldsymbol{u} \\ \boldsymbol{\phi} \end{Bmatrix} = \begin{Bmatrix} \boldsymbol{F} \\ \mathbf{0} \end{Bmatrix} \tag{1}$$

In eq. (1), $\boldsymbol{F}$, $\boldsymbol{u}$ and $\boldsymbol{\phi}$ are the nodal applied force, displacement and voltage amplitude vectors, respectively, while $\mathbf{K}_{uu}$, $\mathbf{K}_{\phi u}$, $\mathbf{K}_{\phi\phi}$ and $\mathbf{M}$ are the global mechanical stiffness, piezoelectric coupling, dielectric and mass matrices, respectively. The element-wise calculation of the matrices are shown in eq. (2).

$$\begin{aligned} \mathbf{K}_{uu}^e &= \int_{\Omega^e} \mathbf{B}_u^T \mathbf{c}^E \mathbf{B}_u \, d\Omega^e \\ \mathbf{K}_{\phi u}^e &= \int_{\Omega^e} \mathbf{B}_\phi^T \mathbf{e} \mathbf{B}_u \, d\Omega^e \\ \mathbf{K}_{\phi\phi}^e &= \int_{\Omega^e} \mathbf{B}_\phi^T \boldsymbol{\varepsilon}^S \mathbf{B}_\phi \, d\Omega^e \\ \mathbf{M}^e &= \int_{\Omega^e} \mathbf{N}^T \rho \mathbf{N} \, d\Omega^e \end{aligned} \tag{2}$$

In eq. (2), the superscript e indicates an element, $\mathbf{N}$ is the matrix that contain the coefficients of the shape linear shape functions, $\mathbf{B}_u$ and $\mathbf{B}_\phi$ are the first order derivative matrices of the shape functions, used to interpolate the displacements and electric potentials, respectively. The piezoelectric material properties $\mathbf{c}^E$, $\mathbf{e}$, $\boldsymbol{\varepsilon}^S$ and ρ are shown in Table 1 for PZT-4. The substrate material is steel, with $E = 200\ GPa$ Young's modulus, $\nu = 0.29$ Poisson's ratio and $\rho = 7860\ kg/m^3$ specific mass.

The boundary conditions are: zero displacements in the clamped portion of the beam; zero electric potential for the piezoelectric-substrate interface; the furthest upper piezoelectric surface nodes have equal electric potential, as well as the lower ones, due to the electrodes. This coupling restriction is met by expanding eq. (1) using a Lagrange matrix $\boldsymbol{\Lambda}$ [13], which contains the equipotential voltage restrictions. Simplifying eq. (1) to $\mathbf{K}_g \boldsymbol{u}_g = \boldsymbol{F}_g$, the following linear system must be solved:

Table 1: PZT-4 properties

Property	**Value**
Elasticity matrix $\mathbf{c}^E$ (constant electric field)	$\begin{bmatrix} 1.390 & 0.778 & 0.743 & 0 & 0 & 0 \\ 0.778 & 1.390 & 0.743 & 0 & 0 & 0 \\ 0.743 & 0.743 & 1.154 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0.256 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.256 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.306 \end{bmatrix} 10^2 GPa$
Coupling matrix $\mathbf{e}$	$\begin{bmatrix} 0 & 0 & -5.2 \\ 0 & 0 & -5.2 \\ 0 & 0 & 15.1 \\ 0 & 12.7 & 0 \\ 12.7 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} C/m^2$
Dielectric matrix $\boldsymbol{\varepsilon}^S$ (constant strain)	$\begin{bmatrix} 6.45 & 0 & 0 \\ 0 & 6.45 & 0 \\ 0 & 0 & 5.62 \end{bmatrix} nF/m$
Specific mass ρ	$7500 kg/m^3$

$$\begin{bmatrix} \mathbf{K}_g & \mathbf{\Lambda}^T \\ \mathbf{\Lambda} & \mathbf{0} \end{bmatrix} \begin{Bmatrix} \boldsymbol{u}_g \\ \boldsymbol{l} \end{Bmatrix} = \begin{Bmatrix} \boldsymbol{F}_g \\ \mathbf{0} \end{Bmatrix} \tag{3}$$

In equation (3), $\boldsymbol{l}$ is a vector that when pre-multiplied by $\mathbf{\Lambda}^T$ represents the internal forces necessary to impose the electrode coupling constraints, and is not used for subsequent calculations.

3 TOPOLOGY OPTIMIZATION

The topology of the piezoelectric harvester is optimized using the soft-kill BESO method[9] in order to maximize the mechanical to electric energy conversion ratio, or rather, minimize its inverse value ζ, as shown in the objective function in eq. (4)[2,3].

The BESO method is a sensitivity based topology optimization method that uses discrete design variables. This is especially advantageous for the thickness profile optimization of piezoelectric harvesters, since the location of the electrode is easily defined by the solid-void boundaries during the optimization process. Checkerboard pattern and mesh dependency are avoided by applying a filter in each iteration.

$$\begin{aligned} &minimize && \zeta = 1 + \frac{\Pi^S}{\Pi^E} \\ &subject\ to && \sum_i x_i V_i = V^* \\ & && x_i = x_{min}\ or\ 1 \end{aligned} \tag{4}$$

In eq. (4), Π^S and Π^E are the dynamic mechanical and electric energies, respectively, calculated as shown in eq. (5). V^* is the target volume.

$$\Pi^S = \boldsymbol{u}^T \left(\mathbf{K}_{uu} - \omega^2 \mathbf{M}\right) \boldsymbol{u} \qquad and \qquad \Pi^E = \boldsymbol{\phi}^T \mathbf{K}_{\phi\phi} \boldsymbol{\phi} \tag{5}$$

Furthermore, in eq. (4), x_i with $i = 1, ...,$ *number of elements* are the design variables, which are equal to 1 if the FE is solid and equal to a small value x_{min}, close to zero, when it is void. To determine if the element should be solid or void, the element sensitivities α_i are calculated, which are equal to the derivative of the objective function with respects to the design variables x_i, as shown in equation (6).

$$\alpha_i = \frac{\partial \zeta}{\partial x_i} = \frac{1}{\Pi^S} \frac{\partial \Pi^S}{\partial x_i} - \frac{1}{\Pi^E} \frac{\partial \Pi^E}{\partial x_i} \tag{6}$$

Where the derivative of the mechanical Π^S and electric Π^E energies with respect to the i-th design variable are calculated using the adjoint method as:

$$\begin{aligned} \frac{\partial \Pi^S}{\partial x_i} &= \left(\frac{1}{2}\boldsymbol{u}^T + \boldsymbol{\lambda}_1^T\right) \left(\frac{\partial \mathbf{K}_{uu}}{\partial x_i} - \omega^2 \frac{\partial \mathbf{M}}{\partial x_i}\right) \boldsymbol{u} + \boldsymbol{\lambda}_1^t \frac{\partial \mathbf{K}_{\phi u}^T}{\partial x_i} \boldsymbol{\phi} + \boldsymbol{\mu}_1^T \frac{\partial \mathbf{K}_{\phi u}}{\partial x_i} \boldsymbol{u} - \boldsymbol{\mu}_1^T \frac{\partial \mathbf{K}_{\phi\phi}}{\partial x_i} \boldsymbol{\phi} \\ \frac{\partial \Pi^E}{\partial x_i} &= \left(\frac{1}{2}\boldsymbol{\phi}^T - \boldsymbol{\mu}_2^T\right) \frac{\partial \mathbf{K}_{\phi\phi}}{\partial x_i} \boldsymbol{\phi} + \boldsymbol{\lambda}_2^T \left(\frac{\partial \mathbf{K}_{uu}}{\partial x_i} - \omega^2 \frac{\partial \mathbf{M}}{\partial x_i}\right) \boldsymbol{u} + \boldsymbol{\lambda}_2^T \frac{\partial \mathbf{K}_{\phi u}^T}{\partial x_i} \boldsymbol{\phi} + \boldsymbol{\mu}_2^T \frac{\partial \mathbf{K}_{\phi u}}{\partial x_i} \boldsymbol{u} \end{aligned} \tag{7}$$

The following linear systems are solved to find the adjoint vectors $\boldsymbol{\lambda}_1$, $\boldsymbol{\mu}_1$, $\boldsymbol{\lambda}_2$ and $\boldsymbol{\mu}_2$, respectively:

$$\begin{aligned} \begin{bmatrix} \mathbf{K}_{uu} - \omega^2 \mathbf{M} & \mathbf{K}_{\phi u}^T \\ \mathbf{K}_{\phi u} & -\mathbf{K}_{\phi\phi} \end{bmatrix} \begin{Bmatrix} \boldsymbol{\lambda}_1 \\ \boldsymbol{\mu}_1 \end{Bmatrix} &= \begin{Bmatrix} -\left(\mathbf{K}_{uu} - \omega^2 \mathbf{M}\right) \boldsymbol{u} \\ \mathbf{0} \end{Bmatrix} \\ \begin{bmatrix} \mathbf{K}_{uu} - \omega^2 \mathbf{M} & \mathbf{K}_{\phi u}^T \\ \mathbf{K}_{\phi u} & -\mathbf{K}_{\phi\phi} \end{bmatrix} \begin{Bmatrix} \boldsymbol{\lambda}_2 \\ \boldsymbol{\mu}_2 \end{Bmatrix} &= \begin{Bmatrix} \mathbf{0} \\ -\mathbf{K}_{\phi\phi} \boldsymbol{\phi} \end{Bmatrix} \end{aligned} \tag{8}$$

In order to implement the sensitivity calculations shown above, the derivative of each stiffness matrix with respects to the design variables have to be defined. In this work, the SIMP material interpolation scheme is used, with a penalization factor for each of the material property. Thus, the element stiffness matrices are:

$$\mathbf{K}_{uu}^e = x^{p_1} \mathbf{K}_{uu0}^e \quad \mathbf{K}_{\phi u}^e = x^{p_2} \mathbf{K}_{\phi u0}^e \quad \mathbf{K}_{\phi\phi}^e = x^{p_3} \mathbf{K}_{\phi\phi 0}^e \quad \mathbf{M}^e = x^{p_m} \mathbf{M}_0^e \tag{9}$$

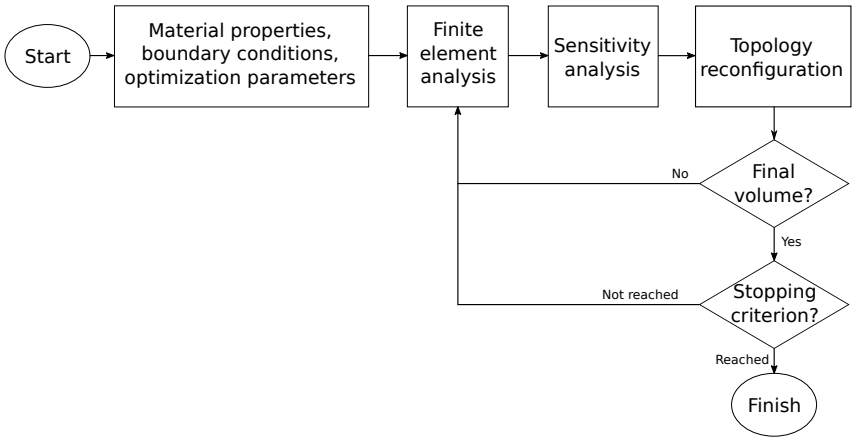


Figure 2: BESO flowchart

The subscript 0 indicates the value when the element is solid, calculated as shown in (2).

Additional weight factors w_S and w_E are used in eq. (6) to improve the algorithm's convergence stability, with $0 < w_E = 1 - w_S < 1$.

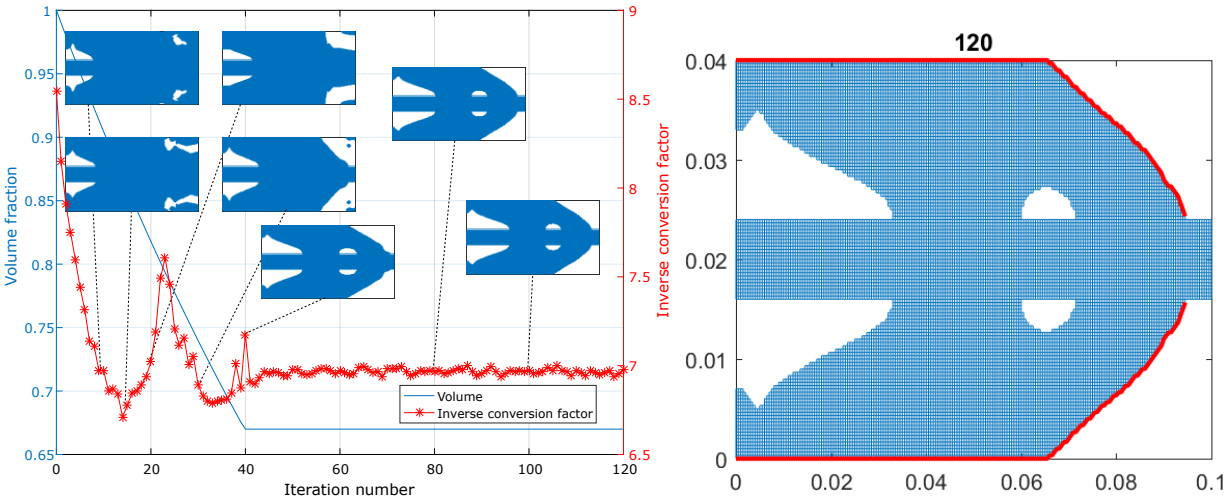
$$\alpha_i = w_S \frac{1}{\Pi^S} \frac{\partial \Pi^S}{\partial x_i} - w_E \frac{1}{\Pi^E} \frac{\partial \Pi^E}{\partial x_i} \tag{10}$$

The cellular topology is obtained by applying a periodicity constraint in the sensitivity calculation and through the subsequent step in the optimization algorithm by, in which the topology is redesigned, by adding or removing a number of elements multiple of the number of cells. In this work, the design domain consists solely on piezoelectric elements.

The initial volume of the design domain is 100%. Figure 2 shows a flowchart of the optimization procedure. After defining the material property values, the boundary constraints and the optimization parameters, the iterative procedure starts. A FE analysis is done, thus obtaining $\boldsymbol{u}$ and $\boldsymbol{\phi}$. Next the sensitivity calculation, filtering and analysis is performed and, based on their values as well as the next iteration's volume, the topology is reconfigured (values of x_i). This loop repeats itself until the target volume is reached and a stopping criterion is met. The stopping criterion is determined by the mean value of the objective function's variation during the last 10 iterations, and has to be less than a certain value, such as $1 \cdot 10^{-7}$.

4 RESULTS

In this section results of the proposed topology optimization algorithm are shown, first considering no periodicity constraint and then with it. The problem optimizes the piezoelectric harvester shown schematically in Fig. 1, which also shows what the boundary conditions are. The applied harmonic point force has a 1 N amplitude. The harvester has a 100 mm length, a 40 mm thickness and an 8 mm thick substrate. As mentioned



(a) Inverse conversion factor ζ

(b) Final topology. The red lines are the electrodes.

Figure 3: Results for no periodicity constraint

previously, the piezoelectric material considered for the analysis was PZT-4, with the properties shown in Table 1, and a substrate was considered steel, with $E = 200\ GPa$, $\nu = 0.29$ and $\rho = 7860\ kg/m^3$. In all cases, the harvester is optimized for low frequency excitation: $\omega = 300\ Hz$. The target volume of the piezoelectric material was 67% of its initial volume.

4.1 No periodicity constraint

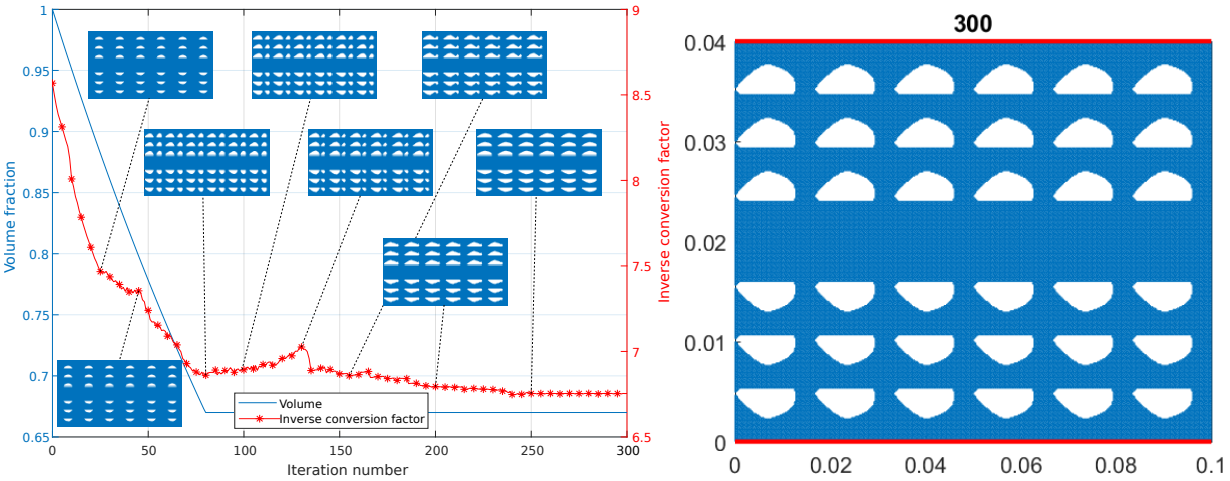
The topology was optimized using a 200 by 120 (24000) element mesh. The evolutionary ratio was 1%, the maximum element addition ratio was 0.5% and the filter radius was 4 mm. The penalization factors p_1, p_2, p_3 and p_m were 3, 2, 1 and 1, respectively. The sensitivity weight factors were $w_S = 62\%$ and $w_E = 38\%$. The results are shown in Fig. 3.

The inverse conversion factor was successfully minimized from 8.56 to 6.95. And the electric potential difference between the upper and lower electrodes decreased from 55.95 mV to 34.15 mV.

4.2 Cellular: 36 cells

The topology was then optimized considering 6 by 6 (36) cells, with a total of 108000 elements. The evolutionary ratio was 0.5%, the maximum element addition ratio was 0.25% and the filter radius was 4 mm. The penalization factors and the sensitivity weight factors were the same as in the no periodicity case. The results are shown in Fig. 4.

The inverse conversion factor was minimized from 8.56 to 6.75. Notice that the inverse



(a) Inverse conversion factor ζ

(b) Final topology. The red lines are the electrodes.

Figure 4: Results for a bimorph piezoelectric harvester with 36 cells

conversion factor's final value is smaller than the value of the optimized non-periodic case. Furthermore, the electric potential difference between the two electrodes decreased from 55.95 mV to 47.79 mV. The electric potential difference is larger than for the non-periodic case, which is more favorable, especially considering that for closed-circuits it is generally desired to maximize the electrical power output, which is directly proportional to the square of this value. It is noticeable how the convergence curve in Fig. 4 is more stable than in Fig. 3.

5 CONCLUSIONS

A two-dimensional bimorph beam-like piezoelectric energy harvesting device with series connection modeled under plain-strain hypothesis was successfully topologically optimized using a soft-kill BESO algorithm for harmonic excitation under open-circuit condition. Two main results were shown: one considering no periodicity constraint; and another with 36 cells.

The results show that the optimal topology for the periodic case yields a inverse conversion factor equal to 6.75 (a measure of mechanical to energy conversion efficiency), which is smaller than that of the optimized topology for the non-periodic case, namely 6.95. Furthermore, the electric potential voltage difference between the electrodes is larger for the cellular optimized topology, which is more desirable, with regards to electrical power output to a closed-circuit.

For future projects, damping effects can be taken into account in the harmonic analysis, base excitation can be considered as the input instead of an applied force and the periodic topology optimization can be done using the inverse homogenization method.

6 ACKNOWLEDGEMENTS

The authors are grateful to FAPESP (São Paulo Research Foundation, grant numbers 2013/08293-7 and 2018/00075-4) and CAPES (Coordination for the Improvement of Higher Education Personnel) for their financial support of this work.

REFERENCES

[1] Erturk, A. and Inman, D.J., Piezoelectric Energy Harvesting. John Wiley & Sons, Ltd (2011).

[2] Zheng, B., Chang, C.J. and Gea, H.C., Topology optimization of energy harvesting devices using piezoelectric materials. Structural and Multidisciplinary Optimization (2008)38(1):17–23.

[3] Noh, J.Y. and Yoon, G.H., Topology optimization of piezoelectric energy harvesting devices considering static and harmonic dynamic loads. Advances in Engineering Software (2012)53:45 – 60.

[4] Lin, Z.Q., Gea, H.C. and Liu, S.T., Design of piezoelectric energy harvesting devices subjected to broadband random vibrations by applying topology optimization. Acta Mechanica Sinica (2011)27(5):730–737.

[5] Kiyono, C.Y., Silva, E.C.N. and Reddy, J.N., Optimal design of laminated piezocomposite energy harvesting devices considering stress constraints. International Journal for Numerical Methods in Engineering (2016)105(12):883–914.

[6] Kim, K., Zhu, W., Qu, X., Aaronson, C., McCall, W.R., Chen, S. and Sirbuly, D.J., 3d optical printing of piezoelectric nanoparticle–polymer composite materials. ACS Nano (2014)8(10):9799–9806.

[7] Bodkhe, S., Turcot, G., Gosselin, F.P. and Therriault, D., One-step solvent evaporation-assisted 3d printing of piezoelectric PVDF nanocomposite structures. ACS Applied Materials & Interfaces (2017)9(24):20833–20842.

[8] de Almeida, B.V. and Pavanello, R., PIEZOELECTRIC HARVESTER TOPOLOGY OPTIMIZATION USING A MULTIPARAMETER MATERIAL MODEL. Proceedings of the XXXVIII Iberian Latin American Congress on Computational Methods in Engineering, ABMEC Brazilian Association of Computational Methods in Engineering (2017) .

[9] Huang, X. and Xie, M., Evolutionary Topology Optimization of Continuum Structures: Methods and Applications. Wiley (2010).

[10] Vicente, W.M., Picelli, R., Pavanello, R. and Xie, Y.M., TOPOLOGY OPTIMIZATION OF PERIODIC STRUCTURES FOR COUPLED ACOUSTIC-STRUCTURE SYSTEMS. Proceedings of the VII European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS Congress 2016), Institute of Structural Analysis and Antiseismic Research School of Civil Engineering National Technical University of Athens (NTUA) Greece (2016) 3565–3582.

[11] Vicente, W., Zuo, Z., Pavanello, R., Calixto, T., Picelli, R. and Xie, Y., Concurrent topology optimization for minimizing frequency responses of two-level hierarchical structures. Computer Methods in Applied Mechanics and Engineering (2016)301:116–136.

[12] IEEE, IEEE Standard on piezoelectricity. ANSI/IEEE Std 176-1987 (1988).

[13] Cook, R.D., Malkus, D.S. and Plesha, M.E., Concepts and Applications of Finite Element Analysis. Wiley (2001).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Design of a Damper for Suborbital Payloads Based on Honey Comb Structures and Additive Manufacture

Eduardo Amaro*, Fernando Velazquez**

*UNAM, **UNAM

ABSTRACT

One of the most critical phases in suborbital flights is guarantee the integrity of the payload. This can suffer severe damage during the landing because of the impact. To solve this issue dampers are implemented for dissipating kinetical energy. However, this implies add mass to the gondola, which reduces the altitude reached during the flight. In this work honey comb structures are applied to design a light damper for suborbital payloads. The main objective is to maximize the energy dissipation while mass is minimized. By changing geometric parameters several structures were proposed and studied by Finite Element Analysis to calculate the energy absorption during impact. Due to the geometric complexity of the structure additive manufacture is used for manufacturing the structure.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Topology Optimisation of Metallic Fins in Adsorbed Natural Gas Tanks

Ricardo Amigo*, Robert Hewson**, Emilio Silva***

*University of Sao Paulo, **Imperial College London, ***University of Sao Paulo

ABSTRACT

Adsorption is a retention mechanism of fluid molecules on solid surfaces that is explored in gas storage applications. Adsorbed Natural Gas (ANG) tanks are constituted by porous materials which accumulates gas molecules by adsorption, reaching storing densities similar to tanks based on compression at much lower pressure. The major drawback of such tanks is the high dependency of the adsorption phenomenon on temperature, which hinders the attainment of the full storage capacity. In this work, the Topology Optimisation Method (TOM) is implemented to distribute metal in adsorbent beds to improve the heat exchange in order to maximise the total mass of gas admitted during tanks filling cycle. FEniCS is used to solve the governing equations of the adsorption problem (continuity, energy balance and adsorption kinetics) and the sensitivities are obtained via the transient adjoint method. Resulting topologies are presented and compared with tank constituted by pure adsorbent beds.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Efficient Topology Optimization with Geometric Nonlinearities Using Reanalysis-based Approaches

Oded Amir*, Matti Spicer**

*Technion - Israel Institute of Technology, **Technion - Israel Institute of Technology

ABSTRACT

Topology optimization is a computational method for finding the optimal distribution of material in a given design domain. It is typically applied for balancing weight and stiffness, and has developed into a widespread computational design approach that is widely used in automotive and aerospace industries. Because the problem is defined and solved on a finite element discretization of the continuum domain, it inherently involves a very large number of state variables (e.g. displacements) that need to be computed in every design cycle. Several approaches have been suggested for reducing the computational effort invested in such sequences of finite element analyses, however they focus on optimization considering linear static responses. The need for efficient procedures is more evident when the underlying structural analysis is nonlinear – this is the focus of the current contribution. In this talk, we will present and discuss efficient solution procedures for nonlinear structural analysis based on reanalysis and reuse of information throughout the optimization process. First, we follow the two schemes proposed in [1]: I) The solution (i.e. displacements) of the nonlinear structural analysis corresponding to a certain design cycle is used as a starting point for the analysis in the next design cycle; II) The factorization (or preconditioner) of the tangent stiffness matrix corresponding to a certain design cycle is reused in subsequent design cycles. Second, we investigate the influence of the problem formulation: In linear static cases, it was shown that reanalysis is more effective for volume minimization than for stiffness maximization due to the advantages of “stiff preconditioning” [2]. The extension of this observation to the case of geometrically nonlinear (GNL) responses will be examined and discussed. Finally, we enhance the procedures presented in [1] by employing reanalysis in the solution of the linear adjoint problem, enabling further computational savings. Preliminary results show that significant computing time can be reduced by applying various combinations of the schemes described above. Furthermore, the effect of “stiff preconditioning” and the consequent benefit of volume minimization are shown to be valid also for the GNL case. Test cases will include the optimization of beams and columns undergoing large deformations and buckling. [1] Amir, O., 2011. Efficient reanalysis procedures in structural topology optimization (Doctoral dissertation, PhD thesis, Technical University of Denmark). [2] Amir, O., 2015. Revisiting approximate reanalysis in topology optimization: on the advantages of recycled preconditioning in a minimum weight procedure. Structural and Multidisciplinary Optimization, 51(1), pp.41-57.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Redox Fuel Cell Capable of Converting Fuels to Electricity at a High Rate

Liang An*

*The Hong Kong Polytechnic University

ABSTRACT

The use of hydrogen peroxide in fuel cells has recently received increasing attention, primarily due to its several unique characteristics when compared with the use of gaseous oxygen. However, there are three issues associated with the use of hydrogen peroxide in fuel cells. Firstly, the actual cathode potential is lower than the theoretical one, which is mainly attributed to the mixed potential resulting from the simultaneous hydrogen peroxide oxidation reaction on the cathode. Secondly, the hydrogen peroxide oxidation reaction releases gaseous oxygen, leading to a two-phase mass transport. Thirdly, the reduction of hydrogen peroxide in fuel cells has to use metal catalysts, such as platinum, palladium and gold. In this work, we propose to create the cathode potential by introducing a redox couple to the cathode while to use hydrogen peroxide to chemically charge to redox ions. The redox cathode not only completely eliminates the mixed-potential problem associated with the direct reduction of hydrogen peroxide, but also enables a faster cathodic electrochemical kinetics even without noble metal catalysts. It has been demonstrated that the direct ethanol fuel cell with a redox couple of V(IV)/V(V) yields a peak power density of 450 mW cm-2 at 60oC, which is 87.5% higher than that of the conventional cell with direct reduction of hydrogen peroxide.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Coupled Atomistics and Discrete Dislocations in 3d (CADD-3d)

Guillaume Anciaux*, Jaehyun Cho**, Till Junge***, Max Hodapp****, Jean-François Molinari*****, William Curtin******

*EPFL, **EPFL, ***EPFL, ****EPFL, *****EPFL, ******EPFL

ABSTRACT

Capturing plasticity at realistic dislocation densities with high configurational complexity requires a continuum-level discrete dislocation dynamics (DDD) description. However, many features controlling dislocation motion are inherently atomistic, such as the interaction of dislocations with solutes, precipitates, cracks, interfaces and nucleation. In two dimensions, modeling these phenomena in a multi-scale manner was possible thanks to the method Coupled Atomistic and Discrete Dislocation dynamics (CADD2d). Here, we present an approach that extends this multiscale coupling in 3d (CADD3d). The algorithm principle will be described in details, where dislocations can be described with atomistic resolution intimately coupled to a surrounding continuum domain in full 3d. In such a case, individual dislocation lines may span both domains simultaneously, therefore forming hybrid dislocations, partially represented with dislocated atoms and partially as discrete lines. Continuum dislocation properties and atomistic dislocation properties need to match closely. An implementation prototype is presented based on the DDD code Paradis and on the MD code LAMMPS, altogether interfaced with the coupling code LibMultiScale. Simulations of the dynamics of a single hybrid dislocation and of a hybrid dislocation loop will illustrate the potential and robustness of the approach for near-seamless motion of dislocations into, across, and out of the atomistic domain. Finally we present the nucleation of dislocation loops emitted from a Frank-Read source and then transformed into DD dislocations, demonstrating the possibilities of our framework.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Higher-Order Finite Element ALE Method with Non-conforming Mesh Refinement

Robert Anderson*, Veselin Dobrev**, Robert Rieben***, Vladimir Tomov****, Jakub Cerveny*****, Tzanio Kolev******

*LLNL, **LLNL, ***LLNL, ****LLNL, *****University of West Bohemia in Pilsen, ******LLNL

ABSTRACT

We present non-conforming adaptive mesh refinement extensions for a higher-order finite element ALE code and methodology that has been under development by Kolev, Dobrev, Rieben, et. al. [1][2]. The underlying ALE methodology is a Lagrange plus remap scheme, and can be characterized as a higher-order generalization of the classical staggered grid Lagrange plus remap hydrodynamics methods. The Lagrangian phase uses continuous finite elements for kinematic variables and the curvilinear mesh, and discontinuous finite elements for thermodynamic variables. The remap phase is based on a conservative, monotonic DG formulation. The AMR extension involves element-by-element, potentially anisotropic h-refinement at a fixed polynomial order. The resulting AMR systems of equations involve constraints on hanging nodes when there are continuity requirements, and in this case the system is solved through variational restriction. The hanging node constraints are specified through a prolongation matrix P, which maps "true" degrees of freedom (DOFs) to the full set of DOFs which are potentially non-conforming if no constraints are applied. The efficient construction of P in parallel is an essential component of the AMR method. Parallel partitioning of the AMR hierarchy is achieved through the use of a space-filling curve, which is then equipartitioned to distribute the elements to MPI ranks to achieve load balance. These methods have been incorporated into the finite element library MFEM, which forms the foundation of the ALE code under development. With the choice of abstractions utilized in MFEM, it is notable that adoption of AMR in the aforementioned ALE code is remarkably unintrusive. With the foundations of an AMR capability in place, we will discuss some initial verification and performance characterization results of the ALE-AMR method, and ongoing research into suitable refinement criteria and the use of dynamic regridding. [1] V. Dobrev, Tz. Kolev and R. Rieben, “High-Order Curvilinear Finite Element Methods for Lagrangian Hydrodynamics”, SISC., Vol. 34, pp. B606-B641, (2012). [2] R. Anderson V. Dobrev, Tz. Kolev and R. Rieben, “Monotonicity in High-Order Curvilinear Finite Element ALE Remap,” IJNMF, Vol. 77, pp. 249-273 (2014).
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Row-Wise Clustering for Sparse and Spatial Local Reduced-Order Bases

Spenser Anderson*, Tina White**, Phil Avery***, Charbel Farhat****

*Stanford University, **Stanford University, ***Stanford University, U.S. Army Research Laboratory, ****Stanford University

ABSTRACT

The construction of a Projection-based Reduced-Order Model (PROM) relies on the precomputation of a Reduced-Order Basis (ROB) representing an approximation subspace that, despite having a dimension much smaller than that of the underlying High-Dimensional Model (HDM), can capture its dominant features. It is common to build this ROB by collecting many solution snapshots from the HDM and compressing them using the SVD. However, for highly nonlinear problems characterized by multiple regimes, a single ROB often needs to be prohibitively large in order to deliver the desired accuracy. This issue was recently addressed by introducing the concept of local ROBs [1]. There, the solution manifold is partitioned into subregions using a clustering algorithm applied to the columns of the snapshot matrix. Local ROBs are constructed by compressing the clustered snapshots, and are assigned to the subregions of the manifold they best represent. Although this approach has demonstrated a significant potential for achieving simultaneously good speed-ups and accuracy, it has room for improvement. To this end, this talk will describe a complementary approach for constructing local ROBs where clustering is performed row-wise or row-column-wise, instead of column-wise. More importantly, it will be shown that row clustering, which can be described as spatial clustering, is an effective approach for sparsifying a ROB and therefore accelerating online PROM simulations. It will also be shown that for problems with localized phenomena, row clustering leads to more effective PROMs than column clustering. Most importantly, row clustering can be combined with column clustering to simultaneously achieve dimensional reduction and sparsification, and therefore to maximize computational efficiency. It is also amenable to existing hyper reduction techniques such as GNAT [2] for CFD, and ECSW [3] for CSD. Finally, the talk will illustrate all stated properties of row clustering with several examples from computational mechanics. 1. D. Amsallem, M. Zahr and C. Farhat, Nonlinear Model Order Reduction Based on Local Reduced-Order Bases, International Journal for Numerical Methods in Engineering, Vol. 92, pp. 891-916 (2012) 2. K. Carlberg, C. Bou-Mosleh and C. Farhat, Efficient Nonlinear Model Reduction via a Least-Squares Petrov-Galerkin Projection and Compressive Tensor Approximations, International Journal for Numerical Methods in Engineering, Vol. 86, pp 155-181 (2011) 3. C. Farhat, T. Chapman and P. Avery, Structure-Preserving, Stability, and Accuracy Properties of the Energy-Conserving Samplingand Weighting (ECSW) Method for the Hyper Reduction of Nonlinear Finite Element Dynamic Models, International Journal for Numerical Methods in Engineering, Vol. 102, pp. 1077-1110 (2015)

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Spanwise Surface Roughness Heterogeneity: Circulation Intensity and a Prognostic Model for Turbulent Secondary Flows

William Anderson*, Kalyan Shrestha**

*UT Dallas, **UT Dallas

ABSTRACT

Spanwise surface heterogeneity beneath high-Reynolds number, fully-rough wall turbulence is known to induce mean secondary flows in the form of counter-rotating streamwise vortices. The secondary flows are a manifestation of Prandtl's secondary flow of the second kind -- driven and sustained by spatial heterogeneity of components of the turbulent (Reynolds averaged) stress tensor. The spacing between adjacent surface heterogeneities serves as a control on the spatial extent of the counter-rotating cells, while their intensity is controlled by the spanwise gradient in imposed drag (where larger gradients associated with more dramatic transitions in roughness induce stronger cells). In this work, we have performed an order of magnitude analysis of the mean (Reynolds averaged) streamwise vorticity transport equation, revealing the scaling dependence of circulation upon spanwise spacing. The scaling arguments are supported by a simulation data. Then, we demonstrate that mean streamwise velocity can be predicted a priori via a similarity solution to the mean streamwise vorticity transport equation. A vortex forcing term was used to represent the affects of spanwise topographic heterogeneity within the flow. Efficacy of the vortex forcing term was established with large-eddy simulation cases, wherein vortex forcing model parameters were altered to capture different values of spanwise spacing.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Modeling of Organic-organic Interfaces and Mixtures for Organic Photovaltaic Applications

Denis Andrienko*

*Max Planck Institute for Polymer Research

ABSTRACT

We will discuss the role of mesoscale order, electrostatic effects, defects, and roughness for charge splitting and detrapping at organic-organic interfaces. We will show how inclusion of mesoscale order resolves the controversy between experimental and theoretical results for the energy-level profile and alignment in a variety of photovoltaic systems, with direct experimental validation [1,2]. We will show how one can predict open-circuit voltages of planar heterojunction solar cells, in excellent agreement with experimental data, based only on crystal structures and interfacial orientation. We will show how long-range molecular order and interfacial mixing generate homogeneous electrostatic forces that can drive charge separation and prevent minority carrier trapping across a donor-acceptor interphase [2]. Comparing several of small-molecule donor-fullerene combinations, we will illustrate how tuning of molecular orientation and interfacial mixing leads to a trade-off between photovoltaic gap and charge-splitting and detrapping forces, with consequences for the design of efficient photovoltaic devices. By accounting for long-range mesoscale fields, we will obtain the ionization energies in both crystalline and mesoscopically amorphous systems with high accuracy [4,5]. References: [1] C. Poelking, M. Tietze, C. Elschner, S. Olthof, D. Hertel, B. Baumeier, F. Wuerthner, K. Meerholz, K. Leo, D. Andrienko, Nature Materials, 14, 434, 2015 [2] C. Poelking, D. Andrienko, J. Am. Chem. Soc., 137, 6320, 2015 [3] M. Schwarze, W. Tress, B. Beyer, F. Gao, R. Scholz, C. Poelking, K. Ortstein, A. A. Guenther, D. Kasemann, D. Andrienko, K. Leo, Science, 352, 1446, 2016 [4] P. Kordt, J. J. M. van der Holst, M. Al Helwi, W. Kowalsky, F. May, A. Badinski, C. Lennartz, and D. Andrienko, Adv. Funct. Mater. 25, 1955, 2015 [5] C. Poelking, D. Andrienko J. Chem. Theory Comput., 12, 4516, 2016

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

FE Modelling of Tensile Deformation of Ductile Cast Iron Using In-Situ 3D Tomography Results as Input and Validation

Tito Andriollo*, Yubin Zhang**, Jesper Thorborg***, Jesper Hattel****

*Department of Mechanical Engineering, Technical University of Denmark, **Department of Mechanical Engineering, Technical University of Denmark, ***Department of Mechanical Engineering, Technical University of Denmark, ****Department of Mechanical Engineering, Technical University of Denmark

ABSTRACT

In key industrial sectors like transportation and energy production there is a strong demand for improving the performance of ductile cast irons, in order to optimize designs for lower weight and longer life. Consequently, research efforts are currently being made to understand quantitatively the mechanisms controlling deformation and fracture at the micro-scale. As emphasized in a recent review paper (Hütter et al. [2015]), a major challenge is represented by the complex material microstructure, which consists of graphite particles embedded in a steel matrix. Remarkably, most of the theoretical models developed so far assume that this microstructure is stress-free at room temperature. However, recent synchrotron-based studies by the present authors have demonstrated that the thermal contraction mismatch between the graphite and the matrix during manufacture leads to localized elastic and plastic deformation (Zhang et al. [2016]). Also, the residual stress field associated with the elastic strain is non-negligible and highly affected by the sub-structure of the graphite particles, which creates stress concentrations in the matrix (Andriollo et al. [2017]). The present work takes these studies to the next step by investigating how this inhomogeneous residual stress field affects the deformation mechanisms of the material at the micro-scale. First, a FE model based on a RVE obtained from micro computed tomography (CT) is developed and used to simulate manufacture and tensile loading of ductile cast iron. Then, the model results are validated by means of digital volume correlation, based on CT scans acquired in-situ during deformation. Finally, the importance of taking residual stress and 3D effects into account is discussed in relation to previous findings from the literature.
REFERENCES: Andriollo, T., Hellström, K., Sonne, M.R., Thorborg, J., Tiedje, N., and Hattel, J. 2018, "Uncovering the local inelastic interactions during manufacture of ductile cast iron: How the substructure of the graphite particles can induce residual stress concentrations in the matrix ", J. Mech. Phys. Solids, 111, 333–357. Hütter, G., Zybell, L., and Kuna, M. 2015, “Micromechanisms of fracture in nodular cast iron: From experimental findings towards modeling strategies – A review”, Eng. Fract. Mech., 144, 118–141. Zhang, Y.B., Andriollo, T., Fæster, S., Liu, W., Hattel, J., and Barabash, R. I. 2016, "Three-dimensional local residual stress and orientation gradients near graphite nodules in ductile cast iron", Acta Mater., 121, 173–180.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Error Estimation and Adaptivity Using Hierarchical Splines with Applications to Fracture Mechanics

Cosmin Anitescu*, Somdatta Goswami**, Timon Rabczuk***

*Leibniz Universität Hannover, **Bauhaus-Universität Weimar, ***Bauhaus-Universität Weimar

ABSTRACT

We present a method for error analysis and adaptivity when the approximation space considered is that of smooth piecewise polynomials. It is well-known that higher-order and higher smoothness bases, such as the ones used in isogeometric analysis [1] provide an efficient way to approximate smooth solutions as well as compatibility with existing CAD models. Nevertheless, we focus on applications to problems with discontinuities, for which adaptivity is needed to efficiently represent the approximate solution. We introduce and compare recovery and residual-based estimators for hierarchical splines, as well as algorithms for performing h- and p- adaptivity. The problems considered involve fracture which is modeled by means of a phase field approach [2]. Several benchmark problems will be considered to demonstrate the performance of the presented method. [1] T.J.R. Hughes, J.A. Cottrell, Y. Bazilevs, Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement, Computer Methods in Applied Mechanics and Engineering, Volume 194, Issues 39–41, 2005, Pages 4135-4195, ISSN 0045-7825, [2] C. Miehe, M. Hofacker, F. Welschinger, A phase field model for rate-independent crack propagation: Robust algorithmic implementation based on operator splits, Computer Methods in Applied Mechanics and Engineering, Volume 199, Issues 45–48, 2010, Pages 2765-2778, ISSN 0045-7825

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Self-organization of Nanostructured Morphologies in Physical Vapor Deposited Phase-separating Multicomponent Alloys

Kumar Ankit*, Rahul Raghavan**

*Arizona State University, **Arizona State University

ABSTRACT

Experiments have demonstrated a rich variety of self-organized nanoscale concentration modulations in physical vapor deposited films of phase-separating alloys. However, a comprehensive model that is capable of predicting the entire spectrum of these self-organized nanostructures as a function of material and processing parameters has yet to be developed. We adopt a phase-field approach to numerically investigate the role of substrates, deposition rates, phase fraction and separation kinetics, on the morphological self-structuring in vapor-deposited alloys. Based on synergies with experimental results, we map out the processing space where the evolution of mixed morphology is favorable. We propose new strategies for morphology control based on the insights gained from our numerical study.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Isogeometric Analysis on Trimmed Volumetric Geometries

Pablo Antolin*, Annalisa Buffa**, Gershon Elber***, Massimiliano Martinelli****, Fady Massarwi*****

*École polytechnique fédérale de Lausanne. Switzerland, **École polytechnique fédérale de Lausanne. Switzerland / Istituto di Matematica Applicata e Tecnologie Informatiche "Enrico Magenes", IMATI - CNR. Pavia, Italy, ***Technion - israel Institute of Technology, ****Istituto di Matematica Applicata e Tecnologie Informatiche "Enrico Magenes", IMATI - CNR. Pavia, Italy, *****Technion - israel Institute of Technology

ABSTRACT

The idea of designing and analyzing methods able to alleviate the remeshing step by directly using the output of CAD is the challenge of Isogeometric analysis (IGA), which was proposed by T.J.R. Hughes and co-authors in 2005. In this work we propose a methodology for treating volumetric geometries (V-reps), constructed using the IRIT modeler through boolean operations and trimming. It allows to use isogeometric discretizations in a Galerkin-like context for 2D and 3D spline trimmed domains in a fully automatic way. When trying to assemble the operators of a discrete variational problem element by element, it is immediately clear that integrals for the Bézier elements affected by the boolean operations are not easily computable. Suitable quadrature formulas that consider only the part of the element inside the computational domain are required. In order to do that we split the geometry in Bézier elements. The elements not affected by trimming operations are processed in a standard way, while for trimmed Bézier elements we present two different approaches. A first approach subdivides the trimmed element into spline patches (tiles), that together are identical geometrically to trimmed Bézier element. Currently, this approach is only applicable for 2D geometries (even embedded in a 3D euclidean space). A second methodology consists in meshing “à la finite elements” every trimmed element. Thus, for every trimmed element a boundary representation (B-rep) is created, then we a create a high-order mesh (in order to approximate correctly the boundary of the B-rep) of the interior using Gmsh. This approach works for both 2D and 3D geometries. In both approaches the quadrature formula of every Bézier element is composed by a set of quadrature formulas, one for every tile. In addition to compute integrals in the interior of the computational domain, this methodology allows to compute integrals on the domain boundary. The degree of the tiles is chosen accordingly to the degree of the spline functions used in the discretization of the unknown variables. We show theoretically that, by using the same degree for both the discretization of the unknowns and the tiles, the method presents optimal approximation properties for any degree. We present numerical results that support the theoretical results and examples involving complex and trimmed geometries that illustrate the potential applicability of the method. Finally, future perspectives are drawn.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Optimum Design of Thrust Bearings for Maximizing the Load Capacity

Olga Antonova*, Alexey Borovkov**, Yuri Boldyrev***, Igor Voynov****

*Peter the Great St.Petersburg Polytechnic University, **Peter the Great St.Petersburg Polytechnic University, ***Peter the Great St.Petersburg Polytechnic University, ****Peter the Great St.Petersburg Polytechnic University

ABSTRACT

One of the most important structural elements of the wide range of the power machines is hydrodynamic thrust bearing which perceives a major part of load. The important operational parameter that characterizes the efficiency of the bearing is the load capacity of an oil wedge, which has nonlinear dependence on gap size. However, reduction of oil film thickness leads to decreasing the bearing stability under dynamic loads. In this study we consider the lubricant layer microgeometry profiling with the aim of optimal design of the hydrodynamic bearing for ensuring the maximum load capacity. Historically the first formulation of the considered problem in one-dimensional case goes back to the work by J.W. Rayleigh published in 1918 [1]. The Rayleigh results were much ahead of his time, were repeated later by S. Y. Maday only in 1967 [2]. In 1975 one of the authors together with V.A. Troitsky considered the spatial variational problem put by Rayleigh to gain the optimal shape profile for the rectangular gap region. Here we enlarge the results of the previous works in relation to the sector thrust bearings based on advanced computing technologies. The special case for one sector of self-aligning acting bearing with profile consisted of two parts: straight line and generalized ellipse was considered. Geometrical parameters witch define profile curvature were used as optimization variables during optimization procedure. Using special code IOSO the optimization problem was solved. As objective function the maximum of pressure integral over the lubricant layer surface was used. To solve the optimization problem, the CFD mesh for investigated domain was generated and hydrodynamics problem, using Navier-Stocks equations was solved on the basis of numerical approach and commercial CFD code ANSYS/CFX. The numerical simulation of the problem was carried out using the St.Petersburg Polytechnic Supercomputer Center. References [1] Lord Rayleigh. Notes on the theory of lubrication, Phil. Mag.35 (1) (1918),p. 1-12. [2] C. J. Maday A Bounded Variable Approach to the Optimum Slider Bearing, Trans. ASME. Ser. F. J. Lubr. Technol. 90(1) (1968), p. 240-242 [3] Yu.Yu. Boldyrev, V.A. Troitsky One spatial variational problem of the theory of gas lubrication, Tidings AS USSR MFG 5(1975), p.34-39

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Modeling Microwave Induced Fragmentation of Heterogeneous Rocks for Mining Applications

Thomas Antretter*, Michael Toifl**, Philipp Hartlieb***, Ronald Meisels****, Friedemar Kuchar*****

*Institute of Mechanics, Montanuniversitaet Leoben, **Institute of Mechanics, Montanuniversitaet Leoben, ***Chair of Mining Engineering and Mineral Economics, Montanuniversitaet Leoben, ****Institute of Physics, Montanuniversitaet Leoben, *****Institute of Physics, Montanuniversitaet Leoben

ABSTRACT

Excavation processes in mining and tunneling are very costly, especially if the rock material is very hard. Only 1% of the invested energy is converted into the creation of new surfaces, i.e., the fragmentation of the rock while almost the entire rest is lost as frictional heat. A more economical alternative is to heat up the rock by means of microwave irradiation thereby creating thermal stresses high enough to generate cracks in the rock so that subsequent mechanical processes already cut into a partly pre-damaged and hence softer material. Quantification of the potential energy savings requires a thorough analysis of the physical phenomena coming into play. This includes a) the propagation of the electro-magnetic waves emitted by a high-power microwave source into the rock-material, b) locally varying heating due to absorption of the microwaves, c) redistribution and evolution of the temperature field due to heat conduction, d) thermal expansion of the differently heated areas followed by mechanical strains and stresses inside the rock that locally exceed the rock's strength thus leading to micro-cracks that eventually coalesce and form a dominant crack. The heterogeneous nature of natural rocks must be taken into account, because the different material properties of the individual constituents of a rock significantly amplify the temperature gradients and stresses hence accelerating the formation of cracks. The theoretical investigations were carried out by a numerical full field analysis of the coupled phenomena a) to d) enumerated above. The electrical material properties, more specifically the permittivity across a wide temperature range, were experimentally measured in a specifically designed oven. The thermal expansion properties were determined using dilatometry on thin rock samples. The numerically obtained crack patterns showed a good agreement with the ones found in full-scale microwave irradiation experiments.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Evolutionary Aseismic Design of Three-Dimensional Structures with Passive Devices

Georgios Apostolakis*, Gary Dargush**

*University of Central Florida, **SUNY at Buffalo

ABSTRACT

Current seismic codes do not incorporate a systematic and well-establish methodology for the topological distribution and properties of passive devices in three-dimensional structures. The issue is further exaggerated when structures are subject to extreme events and operate well within their inelastic range. To overcome the above shortcomings, an evolutionary computational framework was developed to design tall regular and irregular three-dimensional buildings when subjected to a predefined seismic environment (Apostolakis and Dargush, 2012). The framework incorporated Mixed Lagrangian Formalism (MLF) variational principles within an evolutionary compact Cellular Automata-based Genetic Algorithm (CAGA). From the evolutionary process, the optimal placement, strength and size of hysteretic dampers throughout the height of the structures were obtained. The topological distributions of the braces throughout the height of the structure corresponded to patterns that were not seen in common practice. Furthermore, the optimization framework produced optimal designs with reduced drifts while reducing accelerations at the same time, when compared to the original base structure. In this presentation, our previous work is extended to include different type of passive devices (e.g., viscous dampers), enhanced Self-Automated based Genetic Algorithm (SAGA) incorporating deep learning technique to establish the weighted probabilistic gene-by-gene cross-over and mutation operations, and hierarchical multiscale brace architectures where brace topology patterns can span multiple bays/stories (mega-braces). The objectives will be to establish (a) a robust computational framework to yield designs based on ductility demand throughout the height of the yielded structure under seismic loading, (b) identify optimal designs with ductility demand uniformly distributed throughout the height, (c) realize novel three-dimensional multiscale mega-brace architectures, (d) require modest computational and engineering effort well within the range of typical seismic design firms. Apostolakis G, Dargush GF, Filiatrault A (2014) Computational Framework for Automated Seismic Design of Steel Frames with Self-Centering Connections, ASCE Journal of Computing in Civil Engineering, 28(2), 170-181. Apostolakis G, Dargush GF (2012) Optimal Design of Three-Dimensional Structures with Hysteretic Braces, 15th World Conference on Earthquake Engineering (WCEE), 24-28 September, Lisbon, Portugal. Apostolakis G, Dargush GF (2010) Optimal Seismic Design Of Moment-Resisting Steel Frames with Hysteretic Passive Devices, Earthquake Engineering and Structural Dynamics, 39, 355-376.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Hermite and dG Methods for Wave Equations and Their Application to Uncertain and Inverse Problems

Daniel Appelö*, Thomas Hagstrom**, Mohammad Motamed***, Arturo Vargas****, Yunan Yang*****

*University of Colorado, Boulder, **Southern Methodist University, ***University of New Mexico, ****Lawrence Livermore National Laboratory, *****University of Texas at Austin

ABSTRACT

In this talk we report on the development of high order Hermite and dG methods for wave equations in second order form and its applications to forward propagation of uncertainties and the inversion of material parameters from boundary measurements. The Hermite methods come in two flavors, dissipative and conservative. The dissipative method achieves space-time accuracy of order (2m+1), while the conservative method has space-time order (2m). Besides their high order of accuracy in both space and time combined, the methods have the special feature that they are stable for CFL numbers up to and including unity for all orders of accuracy. Curiously, when using CFL equal to one, the orders of both methods increase. Our spatial discontinuous Galerkin discretization of wave equations in second order form relies on a new energy based strategy featuring a direct, mesh-independent approach to defining interelement fluxes. Both energy-conserving and upwind discretizations can be devised. The method comes with optimal a priori error estimates in the energy norm for certain fluxes and we present numerical experiments showing that optimal convergence for certain fluxes. The forward propagation of uncertainties is performed by a new multi-order Monte Carlo algorithm for computing the statistics of stochastic quantities of interest. The method is a non-intrusive technique based on a high (but variable) order discretizations, as those presented. The algorithm is built upon a hierarchy of degrees of polynomial basis functions rather than a mesh hierarchy used in multi-level Monte Carlo. In addition to the convenience of working with a fixed mesh, which is desirable in many real applications with complex geometries, the multi-order method is particularly beneficial in reducing errors due to numerical dispersion in long-distance propagation of waves. To invert for P and S velocities in the elastic wave equation we extend the novel trace-by-trace quadratic Wasserstein metric (W2) technique pioneered by Yang and co-authors. We give examples comparing W2 with the standard L2 misfit.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Lower-Triangular Mass Matrix Approach to Explicit Time Advancement for Continuous Triangular Finite Element Methods

Jay Appleton*, Brian Helenbrook**

*Clarkson University, **Clarkson University

ABSTRACT

When using explicit time advancement with continuous high order finite elements, a mass matrix is formed which must be inverted to advance the solution in time. For the Gauss-Lobatto-Lagrange basis typically used on quadrilaterals, an accurate approximate diagonal mass matrix exists which makes explicit time stepping methods efficient while achieving pth-order spatial convergence rates. No such approach exists for triangular methods. This work introduces an alternative in the form of a lower-triangular method that achieves pth-order convergence. This specific lower-triangular method allows for computationally efficient time advancement without sacrificing spatial accuracy.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Usage of the Discrete Element Method for the Study of Concrete

Antonio Aquino*, Ruben Lopez**, Osvaldo Quintana***

*National University of Asuncion. Faculty of Engineering, **National University of Asuncion. Faculty of Engineering, ***National University of Asuncion. Faculty of Engineering

ABSTRACT

The DEM was applied for the first time to concrete by Bazant and his collaborators (Zubelewicdz & Bazant, 1987; Bazant et al., 1990) based on the DEM previously proposed for the study of granular geomaterials, (Cundall & Strack, 1979). In the current literature, some models represent cement grains by equivalent spheres as an initial state prior to the hydration process (Maekawa et al., 2009). Ulm & Lemarchand (2003), sought to obtain the mechanical properties of cement paste as a function of time during the hydration process from the development of a multiscale model validating their results through experimental data obtaining a very good correlation of them. Within the area of the study of the cement hydration process there is still a limited literature that addresses this process through this numerical technique. On the other hand, in recent times with the use of mass concrete structures in civil construction has been necessary to consider the evolution of temperature in the structure to prevent the formation of cracks of thermal origin in it. This work proposes obtaining a multi-scale model that describes the phenomena associated with the hydration of concrete and applying this model to the analysis of the different types of concrete produced in Paraguay. The model is implemented through the use of the Discrete Elements Method (DEM). To calibrate the implementation of the mechanical component of the model, the Abaqus program was used. For this simulation, the strategy used to initialize the model consisted of specifying the approximate initial position of the particles with some distance between them to allow the particles that accommodate themselves in their position under the action of gravity. The element consists on an only one node element that describes the spherical particle, whose kinematics is modeled as a rigid body and where any adjustment is made in the model constituting the contact between particles. For the calibration of the implementation of the thermal component of the model, the LIGGGHTS program was used, where spherical particles were also used. The obtained results show that the method of the discrete elements is suitable to model a thermo-mechanical problem, in addition, the temperature distributions obtained are comparable with those obtained in a continuous model based on the Finite Element Method.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

The Discontinuity-Enriched Finite Element Method (DE-FEM): New Developments for Fracture and Unfitted Mesh Problems

Alejandro M. Aragón*, Jian Zhang**, Sanne J. van den Boom***, Elena De Lazzari****, Dongyu Liu*****, Max van der Kolk******, Matthijs Langelaar*******, Angelo Simone********, Fred van Keulen*********

*Delft University of Technology, Delft, the Netherlands, **Delft University of Technology, Delft, the Netherlands, ***Delft University of Technology, Delft, the Netherlands, ****Delft University of Technology, Delft, the Netherlands, *****Delft University of Technology, Delft, the Netherlands, ******Delft University of Technology, Delft, the Netherlands, *******Delft University of Technology, Delft, the Netherlands, ********University of Padua, Padova, Italy, *********Delft University of Technology, Delft, the Netherlands

ABSTRACT

Weak and strong discontinuities play an important role in the analysis of a wide range of (multi-physics) problems, such as fracture or multi-phase materials. In standard Finite Element Analysis (FEA), discontinuities are explicitly taken into account by the spatial discretization, by ensuring that any material interfaces, domain boundaries, and/or cracks coincide with element sides. Creating such a matching mesh can be a challenging exercise, especially when dealing with complex 3D geometries. To make matters worse, remeshing has to take place in cases where the problem domain undergoes changes between analysis steps. This occurs, for example, in shape or topology optimization or in fluid-structure interaction. Remeshing is also an important issue in crack propagation, where a special mesh has to be created around crack fronts. The Discontinuity-Enriched Finite Element Method (DE-FEM) [1] was recently introduced as a novel enriched formulation to model weak and strong discontinuities without the need of a matching mesh. In DE-FEM, enriched degrees of freedom are placed only along discontinuities, resulting in a new modelling paradigm with several key properties. Indeed, this allows a hierarchical implementation of enrichment functions, which simplifies the analysis of arbitrary cracked configurations (e.g., n-junctions or cracks traversing material interfaces). Moreover, Dirichlet boundary conditions can be prescribed in a strong manner, which gives DE-FEM an edge over other enriched formulations such as XFEM/GFEM. In this presentation, we will demonstrate the versatility of the method in the context of fracture mechanics, granular materials, immersed domains, and fluid-structure interaction. We illustrate the method for modelling 2D and 3D cracks, and NURBS-enhanced discontinuities. Furthermore, we demonstrate DE-FEM as an immersed boundary (or embedded domain) method for problems in elasticity and in the context of fluid dynamics and fluid-structure interaction. Finally, we show the stability of the method with regards to the condition number of the resulting system matrices.
REFERENCES [1] Aragón AM, Simone A. The discontinuity-enriched finite element method. Int J Numer Meth Engng. 2017;112:1589–1613. https://doi.org/10.1002/nme.5570

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Non-linear Multi-Scale Modeling of 3D Fabric-Rubber Composites

Damian Aranda-Iglesias*, Gaetano Giunta**, Salim Belouettar***, Anne Peronnet-Paquin****, Franco Sportelli*****, Daniel Keniray******

*Luxembourg Institute of Science and Technology, **Luxembourg Institute of Science and Technology, ***Luxembourg Institute of Science and Technology, ****The Goodyear Tire & Rubber Company, *****The Goodyear Tire & Rubber Company, ******The Goodyear Tire & Rubber Company

ABSTRACT

Mechanical testing of complex 3D fabric-rubber composites considering structurally different textiles as reinforcements are expensive and time-consuming. Therefore, it is of benefit to develop mechanical models that allow a better understanding of the interaction between the constituents and of the role played by the different length scales in the complex textile micro-structure. The current study seeks to predict the behavior of 3D fabric-rubber composites using a multi-scale modelling approach. The composite structure is divided into simplified models at different scales and a finite element full field homogenization is conducted at each of these scales. The mechanical response is, then, fitted by appropriate isotropic or anisotropic hyperelastic material models connecting the information in a staggered multi-scale approach. The multi-scale based modeling approach presented in this work is intended to support the development of these new 3D fabric-rubber materials by enabling the optimization of the different constituents to obtain specific mechanical properties.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Hypersonic Spatially-developing Turbulent Boundary Layers via DNS

Guillermo Araya*, Kenneth Jansen**

*University of Puerto Rico-Mayaguez, **University of Colorado-Boulder

ABSTRACT

DNS of compressible spatially-developing turbulent boundary layers is performed at a Mach number of 5 over an isothermal flat plate. Turbulent inflow information is generated by following the concept of the rescaling-recycling approach introduced by Lund et al. (J. Comp. Phys. 140, 233-258, 1998), although, the proposed methodology is extended to hypersonic flows. Furthermore, a dynamic approach is employed to connect the friction velocities at the inlet and recycle stations (i.e., there is no need of an empirical correlation as in Lund et al.). Additionally, the Morkovin's Strong Reynolds Analogy (SRA) is used in the rescaling process of the thermal fluctuations from the recycle plane. Low/high order flow statistics are compared with direct simulations of an incompressible isothermal ZPG boundary layer at similar Reynolds numbers and temperature regarded as a passive scalar. Focus is given to the assessment of flow compressibility on the dynamics of hydrodynamic/thermal coherent structures. Preliminary results have shown that large hydrodynamic turbulent structures are finer and less organized in compressible flow than in the incompressible regime, with less intense "gaps" of high speed fluids in between. A similar conclusion can be drawn for thermal structures. Q2 events are observed to form more elongated and voluminous zone in the incompressible case. Acknowledgement This material is based upon work supported by the Air Force Office of Scientific Research under award number FA9550-17-1-0051. An award of computer time was provided by the Innovative and Novel Computational Impact on Theory and Experiment (INCITE) program and the Theta and Aurora Early Science Programs. This research used resources of the Argonne Leadership Computing Facility, which is a DOE Office of Science User Facility supported under Contract DE-AC02-06CH11357. NSF-CBET Grant #1512393. XSEDE computational allocation #TG-CTS170006.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Multiscale Hybrid-Mixed Method for the Stokes/Brinkman Equations

Rodolfo Araya*

*Departamento de Ingenieria Matematica, Universidad de Concepcion, Concepcion, Chile

ABSTRACT

In this work a Multiscale Hybrid-Mixed method (MHM), applied to the Stokes/Brinkman equations on heterogeneous media, is introduced and analyzed. Given a coarse partition of the domain and using a hybrid formulation, the MHM method consists of independent Stokes/Brinkman local problems bring together by a face-based weak formulation on the skeleton of the partition. The multiple scales of the media are incorporated in the basis functions which are driven by the local problems with prescribed Neumann boundary conditions. Once available (exactly or approximatively), the multiscale basis functions are used to compute the degrees of freedom from a faced-based global variational problem defined on the skeleton of the partition. The numerical solution shares the important properties of the continuum as the local equilibrium with respect to external forces and local mass conservation. Several numerical tests assess the accuracy and the conservative properties of MHM method on academic and highly heterogeneous cases.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A One-dimensional Model for Large Deformation and Materially Nonlinear Analysis of 3-D Structures

Archana Arbind*, J N Reddy**, Arun Srinivasa***

*Advanced Computational Mechanics Laboratory,Department of Mechanical Engineering, Texas A&M; University, College Station, **Advanced Computational Mechanics Laboratory,Department of Mechanical Engineering, Texas A&M; University, College Station, ***Department of Mechanical Engineering, Texas A&M; University, College Station

ABSTRACT

In this study, a general higher-order 1-D theory (i.e., rod theory) is presented to analyze the large deformation of 3-D structures, which have a space curve as their central axis (see Arbind and Reddy [1] and [2]). A general displacement field of the cross-section perpendicular to the reference curve has been considered in the form of Fourier series in the curvilinear polar cylindrical coordinate system. For the framing of the reference curve, Frenet frame (for C3 continuous regular space curve) as well as frame based on relatively parallel field or Bishop frame (see [3]) for more general C1 continuous and piece-wise regular curve are used. A nonlinear finite element formulation has been presented for linear and nonlinear material such as incompressible neo-Hookean and Mooney-Rivlin solids. The incompressibility condition is imposed via the Lagrange multiplier method and the penalty method in two separate finite element models. Also, due to the one-dimensional nature of this formulation, this theory can be easily implemented for the higher-order gradient elasticity, which requires higher-order continuous interpolation function in the fi nite element model; this can be easily achieved by higher-order Hermite interpolation functions in the one-dimensional analysis. Various numerical examples are presented to illustrates the application of the presented theory to analyze the curved pipe or other shell structures, which have application in bio-mechanics. The numerical results have been compared with the shell theory or 3-D fi nite element model of the same problems. Keywords. one-dimensional theory; general higher-order rod theory; Neo-Hookean material; Mooney-Rivlin material; analysis of curved pipe References: [1] A Arbind and JN Reddy. A one-dimensional model of 3-d structure for large deformation: a general higher-order rod theory. Acta Mechanica, pages 1-29, 2017. [2] A Arbind and JN Reddy. A general higher-order one-dimensional model for large deformation analysis of solid bodies. Computer Methods in Applied Mechanics and Engineering, 328:99-121, 2018. [3] Richard L Bishop. There is more than one way to frame a curve. The American Mathematical Monthly, 82(3):246-251, 1975.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

General Constitutive Updating for Finite Strain Formulations Based on Assumed Strains and the Jacobian

Pedro Areias*, Timon Rabczuk**

*CERIS - Instituto Superior Técnico and Universidade de Évora, Portugal, **Bauhaus University, Weimar, Germany

ABSTRACT

Compatibility between element technology featuring assumed (finite)-strains based on least-squares and most constitutive formulations employed in elastic and inelastic contexts is a demanding task. Local frames are required for anisotropic and cohesive laws, some assumed-strain element technologies do not explicitly provide the deformation gradient, and total Lagrangian approaches are often inadequate for advanced plasticity models. Kirchhoff stress-based \bm{F}_{e}\bm{F}_{p} decompositions are also not convenient for ductile damage models. In addition, if rotational degrees-of-freedom are used, as is the case in beams and shells, the adoption of a fixed undeformed configuration entails implementation brittleness. An additional aspect to consider is remeshing by element partition, which precludes the storage of constitutive tensors in local frames, invalidating the stored quantities. Based on seven algorithmic requirements and the corresponding design solutions, we introduce a general constitutive updating algorithm based on the strain and the Jacobian provided by the element. This allows the use of virtually any constitutive law with any finite-strain element formulation while satisfying the seven requirements. In addition, Newton-Raphson convergence properties are extraordinary, at the cost of precision in the strain rate estimation. As a prototype element implementation, we present a stable hexahedron based on least-squares strains. A BFGS secant estimation is employed for the weight in the least-squares so that softening constitutive laws can be adopted without stability issues at the element level.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Lattice Boltzmann Finite Element Methodology for 2D Fluid-structure Interaction with Moving Boundary Conditions

Marco Argenta*, Sara Bueno**

*UFPR, **UFPR

ABSTRACT

This work proposes a methodology for solving two-dimensional incompressible fluid-structure interaction in moving and deformable boundary problems. The proposition is modeling the fluid flow by lattice Boltzmann method (LBM) using BGK formulation (Bathnagar et al, 1954), whose principle is based on mesoscale discretization of the particles with motion on a fixed grid of probabilities, and the moving and deformed boundary using frame finite elements. The LBM has computational advantages in computational cost comparing to the conventional solution based on the Navier-Stokes equations (Guzella et al, 2016). However, even being very efficient, modeling the boundary conditions in the LBM are still a problem for numerical estability when the interactions between fluid and structure take effect, especially when the structure is flexible. In order to simulate this behavior the lattice mesh at each interation is updated creating or destroying lattices according to fluid domain defined by the flexible boundary conditions, moreover an interpolation algorithm for lattices with immersed boundary is proposed. These informations are obtained by mapping the fluid displacements that are consequence of the geometric variation in domain. The novelty of this work is modeling the boundary using finite element method (FEM) considering one-dimensional frame elements restricted to small deformations and rotations. This version is very attractive for solving coupling problems because numerical instabilities are reduced due to the low complexity of the elements formulation with allow a better understanding of the simulation in order to rise the complexibility of the model. Furthermore, using frame elements enables to obtain tensions and deformations results in the walls that hold the fluid in motion. The method is described and it is validated on well-established literature similar two-dimensional cases.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Parametric Study of a Fractal Helmholtz Resonator System

Clara Argerich Martin*, Rubén Ibanez Pinillo**, Anaïs Barasinski***, Emmanuelle Abisset-chavanne****, Francisco Chinesta*****

*GeM, Ecole Centrale Nantes, **ICI, Ecole Centrale Nantes, ***GeM, Ecole Centrale Nantes, ****ICI, Ecole Centrale Nantes, *****ESI Group, ENSAM Paris

ABSTRACT

The Helmholtz resonator is one of the oldest acoustic devices and has been largely exploited in literature. Different acoustic absorption systems have been designed and proposed, acoustic solutions vary from combining different resonators to adding a membrane to widen the sound absorption range , as in [1]. In this work we propose an acoustic system of connected Helmholtz Resonators following a fractal generation based on the 'Cantor Set' fractal formation, which is explained on detail in [2]. A single Helmholtz resonator is able to absorb a specific frequency depending on its geometry: the volume of the cavity and the length and diameter of the pipe. In our proposed system we start with two Helmholtz resonators connected by a pipe, and at each new generation new cavities are added whose geometry depends on the initial one. The main benefit of using a fractal sequence is that the resonance frequencies of the system depend on the initial volume, length and diameter of the pipes and the number of generations. In other words, the stiffness matrix of the dynamic system depends on the initial geometry of the problem and the number of generations, which leads to a parametric eigenvalues problem. Through a non-intrusive resolution of the parametric eigenvalue problem and the subsequent construction of a model relating geometrical parameters with eigenfrequencies, an inverse problem for attenuating certain frequencies present in the incident acoustic loading can be formulated and successfully solved. A deeper machine-learning based analysis should inform on the most relevant geometrical parameters with respect to the wished target, and more particularly the relationship between space curvatures (at the different fractal generations) and time curvatures (frequencies) that could be also put in relation using a model or deep learner. Finally the parametric acoustic problem will be solved in the frequency domain, while including selective linear or frequency-dependent damping, by combining the parametric PGD-rationale with a wavelet based approximation to regularise the solution procedure in presence of highly localized solution around the (parametric) natural frequencies. [1] A.Sanada, N. Tanaka Extension of the frequency range of resonant sound absorbers using two-degree-of-freedom Helmholtz-based resonators with a flexible panel. Applied Acoustics 74 (2013) 509–516 – 2012 [2] Mandelbrot B, The fractal geometry of Nature. New York (NY): W.H. Freeman and Company; 1983.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

General Purpose Finite Element Library for Computation of High-Order Multivariable Sensitivities

Mauricio Aristizabal*, Harry Millwater**, Manuel Garcia***

*Universidad EAFIT, **University of Texas at San Antonio, ***University of Texas at San Antonio

ABSTRACT

Computation of accurate sensitivities of finite element analysis is a necessity for general multiphysics problems. Among different approaches, hypercomplex algebras, i.e. algebras with one or more imaginary units, have been successfully used to compute high order derivatives due to the lack of subtraction cancellation error. This work presents a library that uses the variational formulation of the Partial Differential Equation that model multi-physics problems and computes high order sensitivities with respect to multiple variables using Order Truncated Imaginary (OTI) numbers. These variables include problem parameters, shape derivatives and boundary conditions. The library has been tested with different physical models including the Laplace/Poisson equation, linear elasticity and the stokes equation in 2D. Derivatives with respect to shape (both Lagrangian and Eulerian derivatives), spatial coordinates and/or problem parameters, such as heat transfer coefficient and modulus of elasticity were obtained. All derivatives were computed using only one finite element analysis, hence only required one assembly procedure. Results showed that similar to the solution of the state variable, derivative accuracy is dependent on the mesh discretization. Also, all computed derivatives obtained lower error than the best equivalent finite difference solution. Solution time of the system using LU factorization showed that solving each new derivative takes approximately 2.5% the time it takes to solve the real-only system of equations. As a result, the developed library using OTI algebra allows a more efficient computation of high order derivatives for multivariable sensitivities in the finite element method.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Coupling Mechanical Evolution to Electrochemical Performance in Lithium-Ion Batteries

Craig Arnold*

*Princeton University

ABSTRACT

Because of their high energy densities and high working voltages, lithium-ion batteries are the most suitable energy storage choice for a variety of applications from large scale battery electric vehicles to small scale implantable medical devices. These systems are well-known to experience both mechanical and electrochemical phenomena and in this presentation, we discuss how the evolution of internal and external mechanical stress affects the electrochemical performance over the lifetime and how the electrochemical state of the system influences its mechanical properties. Based on a detailed understanding of mechanical and electrochemical coupling, we find that spatially localized phenomena which create non-uniform ionic transport across the electrode materials have the most significant effect on system lifetime and safety. Using numerical models as well as experimental measurements, we identify the critical length scale for localization and suggest methodologies for mitigating such phenomena in real-world battery systems.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Updating Nonparametric Probabilistic Models in Structural Dynamics by Bayesian Statistical Inversion of Symmetric Positive Definite Matrices in High Dimension

Maarten Arnst*, Christian Soize**

*University of Liège, **Université Paris-Est

ABSTRACT

This work is concerned with the updating of probabilistic models for the dynamical behavior of structures and their associated parametric and model uncertainties. Whereas much research in structural dynamics has already addressed the Bayesian statistical inversion of mechanical parameters of structural-dynamics models, the present work focuses on the Bayesian statistical inversion of reduced matrices of reduced-order models. In [1], Soize had introduced a nonparametric probabilistic modeling approach, which uses the maximum-entropy principle to construct a probability distribution capable of representing parametric and model uncertainties in reduced matrices of reduced-order models. In the present work, this probability distribution serves as the prior probability distribution, which is then updated by using Bayes' formula to accommodate data relevant to the dynamical behavior of the structure in a posterior probability distribution. This Bayesian statistical inverse problem is computationally challenging because the support of the posterior is restricted to the symmetric positive definite matrices and because it is of high dimension. In [2], Soize had introduced an Ito-SDE-based MCMC method for sampling from maximum-entropy probability distributions in high dimension. In the present work, this method serves as a basis to propose a method for sampling from the Bayesian posterior. The proposed method exploits a transformation of measure to set up the Markov chain in terms of state variables whose distribution is standard Gaussian under the prior probability distribution but non-Gaussian under the posterior probability distribution. It inherits computational efficiency from the fact that it can exploit the gradient and the Hessian of the distance that the Bayesian update uses to gauge the fit between the reduced-order model and the data. At the conference, we will present the proposed Bayesian statistical inversion, its computational aspects, and its application to an illustration from structural dynamics. [1] C. Soize. A nonparametric model of random uncertainties for reduced matrix models in structural dynamics. Probabilistic Engineering Mechanics, 15:277-294, 2000. [2] C. Soize. Construction of probability distributions in high dimension using the maximum entropy principle: Applications to stochastic processes, random fields and random matrices. International Journal for Numerical Methods in Engineering, 76:1583-1611, 2011.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Computational Approximation of Mesoscale Field Dislocation Mechanics at Finite Deformation

Rajat Arora*, Amit Acharya**

*Carnegie Mellon University, **Carnegie Mellon University

ABSTRACT

Dislocation, being the primary carriers of plastic deformation, play a pivotal role in determining the strength and mechanical properties of engineering materials. The use of first principles to understand complex dislocation interactions occurring at extremely small spatial and temporal scales has been successful in modeling material behavior. However, the steep computational cost associated with these methods limit the system sizes and simulation times that can be achieved in practice. Hence, a continuum scale 'fundamentally accurate' model that enables a predictive understanding of dislocation-mediated deformation serves a complementary purpose. We describe finite deformation results of a Partial Differential Equation (PDE) based model, termed as Mesoscale Field Dislocation Mechanics (MFDM), to understand meso-macroscale plasticity in solids as it arises from dislocation motion / nucleation within the material. The potential and generality of MFDM are demonstrated by applying it to study some (initial) boundary value problems. We demonstrate the stress-field path followed in a body corresponding to a sequence of dislocations starting from a single dislocation to a stress-free dislocation wall constituting a grain boundary. Another example that will also be presented is to quantify the change in the volume in the body upon introduction of dislocations dating back to Toupin and Rivlin's seminal work. Size effects and development of strong in-homogeneity in the simple-shearing of physically constrained and unconstrained grains in the material up to large strains will also be demonstrated. The mechanical structure and the thermodynamical framework of MFDM provide the driving force for the dislocation velocity which has the property that the curve moves perpendicular to itself in space when the dislocation density field is localized. Adopting this as a kinematical implication, we also present a simple example demonstrating longitudinal shear band propagation through essentially the motion of its tip wherein the driving force is uncoupled to the stresses.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Modelling the Round Window Membrane of the Guinea Pig: An Experimental Characterization of Fiber Distribution Based on Microscopic Imaging

Miguel Arriaga*, Daniel Arteaga**, Xun Wang***, Wenbin Wang****, Dimitrios Fafalis*****, Karen Kasza******, Anil Lalwani*******, Jeffrey Kysar********

*Columbia University, **Columbia University, ***Columbia University, ****Columbia University, *****Columbia University, ******Columbia University, *******Columbia University, ********Columbia University

ABSTRACT

The round window membrane (RWM) is a biological membrane separating the perilymph fluid-filled inner ear from the air-filled middle ear cavity, protecting the inner ear from middle ear pathology and modulating changes in perilymphatic pressure produced by the movement of the stapes. While the integrity of the RWM is essential for normal hearing, it is also the only easily accessible portal to the inner ear and therefore the ideal candidate for delivery of medicine and collection of samples for diagnosis. This access is a significant challenge for the current medical technology since the RWM is small (diameter <2mm), thin (thickness<100μm) and pre-stressed, thus easily tearing when perforated with standard surgical tools. To aid in the development of new surgical tools for a structurally safe access through the RWM, a robust modelling of the mechanical behavior of the RWM is necessary. The RWM possesses a layer of connective tissue (collagen and elastic fibers) that endows it with most of its mechanical strength and therefore characterization of the distribution and orientation of these fibers is essential. Confocal microscopy was conducted on intact RWMs isolated from Hartley guinea pigs to characterize for the first time the distribution of collagen and elastic fibers. The fibers were imaged by capturing the emitted signals due to second-harmonic-generation, auto-fluorescence and Rhodamine-B staining. A quantitative analysis of both orientation and dispersion was done such that a structure tensor approach modelling of the fibers was possible. Experimental tests of pressure bulging and micro-indentation were conducted to validate the numerical model and to estimate the hyperelastic parameters of the membrane.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Automatic Boundary Condition Model Parameterisation in Computational Haemodynamics

Christopher J Arthurs*, C Alberto Figueroa**

*King's College London, **University of Michigan; King's College London

ABSTRACT

Finding appropriate parameter values for boundary condition models remains one of the most difficult and time-consuming tasks when creating multi-scale models of haemodynamics. Typically, before any clinical or scientific questions can be addressed, a computational baseline model must first reproduce some carefully-defined target metrics, derived both from a combination of patient-specific and population data [1]. Practically and typically, this task amounts to finding appropriate values of resistances, compliances and inertances within lumped parameter network models of the vasculature beyond the boundaries of the three-dimensional portion of the model. Due to the time-consuming nature of this task, methods for automatic parameterisation by assimilation of patient data are of great interest. It has been shown how reduced-order unscented Kalman filtering (ROUKF), a sequential parameter estimation technique which makes use of an ensemble of simulation “particles” to construct a continuously-updated best estimate of a set of model parameters can be used to determine suitable parameter values for reproducing patient data [2]. However, these methods have only been applied to simple cases such as three-element Windkessel models, and cannot be directly applied to more complex boundary condition models due to the fact that such models have internal state, both present and historical, which must remain consistent with the particles. In the present work, we demonstrate how ROUKF can be applied to more complex models using a least squares approach to generate an internal boundary condition state which is consistent with the particle to which it belongs. We examine the particular case of finding the parameters of a coronary microvascular circuit in the presence of periodic extramicrovascular compression due to myocardial contraction, demonstrating that all five state parameters can be estimated from two continuous observations in the three-dimensional domain: one of pressure and one of volumetric flow. References [1] Arthurs C J , Agarwal P, John A V, Dorfman A L, Grifka R G and Figueroa C A. Reproducing Patient-Specific Hemodynamics in the Blalock–Taussig Circulation Using a Flexible Multi-Domain Simulation Framework: Applications for Optimal Shunt Design. Front Pediatr. 2017; 5: 78. DOI: 10.3389/fped.2017.00078 [2] Xiao, N. Simulation of 3-D Blood Flow in the Full Systemic Arterial Tree and Computational Frameworks for Efficient Parameter Estimation. PhD Thesis, Stanford University. December 2013.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Computational Swine Model for Regional Contractility in Ischemia with Left Bundle Branch Block

Jayavel Arumugam*, Lik Chuan Lee**, Ghassan Kassab***

*Michigan State University, **Michigan State University, ***California Medical Innovations Institute

ABSTRACT

Cardiac Resynchronization Therapy (CRT) non-responder rate sustains at 30% over two decades [1]. The reasons for therapy non-response remain unclear. The ability of the myocardium, with reduced myocardial perfusion and left bundle branch block (LBBB), to contract in response to the therapy is confounding [2]. We present our investigations on the interplay between ischemia and LBBB during bi-ventricular (BiV) pacing using a computational swine cardiac electro-mechanics (EM) model. The EM model accounts for signal conduction and mechanics. The signal conduction is described by the modified FitzHugh-Nagumo equations. The mechanics model comprises of a Fung-type passive constitutive model and an active stress constitutive model. Simulations are performed on a realistic biventricular geometry using the finite element method. Mechanical boundary conditions are applied using a lumped-parameter Windkessel model for systemic and pulmonic circulation. LBBB and different pacing conditions are simulated by varying the conduction velocity and applied electrical stimulus. Ischemia is simulated by decreasing contractility in the ischemic regions [3]. Pacing response and metabolic demand are quantified using cardiac output and regional fibre stress-fibre strain area, respectively. Our investigations using the computational model suggest that the metabolic demand with LBBB significantly increases in the presence of ischemia. This is consistent with previous experimental studies and clinical observations [1, 2]. Thoroughly validated refinements of the EM model are expected to be useful in predicting subject-specific CRT response during different pacing conditions. Further, extending the EM model to account for myocardial perfusion will enhance the utility of the model. [1] Kerckhoffs R.C.P., Lumens J. K., et al. Progress in Biophysics and Molecular Biology (2008) 97: 543-561. https://doi.org/10.1016/j.pbiomolbio.2008.02.024 [2] Svendsen M., Prinzen F.W., et al. Experimental Biology and Medicine (2012) 237-6: 644-651. https://doi.org/10.1258/ebm.2012.012023 [3] Lee L.C., Wenk J.F., et al. Journal of Biomechanical Engineering (2011) 133: 094506 1-5. doi:10.1115/1.4004995

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Implementation of Probabilistic Calculation of Tsunami Hydrodynamic Force

Rafael Aránguiz*, Pedro Osvaldo Rossel**

*Universidad Catolica de la Santisima Concepción, **Universidad Catolica de la Santisima Concepción

ABSTRACT

The design of port facilities at risk of tsunami attack requires tsunami forces to be estimated. These forces can be classified as impact, hydrodynamic, buoyancy, hydrostatic, and debris-induced, among other types. In general, two approaches can be used to estimate tsunami forces, namely, deterministic and probabilistic. While the former requires few tsunami scenarios such that maximum force values are selected, the latter requires hundreds or thousands of them and the adjustment of probabilistic density functions. In the present work, the hydrodynamic forces on a single structure in a fishing port are estimated using the probabilistic approach. Since hydrodynamic force depends on both sea surface elevation and current velocity, these variables need to be properly calculated. First, a synthetic earthquake catalog was generated and then a stochastic slip distribution was defined for each earthquake scenario in order to obtain the tsunami initial condition. To run the numerical tsunami simulations, the NEOWAVE (Non-hydrostatic Evolution of Ocean WAVEs) model was utilized. This model is based on the nonlinear shallow-water equation with a vertical velocity term to account for weakly dispersive waves. The vertical velocity term facilitates modeling of tsunami generation and transfer of kinetic energy from seafloor deformation. When the kinematic source mechanism is implemented, it is possible to complement the non-hydrostatic formulation to provide an accurate description of the wave dynamics. During the 2011 Japan tsunami, tide gauges across Hawaii and an ADCP off the Honolulu coast allowed both the computed surface elevation and current velocity to be validated. Several random variables were defined for computation of tsunami scenarios such as event location, slip distribution, focal depth and rise time, while the other seismic parameters were set to be fixed according to geological configuration. Three nested grids were defined to run the simulations and the integration time steps and roughness coefficients were defined and tested in order to avoid any instability. An automatic algorithm was developed to construct the stochastic scenarios, run the simulations and extract hydrodynamic variables at the given location; thus, a synthetic database of hydrodynamic force is constructed and the probabilistic analysis is assessed. At the conference, we will show the numerical setup for tsunami simulations and preliminary results of stochastic tsunami source models.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Physical Simulation Based Earthquake Scenario and a Multi-scale Tsunami Simulation

Mitsuteru Asai*, Naoki Nakaya**, Ryoichiro Agata***, Takane Hori****, Toshitaka Baba*****

*Kyushu university, **Kyushu University, ***JAMSTEC, ****JAMSTEC, *****Tokushima University

ABSTRACT

In our study, a multi-scale earthquake and tsunami simulation has been developed. The Level-1 tsunami simulation is the same as the practical tsunami simulation made using a two-dimensional (2D) shallow water equation, which is mainly solved by the finite difference method. The main purpose of the Level-1 tsunami simulation is to make an immediate prediction of the tsunami magnitude. The stabilized incompressible SPH (ISPH) method [Asai et al., (2012)] is used for the 3D tsunami inundation simulation as the Level-2 tsunami simulation. These 2D and 3D tsunami simulations are coupled by a virtual wave maker [Asai et al. (2015)]. The virtual wave maker generates a virtual wave in the 3D particle simulation space to smoothly connect from the pre-simulated 2D tsunami simulation result. Before we perform these multi-scale tsunami simulations, we need to estimate an earthquake scenario. Then, an earthquake scenario simulation [Hyodo and Hori (2011)] is done by using a high performance finite element code; GAMERA [Ichimura (2017)]. The physical based earthquake simulation, in which a high-fidelity heterogeneous geographical layer is assumed to make the FEM model, gives the transient crustal deformation and these simulation results become the inputs of the above tsunami simulation. The physical simulation based earthquake and tsunami simulation result is compared with an analytical solution based earthquake and tsunami simulation result. Finally, we discuss the necessity of the high fidelity earthquake scenario simulation. Reference [1] Asai, M. et al.: A Stabilized Incompressible SPH Method by Relaxing the Density Invariance Condition International Journal for Applied Mathematics, Vol.2012, Article ID 139583, 24 pages, 2012. [2] Asai, M. et al. : Coupled tsunami simulation based on a 2D shallow-water equation-based finite difference method and 3D incompressible smoothed particle hydrodynamics, Journal of Earthquake and Tsunami, Vol. 10, 2016 [3] Hyodo, M. and Hori, T. : An interpretation of crustal deformation associated with the 2011 tohoku earthquake, The seismological Society of Japan 2011 Fall Meeting, pp.2-12, 2011 [4] Ichimura, T. et al. Tsunami Analysis Method with High-Fidelity Crustal Structure and Geometry Model, Jornal of Earthquake and Tsunami, Vol.11, No.5, 2017

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Multiscale Modeling of Pure Nickel

Imran Aslam*, Shane Brauer**, Andrew Bowman***, Bradley Huddleston****, Justin Hughes*****, Daniel Johnson******, William Lawrimore*******, Luke Peterson********, William Shelton*********, Mark Horstemeyer**********

*Mississippi State University, **Mississippi State University, ***Mississippi State University, ****Mississippi State University, *****Los Alamos National Laboratory, ******Mississippi State University, *******U.S. Army Engineer Research and Development Center, ********Mississippi State University, *********Louisiana State University, **********Mississippi State University

ABSTRACT

A physically-based, multiscale modeling approach has been applied, in tandem with uncertainty quantification, to simulate three-point bending of pure nickel. Downscaling requirements are driven by the complex stress state induced by the three-point bend, which is experimentally obtained as a force-displacement. Those requirements are then met by upscaling from the atomistic length scale to the macroscale. Density functional theory was utilized at the electronic principal's scale to determine the lattice parameter and equilibrium energy of nickel (Ni), which were then upscaled to the atomistic scale. At the atomistic length scale the Modified Embedded Atom Method was used to calibrate the nickel energy potential curve, which was then used to simulate the motion of a dislocation and, subsequently, to determine the dislocation velocity. The dislocation velocity was then upscaled to the microscale to evaluate the hardening constants of nickel by utilizing Multiple Dislocation Dynamics Plasticity simulations. The hardening constants are upscaled as parameters used in Crystal Plasticity simulations to obtain the stress-strain curves for the three stress states, compression, tension, and shear. The stress-strain curves are upscaled to the macroscale and calibrated using the MSU-ISV Plasticity-Damage Model. The macroscale calibration is fed into Abaqus as a user material model in order to accurately replicate the three-point bending of a thin sheet of pure nickel. Uncertainty was quantified at each length scale as well as propagated throughout the length scales. The force-displacement data obtained from Abaqus is in good agreement with the experimental result.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Numerical Modeling of Coupled Thermo-Mechanical Behavior of Ni-Ti Shape Memory Alloys for Large Deformations

Ozgur Aslan*, Vahid Rezazadeh**

*Atilim University, **Middle East Technical University

ABSTRACT

Shape memory alloys (SMAs) hold a significant importance in different areas of engineering such as aeronautics, adaptive structures, oil/gas down-hole, and high-temperature applications of automobile industry and there is a growing effort to produce mathematical models in order to imitate the related behaviors in a precise manner. This work utilizes a numerical model based on the finite strain framework of continuum mechanics to establish a thermodynamically consistent theory for SMAs. With the martensitic volume fraction as the internal variable evolving with phase transformation, the thermo-mechanically coupled theory both captures the rate and temperature dependency. The model is implemented in a commercial finite element program by writing a user-material subroutine and both isothermal and coupled simulations conducted on different 2-D and 3-D model problems are shown to demonstrate the high capability in capturing various qualitative behavior of Ni-Ti SMA such as pseudoelasticity, one-way shape memory effect and thermomechanical behavior under cyclic thermal loading together with their good agreement with the experimental findings.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

The Role of Aortic Biomechanics in the Initiation of Angiotensin-II Induced Dissecting Aortic Aneurysms

Lydia Aslanidou*, Mauro Ferraro**, Patrick Segers***, Bram Trachet****, Nikos Stergiopulos*****

*EPFL, **EPFL, ***Ghent University, ****EPFL; Ghent University, *****EPFL

ABSTRACT

Angiotensin-II infusion on ApoE-/- mice is a popular model of aortic aneurysm and dissection. We have recently demonstrated that the dissecting aneurysmal lesions in these mice start with a medial tear near the ostia of celiac and mesenteric arteries. Given the location-specific nature of the disease, we hypothesized that the local mechanical equilibrium may drive disease initiation. To this end we developed a novel computational approach to evaluate the in-vivo strain field in the abdominal aorta. Combining ex vivo synchrotron images with in vivo micro-CT, we incorporated model features such as non-uniform aortic wall thickness, non-uniform stretch field and the inclusion of small aortic side branches into our computational models and showed how these often overlooked features impact the location of hotspots in the computed strain field [1]. In this work we validate these simulations with image-guided histology in order to investigate whether regions of high strain collocate with sites of micro-structural damage. N=10 ApoE-/- mice were infused with Angiotensin-II for 3 days and underwent a contrast-enhanced micro-CT scan prior to euthanasia. The aorta was imaged ex-vivo using Phase-contrast X-Ray Microscopy (PCXTM) at 6.5 um isotropic resolution. The same protocol was followed for n=6 saline-infused controls. An in-house automated framework was implemented to morph the non-pressurized non-stretched ex-vivo PCXTM geometry onto the pressurized stretched in-vivo micro-CT geometry [1]. For each animal the output was a mouse-specific structural finite element simulation. Contrast agent infiltration in the aortic wall was used to detect the location of micro-ruptures in the tunica media [1] and image-guided histology in these locations was performed to validate and quantify the vascular damage. Preliminary results show good agreement between hotspots of early vascular damage and hotspots of computed maximal strain. The highest strain values occurred invariably in the vicinity of the celiac and mesenteric arteries and collocated with intramural micro-ruptures and leukocyte infiltration. Moreover, the inter-subject variability of the maximal strain locations (cranial/caudal or right/left of the ostium) corresponded qualitatively to the inter-subject variability of PCXTM-detected contrast agent leakage. We conclude that strain concentrations near side branches could partially explain the focal nature of the disease. References [1] Ferraro, M., Trachet, B., Aslanidou, L., Fehervary, H., Segers, P., and Stergiopulos, N., "Should we ignore what we cannot measure? How non-uniform stretch, non-uniform wall thickness and minor side branches affect computational aortic biomechanics in mice. " Ann Biomed Eng (2017).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Vibroacoustics Modeling of Complex Structures with Attached Heterogeneous Noise Control Materials Using a Hybrid Finite Elements - Transfer Matrix Method

Noureddine Atalla*, Luca Alimonti**

*Université de Sherbrooke, **ESI US R&D;

ABSTRACT

This paper discusses the modeling of the vibration and acoustic responses of structures with attached sound packages, using hybrid FE-TM (Finite Elements - Transfer Matrix) methods. It consists of two parts. In the First, a general framework to calculate the absorption and transmission coefficients of a periodic representation of the structure and its sound package is presented. The approach assumes oblique plane wave excitation and accounts for fluid coupling with the excitation and receiving fluid domains. Several examples are presented to demonstrate the accuracy of the approach. A special attention is given to complex structures (e.g. sandwich composites, highly damped structures, ribbed panels, curved structures) and heterogeneous sound packages (metamaterials in particular). In the second part, the ability of the classical Transfer Matrix Method (TMM) to model these same structures is investigated. Firstly, a simple approach to derive the frequency and heading dependent transfer matrices from the periodic model of the system is presented. Next, its use within the classical TMM is presented. Finally, the range of applicability and usefulness of the presented hybrid method is discussed by a systematic comparison with the results of part 1.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

The Shifted Boundary Method for Embedded Domain Computations: Application to Solid Mechanics

Nabil Atallah*, Alex Main**, Guglielmo Scovazzi***

*Duke University, **Duke University, ***Duke University

ABSTRACT

Embedded/immersed boundary methods cicumvent the challenge of representing complex geometries through their ease in mesh generation. On the other hand, with such a decision arises the need to integrate over the cut elements. To counter this dilemma and maximize on the advantages of embedded methods, we propose a novel approach, named "shifted boundary method ". The proposed method obviates the need to integrate over the cut boundary elements by weakly imposing an equivalent boundary condition on its surrogate (formed of un-cut elements) counterpart. We start by presenting the method for the Poisson problem along with its associated Lagrangian on the surrogate domain and its corresponding boundary. We then present the method in light of elasticity problems whereby we study stability and convergence of the method with the support of a series of tests that display the robustness and accuracy of the method.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

The Future for Predicting Response for Extreme Environments Using a Combination of Experimental Techniques and Numerical Simulations

Stephen Attaway*

*Sandia National Labs

ABSTRACT

Many challenges remain in the search for numerical models that are predictive for extreme events. This talk will provide some examples of extreme events that require a combined approach for modeling and simulation with tests and evaluation. Most structures are designed for a functional life that keeps their behavior in the linear elastic, small deformation range. When buildings are subjected to extreme loads from earthquakes, fires, or terrorist attacks, the tools used for structural designs often fail to provide a technical basis for risk. Using a combination of modeling and simulation with tests and evaluation can provide the technical basis for high-consequence decisions relative to system safety and performance margins. The emergence of exascale computers with millions of cores allows simulations of transient dynamics phenomena at unprecedented scales and fidelity. Even with this increase in compute power some simulations are too costly to directly model all of physics. Full scale testing for many problems is often too costly or impractical. Both modeling and simulation combined with tests and evaluation are needed to reduce uncertainty and provide a technical basis for risk acceptance in extreme events.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Meshless Methods for Manifolds: Hydrodynamics of Curved Fluid Interfaces and Related Applications

Paul Atzberger*, Ben Gross**, Nathan Trask***

*University California Santa Barbara, **University California Santa Barbara, ***Sandia

ABSTRACT

We discuss recent advances in the development of meshless methods for solving partial differential equations on general manifolds. We present a discretization framework based on Generalized Moving Least Squares (GMLS) and exterior calculus formulation of the pdes. Motivated by applications arising in soft condensed matter physics and biophysics, we show how our approaches can be used to solve hydrodynamic equations on curved fluid interfaces. We also present convergence results comparing our GMLS methods with a spectral solver in the case of radial manifolds. We then show some advantages of our GMLS methods demonstrating the capability to handle quite general manifold topologies and to adapt numerical resolution. We conclude by presenting results for hydrodynamic interactions in drift-diffusion dynamics of particle inclusions within a curved fluid interfaces showing some of the important roles played by topology and geometry.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Interplay between Mechanical, Electrostatic and Electronic Nonlinearities inside a MEMS Converting Cardiac Vibrations to Electric Power with Pacemaker Applications

Denis Aubry*, Bogdan Vysotskyi**, Philippe Gaucher***, Fabien Perrain****, Elie Lefeuvre*****

*Ecole CentraleSupelec, **MSSMat/C2N-Site d'Orsay, ***MSSMat., ****C2N-Site d'Orsay, *****C2N-Site d'Orsay

ABSTRACT

In this talk, we intend to present the numerical simulation of a MEMS which converts heart beating movements to electrical power and is thus able to charge the battery of a pacemaker. Mechanical nonlinearities cannot be avoided because the heart vibration spectrum is not favorable to power production and higher frequencies must be generated. Electric current comes from electrostatic charges and the deformable capacity versus current relationship is also highly non-linear. Finally energy harvesting implies the use of electronic components such as diodes whose behavior is extremely nonlinear. We sho that the numerical control of these nonlinearities is mandatory and must be finely tuned and controlled to prove the efficiency of the system and its sensitivity. Comparison between the predicted and experimental power production of a newly design MEMS demonstrates the essential role of these considerations.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Tangential Adaptivity in Volume Boundary Layer Mesh Generation

Romain Aubry*

*United States Naval Research Laboratory

ABSTRACT

Boundary layer mesh generation traditionally extrudes the no-slip surfaces into the volume. While this may provides an accurate ge- ometry, the surface curvature distorts without control the prescribed size at the surface. Even on flat surfaces, the extrusion maintains the same mesh size, while the user prescribed size may vary for thick boundary layers in the volume. This causes numerous practical issues, such as the transition between boundary layer mesh and the isotropic mesh, the collision of front of different sizes. In order to remedy these pitfalls, we propose to adapt in the tangential direction the boundary layer to maintain a size consistent with the prescribed one, as well as a seamless transition with the isotropic part.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Modelling Seabed Ploughing Using the Material Point Method

Charles Augarde*, Andrew Brennan**, William Coombs***, Michael Brown****, Michael Cortis*****, Scott Robinson******

*Dept of Engineering, Durham University, UK, **Civil Engineering, Dundee University, UK, ***Dept of Engineering, Durham University, UK, ****Civil Engineering, Dundee University, UK, *****Dept of Engineering, Durham University, UK, ******Civil Engineering, Dundee University, UK

ABSTRACT

Ploughing is a complex process for which to devise numerical models since it involves material and geometric nonlinearity and is truly 3-dimensional. The Material Point Method (MPM) seems to be a good contender for this modelling since it decouples the deformation of the problem domain from the discretisation framework. This presentation describes recent UK research that has paired numerical modelling of ploughing using the MPM with laboratory experimentation, the latter to provide string validation to the former. Various issues that have been met with in the development of the MPM to provide the ploughing model are discussed, such as dealing with essential boundary conditions and proper implementation of plasticity models. The standard MPM is shown to be a robust choice in comparison to more complex approaches, such as the GIMP and CPDI methods, which seek to reduce the cell-crossing instability but bring additional problems or complexities.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Computational Heart Model of Pulmonary Arterial Hypertension

Reza Avaz*, Emilio Mendiola**, Joao Soares***, Richard Dixon****, Michael Sacks*****

*University of Texas at Austin, **University of Texas at Austin, ***Virginia Commonwealth University, ****Texas Heart Institute, *****Virginia Commonwealth University

ABSTRACT

Pulmonary arterial hypertension (PAH) imposes a pressure overload on the right ventricular free wall (RVFW), leading to substantial growth of muscle cells and remodeling in fiber architecture. The effects of these alterations on the biomechanical behavior of the RVFW and the organ-level cardiac function remain largely unexplored. Recent experimental studies on the mechanical and morphological properties of normal and hypertensive RVFW myocardium suggest that myocardial wall stress is the primary mediator of RVFW growth and remodeling (G&R) responses. An accurate quantification of the wall stress evolution during the development of PAH is needed to determine the correlation between the wall stress and G &R mechanisms. To this end, there is a need to develop a detailed computational heart model that can accurately simulate the effect of PAH in the heart, and thus can be used to understand pathophysiology of RVFW remodeling, its connection to wall stress alterations, and its impact on organ-level cardiac function. We have developed a high-fidelity finite-element (FE) heart model of PAH using extensive time-course datasets from a normal rat heart and from a hypertensive rat heart simulating the pressure overload in the right ventricle (RV). We have implemented a pipeline that integrates a meshed geometry from a high-resolution image of the rat heart, detailed imaging data on the fiber structure of the same heart, and a novel compressible hyperelastic material model accounting for both passive and active behaviors of myocardium. The developed heart model offers a high performance capability for inverse problems such as fine-tuning the active properties of myocardium and characterizing shape change patterns of the RV. We used our model to investigate the correlations between the alterations in the wall stress, the remodeling of the RVFW microstructure, and the shape changes in the RV during the development of PAH. The detailed description of organ-level remodeling patterns can replace the traditional measures of RV dimensions and volume that often lead to gross and limited information on cardiac performance. Ultimately, development and implementation of our model in patient-specific organ-level simulations will allow investigation of optimal diagnosis and new individualized stem-cell interventions for PAH.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Link Shape Synthesis for Dynamic and Structural Requirements

Pedro Enrique Avila-Hernandez*, Fernando Velazquez-Villegas**, Francisco Cuenca-Jimenez***

*Engineering Faculty, UNAM, **Engineering Faculty, UNAM, ***Engineering Faculty, UNAM

ABSTRACT

In the last three decades, different methods of link shape synthesis for balanced linkages have been proposed. However, any of them has considered the mechanical properties of links material. This paper presents for first time the shape synthesis of a four-bar mechanism link that takes into consideration the mechanical properties of its material. This method adapts through Multi-Objective Genetic Algorithm (MOGA), the optimum topologic methods Solid Isotropic Microstructure with Penalization (SIMP) and Evolutionary Structural Optimization (ESO) to determine the shape of a link that satisfies structural and dynamic (balancing) requirements. The method is able to process all the requirements in parallel to determine the link shape. The results show that a link shape that balances a mechanism can be obtained without determining its inertial parameters previously.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Finite-element Predictions of Human Aortic Root Enlargement Based on the Homogenized Constrained Mixture Model

Stephane Avril*, Joan Laubrie**, Jamal Mousavi***

*Université de Lyon, **Université de Lyon, ***Université de Lyon

ABSTRACT

Recently, growth and remodeling (G &R) has been increasingly approached based on the constrained mixture theory (CMT) to predict a variety of arterial mechanobiological behaviors [1, 2]. Most of previously published work has been limited to simplified cases as isotropic growth, axisymmetric motions, mono-layer wall and/or membrane approximations. Although such models have increased our insights in vascular adaptation, a 3D anisotropic bilayer model has the potential of considering more complex cases of arterial G &R such as aortic root enlargement. Therefore, herein, a 3D numerical model based on homogenized CMT is implemented in ABAQUS through a coupled UEL to predict anisotropic G &R of arteries. At the Gauss points level, the passive behavior is assumed hyperelastic and a strain energy function (SEF) is assumed for each constituent with decoupled contributions of the purely volumetric and isochoric parts. Although the same SEF is assumed for every element across the geometry of the artery, different material properties and mass fraction can be applied at each layer. It is considered that the arterial wall is composed of a constrained mixture of elastin, collagen fibers and smooth muscle cells (SMC) and includes the in situ stresses existing in the reference configuration. Four collagen fibers with different mass fractions in media and adventitia in the axial, circumferential and angular directions are considered. The contractility of SMC and turnover of collagen fibers are assumed stress dependent. Simulations are performed on a bilayer thick-wall geometry reconstructed from the CT scan of a patient harboring an ascending thoracic aortic aneurysm (ATAA), subjected to boundary conditions in homeostatic conditions. Two different mechanisms are considered for the initiation of aneurysm enlargement, namely loss of SMC contractility and damage of elastin. Different gain parameters for collagen turnover are considered. The models are able to predict realistic aortic root enlargement as confirmed by a follow-up MRI performed on the same patient. Our findings confirm the determinant role of SMC contractility during ATAA growth. References [1] F.A. Braeu, A. Seitz, R.C. Aydin and C.J. Cyron. Holzapfel. Homogenized constrained mixture models for anisotropic volumetric growth and remodeling. Biomech Model Mechanobiol, 29(8): 16(3):889–906, 2017. [2] A. Valentín, J.D. Humphrey and G.A. Holzapfel. A finite element-based constrained mixture implementation for arterial growth, remodeling, and adaptation: theory and numerical verification. Int J Numer Method Biomed Eng, 29(8):822–49, 2013.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Thermo-mechanical Process Modelling for Selective Laser Melting

Can Ayas*, Yabin Yang**

*Delft University of Technology, **Delft University of Technology

ABSTRACT

Selective laser melting (SLM) is a powder based additive manufacturing method suitable for metallic components. In SLM the part is built utilising a laser beam which scans over the powder bed in order to selectively melt and consolidate thin sections of a solid part in a layer-by-layer fashion. Although SLM enables manufacturing of topology optimized, geometrically complex designs which cannot be realised by traditional subtractive manufacturing techniques, it suffers from distortion of the part and residual stresses induced. Distortion of the part can result in out of tolerance components and residual stresses can cause failure during the built. It is well-known that both part distortions and residual stresses are induced due to heating/cooling cycles associated with laser melting and the corresponding thermal expansion/contraction leading to displacement and stress fields. Therefore it is of great interest to identify process parameters such as laser power and scanning speed and scanning strategies that minimize the detrimental part distortion and residual stresses of a design to be built by SLM. For this purpose, we present a thermo-mechanical modelling framework that is able to predict the temperature transients and the corresponding evolution of mechanical field quantities during the build process. The former is calculated using a computationally efficient semi-analytical method where the closed form analytical solutions of line heat sources describing scanning lines are superimposed with numerically calculated image fields to enforce boundary conditions of the design at hand. The latter requires a one way coupled thermo-mechanical coupling where the temperature induced strain alongside the elastic and plastic strain is calculated leading to the stress state of the component. Temperature dependent J2 elasto-plastic material with kinematic hardening is considered. Several case studies are investigated by the proposed model. The residual stresses and part deformations are investigated as a function of different scanning strategies at different layers. The predictions of the model are compared with experimental findings and existing approximate modelling schemes available in literature.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Discrete Tangent Vector Fields and PDEs on Surfaces

Omri Azencot*, Mirela Ben Chen**

*UCLA, **Technion - Israel Institute of Technology

ABSTRACT

Tangent vector fields are widely used in computer graphics, where they are applied to various tasks such as texture generation on surfaces, and physical simulation for animation. In this talk we will describe a new discretization of tangent vector fields on triangle meshes that is inspired by the classic point of view in differential geometry, namely that vector fields are linear operators on scalar functions. Taking this approach allows us to numerically simulate various PDEs on discrete surfaces, such as function advection and fluid flow, in an efficient and stable manner, with theoretical guarantees. We will show the application of this approach to the problem of simulating thin films on curved triangle meshes. In this problem the motion is governed by a fourth-order nonlinear PDE, which involves geometric quantities such as the curvature of the underlying surface, and is therefore difficult to discretize. Inspired by a recent variational formulation for this problem on smooth surfaces, we present a corresponding model for triangle meshes. We provide a discretization for the curvature and advection operators which leads to an efficient and stable numerical scheme, requires a single sparse linear solve per time step, and exactly preserves the total volume of the fluid. We validate our method by qualitatively comparing to known results from the literature, and demonstrate various intricate effects achievable by our method, such as droplet formation, evaporation, droplet interaction and viscous fingering. The talk is based on the papers [1], [2], where [1] has received one the three best paper awards at SCA. References: [1] Functional Thin Films on Surfaces, Omri Azencot, Orestis Vantzos, Max Wardetzky, Martin Rumpf and Mirela Ben-Chen. Proceedings of ACM Symposium on Computer Animation, Los Angeles, 2015. [2] Functional Thin Films on Surfaces. Orestis Vantzos, Omri Azencot, Max Wardetzky, Martin Rumpf and Mirela Ben-Chen. IEEE Transactions on Visualization and Computer Graphics 23(3), 2017.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Computational Bio-Chemo-Mechanical Model of Inflammation for Tissue Engineering Vascular Grafts

Abhay B. Ramachandra*, Ramak Khosravi**, Jason Szafron***, Jay Humphrey****

*Yale University, **Yale University, ***Yale University, ****Yale University

ABSTRACT

The limited availability of autologous vessels for cardiovascular surgeries has highlighted the need for optimally engineered vessels. Tissue engineered vascular grafts (TEVGs) have shown promise as alternatives to autologous vessels, but post-operative complications remain. The complex interplay in vivo amongst biological, chemical, and mechanical factors governs the outcome of an implanted TEVG, with inflammation playing a critical role [1], and creates design challenges for polymeric scaffolds used in these applications. To gain insights into roles of inflammation in the development and failure of TEVGs, and to design of better scaffolds, we propose a bio-chemo-mechanical computational model of inflammation and tailor it for TEVGs. For illustrative purposes, we model the inflammatory response by focusing on cells and pathways most relevant to TEVGs. Specifically, the biochemical part of the inflammation model consists of inflammatory cells (e.g., Ly6C+/ Ly6C- monocytes, classically and alternately activated macrophages and tissue resident macrophages), cytokines (e.g., TGFbeta, iNOS, IL-10), cells (e.g., endothelial, inflammatory, and synthetic), extracellular matrix constituents (e.g., collagen) and proteases (e.g., MMPs). The kinetics of the inflammatory model are modeled using Michaelis-Menten kinetics. The polymer degradation, derived from experimental data, drives the inflammation while circumferential wall and shear stresses, predicted from a constrained mixture model of growth and remodeling of a TEVG [2], influence (via constitutive equations) the turnover of synthetic smooth muscle, stress mediated collagen, and TGFbeta. Thus, the proposed model is immuno-driven and mechano-mediated. The model is calibrated against existing experimental data from the literature. The complexity of the model yields an abundance of parameters. Bayesian methods and simplex optimization routines are used to estimate the parameters. We also report results of system identification for this data-poor system. The results not only help to gain insights into the role of inflammation in the development and failure of TEVGs, they also promise to help guide future experiments. [1] Roh, Jason D., et al. "Tissue-engineered vascular grafts transform into mature blood vessels via an inflammation-mediated process of vascular remodeling. " Proceedings of the National Academy of Sciences 107.10 (2010): 4669-4674. [2] Miller, Kristin S., et al. "Computational model of the in vivo development of a tissue engineered vein from an implanted polymeric construct. " Journal of Biomechanics 47.9 (2014): 2080-2087.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Enhanced Electroosmotic Flow and Ion Selectivity through a Patterned Soft Channel with pH-Regulated Uncharged Grooves

NAREN BAG*, SOMNATH BHATTACHARYYA**

*INDIAN INSTITUTE OF TECHNOLOGY KHARAGPUR, **INDIAN INSTITUTE OF TECHNOLOGY KHARAGPUR

ABSTRACT

This article deals with the modulation of electroosmotic flow (EOF) through the parallel plate soft nanochannel where the grooves are filled with polyelectrolyte layer (PEL). The PEL of the grooves containing both acidic and basic functional groups. The solid walls of the channel are assumed to be maintained at a constant surface charge density and the surface of the grooves are assumed to be a zero surface charge density. A nonlinear model based on the nonlinear Poisson-Nernst-Planck equation coupled with the Darcy-Brinkman equation is adopted. Going beyond the widely employed Debye-Huckel linearization, we adopt a sophisticated numerical tool to study the effect of pertinent parameters on the modulation of EOF through the soft periodic groove nanochannel. We have illustrated the effect of PEL and surface charge density, electrolyte concentration, softness parameter, periodic length of the groove channel and electrolyte pH. Several interesting key features, including the flow enhancement factor and occurrence of zero flow rate, are studied by regulating the charges entrapped within the PEL and the surface charge distributed along the channel walls. In addition to the flow modulation, we have also demonstrated the selectivity of the mobile ions through the soft nanochannel. The results indicate that the channel can be cation-selective, an anion-selective as well as non-selective based on the nature of the charges within the PEL and walls charge. In order to validate our numerical code, we have compared our computational average velocity in a soft nanochannel with flat walls corresponding to the analytic solution based on Poisson-Boltzmann linear model with Debye-Huckel approximation. The computed results differ from the analytic solution for thicker Debye layer when PEL is either uncharged or the charge of the PEL and walls have the same sign, while for the case of oppositely charged PEL and walls, analytic solution differs from the numerical solution when Debye layer is thinner. We have also seen that the average velocity of the present result approaches to the analytic solution for higher values of the periodic length. The present study also shows that the flow reversal and zero ion selectivity i.e., a non-selective channel for an oppositely charged PEL and walls. References 1. Wang, C. 2003 Flow over a surface with parallel grooves. Phys. Fluids. 15(5), 1114-1121. 2. Matin, M. H. & Ohshima, H. 2015 Combined electroosmotically and pressure driven flow in soft nanofluidics. J. Colloid Interface Sci. 460, 361-369.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Non-local Modeling: Macroscopic Behavior of a Randomly Voided Material and Influence of Void Morphology on the Elastic Properties Gradient

Sami BEN ELHAJ SALAH*, Carole Nadot-Martin**, Mikaël GUEGUEN***, Azdine Nait-Ali****

*Institut Pprime, ISAE-ENSMA, **Institut Pprime, ISAE-ENSMA, ***Institut Pprime, ISAE-ENSMA, ****Institut Pprime, ISAE-ENSMA

ABSTRACT

Keywords: homogenization theory, non-local theory, second gradient theory The asymptotic expansion analysis was developed in the framework of homogenization technique, which is applicable for three-dimensional composites made up of inclusions randomly embedded within a matrix. The so-called asymptotic expansion homogenization (AEH) method was developed by Francfort [1] for the case of linear thermoelasticity in periodic structures. The AEH method has been employed to calculate the homogenized thermomechanical properties of composite materials (elastic moduli and coefficient of thermal expansion). This technique of homogenization enables to replace heterogeneous materials by a homogeneous equivalent medium including second-order displacement gradients [2]. The displacement vector and the stress tensor are considered as functions of macroscopic (x) and microscopic (y) variables. They may be expanded in a series of powers of small (material) parameter “eta”, which is the ratio between macroscopic and microscopic scales. More precisely, the present work is devoted to linear stochastic homogenization and Gamma-convergence problems for variational functional. This Gamma-convergence allows us to study the corresponding variational problem and to prove the convergence of the minimums and of the minimizers. By combining variational convergence with ergodic theory, we study the macroscopic behavior of linear elastic heterogeneous materials. The inclusions are randomly distributed within a matrix, their size is of order “eta”. The variational limit functional energy obtained when “eta” tends to 0 is deterministic and non-local [3]. By including the characteristic displacement vectors, or correctors, the problem can be solved in order to evidence some links with second gradient theory. Computational results in periodic and stochastic cases will be exposed and discussed. This work shows that the asymptotic expansion homogenization method has a strong history of development in the mathematical and engineering fields and it is an accurate and efficient tool not only to predict the mechanical properties of voided materials but also as a vehicle for enabling multistate analysis. An extension of this study will be devoted to the construction of non-local damage model that consists in introducing the gradient of damage (grad Alpha). References [1] Francfort, G., “Homogenization and linear thermoelasticity”, SIAM J Math Anal; 14(4), 696-708 (1983). [2] Forest, S., Cardona, JM., and Sievert, R., “Thermoelasticity of second-grade media”, Continuum Thermomechanics, 163-176 (2000). [3] Michaille, G., Nait-Ali, A., and Pagano, S., “Macroscopic behavior of a randomly fibered medium”, Journal of Pure and Applied Mathematics, 96(3), 230-252 (2011).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Simulation of Coupled Thermal and Mechanical Effects Induced by the Metallurgical Phase Changes in the Welding of Large Components for the Nuclear Industry

Clement BERTHINIER*

*CEA - SEMT/LM2S (Saclay, France)

ABSTRACT

Many industrial metals (such as 16MND5 steel) are subject to allotropic phase transformations during a thermal heating and cooling cycle. These thermal cycles are observed when welding large components that are the pipes of the cooling circuits in the nuclear industry. At first, the objective of this work is to achieve in Cast3M the coupling between the resolution of thermal, metallurgy and mechanics. The metallurgical phase changes proposed in this work are based on two models: the Koistinen-Marburger model and the Leblond-Devaux model. On one hand, these phase changes, have an impact on the thermal and mechanical properties of the different parts (materials properties modifications) and on the other hand induced a plasticity phase change source term. The implementation of these models in Cast3M is verified and validated by comparisons to analytical solutions and numerical solutions from other finite element software (Sysweld and Code_ASTER). In a second step, these developments are used to evaluate the stress and deformation state of two tubes after a predetermined welding sequence. The modeling carried out is in 3D. The parameters injected into the phase change models are chosen to correspond to the TRC diagram of 16MND5 steel. The effects and interest of thermal-mechanical-metallurgical coupling are discussed.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

SFE Methods Applied to Nuclear Containment Buildings Behavior

David BOUHJITI*, Frédéric DUFOUR**, Benoît MASSON***, Julien BAROTH****

*Industrial chair PERENITI (3SR LAB, EDF-SEPTEN), **PERENITI Chairholder (3SR LAB, EDF-SEPTEN/DTG/CIH), ***EDF-SEPTEN, ****Univ. Grenoble Alpes, CNRS, Grenoble INP , 3SR, F-38000 Grenoble, France

ABSTRACT

The aim of this work is to investigate the pertinence of SFE methods when dealing with concrete behavior at the scale of large reinforced and prestressed structures such as Nuclear Containment Buildings. Their simulation involves the use of strongly non-linear behavior laws requiring hefty computational time and a considerable number of parameters (more than 50) affecting their response to the simultaneous Thermo-Hydro-Mechanical (THM) loads. Being a heterogeneous and multiphasic material, concrete properties show intrinsically spatio-temporal variations (in addition to epistemic and ontological ones related to the mixing, casting and curing processes) affecting the aging process in terms of cracking, drying, creep and tightness. In opposition to classical deterministic approaches - which are not sufficient when dealing with random phenomena such as size effects, cracking and permeability -,the introduction of such variations in numerical models is a mandatory step for better assessment of their present behavior and accurate prediction of their future one. The main question remains: which is the most efficient strategy in order to optimize the computational time and still be able to perform an accurate sensitivity analysis (up to what order ?) and uncertainties quantification/propagation through the various THM and leakage calculation steps ? In this contribution concrete cracking patterns are defined according to a stochastic size effect law and a regularized, local and damage-based model. The spatial heterogeneity of concrete at the Representative Structural Volume scale is described using Random Fields and the aging effects on concrete 's long term behavior (uncertainties propagation) is assessed using non-intrusive methods such as: perturbation/quadrature methods and projection methods namely the polynomial chaos expansion approaches. Depending, on the output of interest (mean, coefficient of variation, n-ith statistical moment, pdf) a comparative analysis is performed for the required computational time vs. the error estimation of each output using the results from Monte Carlo approach as a reference.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Computational Damage Approach for Localized Failure in Quasi-brittle Materials

TINH QUOC BUI*, SOHICHI HIROSE**

*TOKYO INSTITUTE OF TECHNOLOGY, **TOKYO INSTITUTE OF TECHNOLOGY

ABSTRACT

In this talk, we present a computational approach based on a novel smoothing gradient-enhanced damage model for localized failure problems in quasi-brittle materials. This approach is particularly tailored to low-order finite elements (e.g., Q4 or T3). In this model, the characteristic length is a stress level dependent parameter. The displacements and nonlocal equivalent strain fields are approximated in the framework of low-order finite elements, i.e., the same interpolation functions are used for both primary variables. A novel modified evolving gradient parameter, which heavily depends on the principal stress and equivalent strain states, serving to reduce the impact of localized deformation, is introduced. Consequently, the spurious damaged zones and stress oscillation induced by the standard gradient damage models can be overcome. Numerical examples in one- and two-dimensions with shear band analysis for quasi-brittle materials are analyzed.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Aggregated Unfitted Finite Element Methods for Large Scale Simulations on Octree Meshes

Santiago Badia*, Francesc Verdugo**, Alberto Martín***

*Universitat Politècnica de Catalunya / CIMNE, **CIMNE, ***CIMNE

ABSTRACT

The use of unfitted finite element methods (FEMs) is an appealing approach for different reasons. They are interesting in coupled problems or to avoid the generation of body-fitted meshes. One of the bottlenecks of the simulation pipeline is the body-fitted mesh generation step and the unstructured mesh partition. The use of unfitted methods on background octree Cartesian meshes avoids the need to define body-fitted meshes, and can exploit efficient and scalable space-filling curve algorithms. In turn, such schemes complicate the numerical integration, imposition of Dirichlet boundary conditions, and the linear solver phase. The condition number of the resulting linear system does depend on the characteristic size of the cut elements, the so-called small cut cell problem. In this work, we will present a parallel unfitted framework that relies on adaptive octree background meshes and space-filling curve partitioners. In order to solve the small cut cell problem, we will consider a re-definition of the finite element spaces that solves this issue, leading to condition number bounds as the ones for body-fitted schemes without any kind of perturbation/stabilization of the Galerkin formulation. We will also define appropriate iterative linear solvers based on domain decomposition preconditioning that are robust and scalable.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Single Chain Polymer Nanoparticles as Building Blocks for A New Class of Polymers

Suwon Bae*, Meredith Silberstein**

*Cornell University, **Cornell University

ABSTRACT

Incorporating intra-chain crosslinks into a single polymer chain is a powerful way to tailor the thermo-mechanical properties of the polymer chain. Intra-chain crosslinks restrict the motion of constituent monomers and modify polymer chain configuration. When induced under moderate to bad solvents these crosslinks lock the polymer chains into collapsed conformations, forming single chain polymer nanoparticles (SCPNs). The thermo-mechanical properties of individual SCPNs can be tuned by means of the crosslinking ratio. In addition to individual SCPNs, bulk polymer synthesized with SCPNs as its building blocks shows a response different than that synthesized with linear chains. Here a molecular dynamics (MD) approach is adopted to investigate the effect of intra-chain crosslinking on both individual SCPNs and bulk polymers formed from assembly of SCPNs. Firstly, we explore the mechanics of SCPNs as individual units. We use a coarse-grained model of a polyethylene-like polymer with Dreiding potential. The dependence of the properties of individual SCPNs on chain length and crosslinking ratio is studied by varying the degree of polymerization and the number of intra-chain crosslinks. While the response is almost independent of the chain length, the response does depend on the crosslinking ratio. As the crosslinking ratio is increased, the glass transition temperature increases and the motion of monomers is more restricted. When subjected to flat plate compression, all SCPNs exhibit behaviors similar to that of a foam with the stress growing rapidly after the structure was compacted. The foam effect was most pronounced in the behavior of SCPNs with the highest cross-linking ratio. We then present how intra-chain crosslinking can be used to tune the thermo-mechanical properties of a bulk polymer assembled from SCPNs. Because of the intra-chain crosslinks within each single chain polymer, only limited portions of each polymer chain interact with other chains. When subjected to uniaxial tension, the bulk with a higher crosslinking ratio shows higher strength and earlier fracture. This computational result is supported by our previous experimental work. We will discuss in detail how the kinematics and energetics of the SCPN assembly differs from those of a bulk linear polymer.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Coupled Shock-Plasticity-Damage Modeling of Explosive Welding by RKPM

Jonghyuk Baek*, Guohua Zhou**, J. S. Chen***, Michael Hillman****

*University of California at San Diego, **The Pennsylvania State University, ***University of California at San Diego, ****The Pennsylvania State University

ABSTRACT

The explosive welding (EXW) process entails shock waves, large plastic deformation, and fragmentation around the collision point, troubling the traditional mesh-based methods for reliable solution. In this work, a computational framework based on the semi-Lagrangian reproducing kernel particle method (SL-RKPM) [1] is introduced for the modeling of EXW. For modeling shocks in plastically deformed solid, a Godunov-type shock algorithm formulated under the stabilized non-conforming nodal integration (SNNI) framework [2] is employed, where the Godunov scheme is embedded in the volumetric strain energy via a purely node-based flux gradient evaluation which ensures the linear momentum conservation. The Gibbs instability is controlled through the smoothed flux divergence in SNNI. The effects of high strain-rate and high temperature on plasticity and damage in the metals are taken into consideration in the material law. The kernel stability in SL-RKPM to accurately capture excessive plastic flow and metal jetting is ensured by introducing a strain rate dependent kernel support update. Adaptive refinement strategies near the contact interface are also introduced. The jet formation, smooth to wavy interface morphologies transition, and the welding condition along the metal interface are compared to several experimental results to validate the effectiveness of the proposed methods for EXW modeling. References [1] Guan, P., Chen, J. S., Wu, Y., Teng, H., Gaidos, J., Hofstetter, K., Alsaleh, M. Semi-Lagrangian reproducing kernel formulation and application to modeling earth moving operations. Mechanics of Materials 2009; 41(6):670–683. [2] Zhou, G., Chen, J. S., and Hillman, M. A Godunov-type Semi-Lagrangian Galerkin Meshfree Method for Modeling Shocks in Solid and Fluid, to be submitted.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Optimal Design of RVE of Polymer Nanocomposites Based on Fouier Transform Approach: A Multiscale Homogenization Analysis

Kyungmin Baek*, Hyunseong Shin**, Maenghyo Cho***

*Seoul National University, **Korea Electronics Technology Institute, ***Seoul National University

ABSTRACT

Representative volume element (RVE) is a unit structure that represents the overall behavior of materials, and is widely used in the field of computational mechanics to characterize the physical properties of material. Polymer nanocomposites, which are composed of various nano-fillers and polymer matrix, have dependency of polymer chain state, particular agglomeration, and volume fraction of particles for determination of RVE size. While there are sufficient studies to analyze the mechanical and thermal behaviors of polymer nanocomposites by arbitrarily selecting RVE [1], it has been challenging to determine the size of RVE that can accurately describe the behaviors of nano-structured materials. Even though some experimental method have been established for woven composites [2], it cannot be applied properly to the polymer nanocomposites because of local uncertainties caused by interaction between the polymer matrix and nanoparticles. In this study, a new numerical approach-based on Fouier transform is proposed to determine optimal RVE size of polymer Nanocomposites. The space domain information for the distribution of nanoparticles is transformed to frequency domain. After that, we determine optimal design of RVE to represent overall behavior of the global structures analyzing the wave length of frequency. Furthermore, the multiscale analysis are conducted to investigate the mechanical behaviors of the polymer nanocomposites. In this study, the multiscale bridging methodology in which the molecular dynamics (MD) simulation information is up-scaled to the continuum finite element model is applied to reflect the mechanical properties of interphase zone depending on the agglomeration of nanoparticles. The mechanical properties of polymer nanocomposites can be effectively obtained by asymptotic homogenization method [3]. We expect that the proposed scheme can broaden the applicability of the computation mechanics in fields of complex materials and structures. Acknowledgements This work was supported by a grant from the National Research Foundation of Korea (NRF) funded by the Korea government (MSIP) (Grant No. 2012R1A3A20488 41). References [1] H. Shin, K. Baek, J.-G. Han, M. Cho, Compos. Sci. Technol. 2017, 138, 217-224. [2] B. Koonbor, S. Ravindran, A. Kidane, Opt. Laser. Eng. 2017, 90, 59-71. [3] M. Cho, S. Yang, S. Chang, S. Yu, Int. J. Numer. Meth. Eng. 2011, 85, 1564-1583.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Material Defect Evaluation Based on Lattice Defect Dynamics and Machine Learning

Abdollah Bagheri*, Peter Chung**

*University of Maryland-College Park, **University of Maryland-College Park

ABSTRACT

In this paper, a computational method is presented to evaluate material defects using lattice defect dynamics and machine learning. For generating training data for machine learning, the dynamical matrix for defective lattices is calculated from the pristine lattice using linear operators which require less computational efforts; then, the phonon density of state is computed for each defect case. In training data, we assume the defect as two vacancies in a lattice with different distances between vacancies. An artificial neural network is designed and trained with the training data to predict defects from the phonon density of sate. For the verification of the method, the effect of defects in the phonon density of state of Si is studied and defects are then estimated by the machine learning method.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Accurate Adaptive Eulerian Framework for Liquid-gaz-solid Interactions

Chahrazade Bahbah*, Mehdi Khalloufi**, Youssef Mesri***, Elie Hachem****

*MINES ParisTech - CEMEF - CFL research group, **MINES ParisTech - CEMEF - CFL research group, ***MINES ParisTech - CEMEF - CFL research group, ****MINES ParisTech - CEMEF - CFL research group

ABSTRACT

We propose an accurate adaptive Eulerian framework for multiphase flows. It consists in combining an a posteriori error estimator that minimizes the interpolation error of the finite element solution followed by an interpolation with restrictions method that conserves physical properties of the field being interpolated. Momentum and mass equations have been solved using the Variational MultiScale method, coupled with an implicit treatment of the surface tension and anisotropic meshing. A convective self-reinitialization Level-Set method is used as a tool for describing the interface evolution. Several numerical examples and new benchmarks, in 2D and 3D, will be presented to illustrate the efficiency of the approach. Finally, we show that the extension of this framework to heat transfer and phase change allows simulating liquid-gaz-solid interactions and thus the complex boiling phenomena.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Homogenization and Stochastic Fracture Simulation of Quasi-brittle Materials

Bahador Bahmani*, Ming Yan**, Philip Clarke***, Katherine A. Acton****, Anand Nagarajan*****, Soheil Soghrati******, Sarah C. Baxter*******, Robert B. Haber********, Reza Abedi*********

*University of Tennessee Knoxville (UTK)/ Space Institute (UTSI), **The Ohio State University, ***University of Tennessee Knoxville (UTK)/ Space Institute (UTSI), ****University of St. Thomas, *****The Ohio State University, ******The Ohio State University, *******University of St. Thomas, ********University of Illinois at Urbana-Champaign, *********University of Tennessee Knoxville (UTK)/ Space Institute (UTSI)

ABSTRACT

Microstructural architecture strongly affects the response of brittle and quasi-brittle materials. Models that assume spatially uniform fracture strength do not capture the influence of microscale inhomogeneities on crack patterns and on observed values and scatter in critical macroscopic measures such as ultimate load and absorbed energy. In this work, we present stochastic models and homogenization methods that generate macroscopic fracture strength fields which incorporate the effects of microscale flaws. We use two methods to generate Statistical Volume Elements (SVEs) in this work. In the first, we use Conforming to Interface Structured Adaptive Mesh Refinement (CISAMR) [1] to generate a 2D finite element mesh from microstructure images that exactly tracks inclusion boundaries. In the second, we use a Voronoi-tessellation-based method [2] to generate SVEs that, in contrast to the first approach, are not square-shaped and do not cut through inclusion boundaries. We compare results from the two methods and discuss the effects of boundary conditions and SVE size on homogenized elastic and fracture properties. We use the statistics of the fracture strength field and the Karhunen-Loeve method to generate consistent realizations of the homogenized fracture-strength field for use in dynamic fragmentation simulations based on alternative macroscopic fracture models. In the first fracture model, an interfacial damage model explicitly represents crack nucleation from weak points in the material as well as subsequent crack propagation. The second uses a rate-dependent bulk model to represent material degradation implicitly. An asynchronous spacetime discontinuous Galerkin method [3] with advanced adaptive meshing capabilities tracks crack paths and captures sharp moving fronts in dynamic simulations based on the two fracture models. We present numerical results demonstrating the effects of loading rate, underlying SVE size, and the chosen fracture model on macroscopic measures such as fracture pattern and fracture-energy dissipation. References: [1] S. Soghrati, A. Nagarajan, and B. Liang. “Conforming to interface structured adaptive mesh refinement technique for modeling heterogeneous materials.” Computational Mechanics, 125:24-40, 2017. [2] K.A. Acton and and S.C. Baxter. "Characterization of Random Composite Properties Based on Statistical Volume Element Partitioning. " Journal of Engineering Mechanics 144.2 (2017): 04017168. [3] R. Abedi, R.B. Haber, and P.L. Clarke. "Effect of random defects on dynamic fracture in quasi-brittle materials. " International Journal of Fracture 208.1-2 (2017): 241-268.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Multiscale Analysis of Heterogeneous Systems with Randomly Distributed Inclusions and Defects

Mahesh Bailakanavar*

*Thornton Tomasetti, Inc.

ABSTRACT

Generation of RVE's is a vital step in the multiscale analysis of heterogeneous materials. Unlike materials with periodic microstructure, generation of morphological details of materials with randomly distributed inclusions, such as defects in ceramics, hard and soft domains in polymers and chopped fiber composites pose various challenges such as: (i) Accurate representation of the inclusion shape, size, volume fraction and spatial orientation and distribution of the inclusions to minimize geometric approximation errors (i) Generation of unit cells with packing fraction as high as 45%, typically found in industrial grade composite materials (ii) Determination of the unit cell size that constitutes a macroscopically homogeneous material (iii) Generation of unit cells in quick succession with maximum computational efficiency for utilization in a stochastic multiscale framework. A Hierarchical Random Sequential Adsorption (HRSA) based algorithm is developed with the following features (i) Robustness - can generate RVE's with volume fraction of up to 45% for aspect ratios as high as 20 (ii) Versatility - able to generate unit cells with inclusions of varying shapes and sizes (iii) Efficiency - hierarchy of algorithms with increasing computational complexity A statistical study aimed at determining the effective size of the unit cell with randomly distributed chopped fibers is conducted for two material systems, namely 35% by volume randomly distributed glass fiber microstructure and a 35% by volume randomly distributed carbon fiber microstructure geometry. The results suggest that for material system with randomly distributed inclusions the optimal size of the unit cell depends upon the relative stiffness of the phases comprising the microstructure. Next, the HRSA algorithm is used in generating the RVE of matrix phase of a CMC system consisting of process-induced defects at crossover points, matrix voids, shrinkage cracks and interlaminar separation. The computed effective matrix properties suggest that the manufacturing induced defects have the most pronounced effect on the through thickness elastic modulus of the matrix. The results suggest that accounting for the defects induced matrix anisotropy is crucial for accurately modeling the damage and failure in CMC systems.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Coupled Multiscale Approach to Modeling Aortic Valve Leaflet Tissue

Ahmed Bakhaty*, Sanjay Govindjee**, Mohammad Mofrad***

*University of California, Berkeley, **University of California, Berkeley, ***University of California, Berkeley

ABSTRACT

Cellular mechanotransduction is the process by which biological cells respond to mechanical stimuli and activate biochemical pathways. Due to the importance of the microscale behavior in biological systems, traditional biomechanical modeling is limited in its capabilities. Multiscale modeling techniques, such as computational homogenization[1] (also known as “FE^2”), however, can be used to investigate the micromechanical behavior of cells in biological systems, and hence mechanotransduction. Huang[2] proposed the valvular interstitial cells (VIC) aspect ratio as a mechanical measure of cellular mechanotransduction activity and performed experiments that investigated the metric in response to physiological loading of aortic valve leaflet tissue. Numerical simulations that mimic these experiments were carried out but limited to 2D and uncoupled 3D models (i.e., no interaction between the macroscale and microscale). In this study, we apply FE2 to aortic valve leaflet tissue in 3D to study the mechanical behavior of the VIC in response to organ-scale mechanical loading. The modeling scheme importantly utilizes self-consistent material models based on layer-wise experimental data from aortic valve tissue.[3] Our simulations demonstrate a viable method for fully multiscale modeling of aortic valve tissue. We find that the “apparent” VIC aspect ratio observed in experiments may not necessarily be consistent with the actual 3D deformations of the cells. [1] Kouznetsova, V., Brekelmans, W.A.M. and Baaijens, F.P.T., 2001. An approach to micro-macro mod- eling of heterogeneous materials. Computational Mechanics, 27(1). [2] Huang, H.Y.S., Liao, J. and Sacks, M.S., 2007. In-situ deformation of the aortic valve interstitial cell nucleus under diastolic loading. Journal of biomechanical engineering, 129(6). [3] Bakhaty, A.A., Govindjee, S. and Mofrad, M.R., 2017. Consistent trilayer biomechanical modeling of aortic valve leaflet tissue. Journal of biomechanics, 61, pp.1-10.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Prediction Modeling of Exergy Destruction Rates of Turboprop Engine Components by the Use of Genetic Algorithm Based Artificial Neural Networks

Tolga Baklacioglu*, Onder Turan**, Hakan Aydin***

*Anadolu University, **Anadolu University, ***Tusas Engine Industries

ABSTRACT

This study illustrates a deep learning approach supported by metaheuristic design, targeting the foremost features and parameters of artificial neural network (ANN) framework used in predicting the rate of exergy destruction attainable in various components of an experimental turboprop engine. The development of deep ANN architectures comprising of three-hidden layers, using data obtained during real experimentation considering multiple engine parameters was accomplished in this regard. The employed engine parameters included gas generator speed, torque, power, airflow, and fuel mass flow obtained through turboprop engine runs. Once the deep learning ANN frameworks were hybridized with a metaheuristic approach, such as genetic algorithms (GAs), the optimization of the features of the initial network was facilitated. The features include biases, momentum factor, step-size, and weights for the back-propagation (BP) learning model, in addition to the number of neurons that are located in the hidden layers in terms of network topology design. The analysis of errors revealed a close fit involving the predicted values of the model and references made on real data in exergy destruction rates for the engine components. The use of appropriately chosen values in preceding networks weights produced more accurate testing results (R values of 0.998986, 0.998315, 0.996497, and 0.996649 for combustor, compressor, gas turbine, and power turbine, respectively) in networks using three hidden layers compared to those using lower hidden layers. Furthermore, optimizing deep ANNs using the GAs delivers not only further improved accuracy (R values of 0.999656, 0.999641, 0.998929, and 0.999966 for the previously mentioned engine components, respectively) but also an effective utilization of time in the resulting models.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Controlling Electronic Properties of Two-dimensional Organic-inorganic Halide Perovskites

Ganesh Balasubramanian*

*Lehigh University

ABSTRACT

Organic-inorganic halide perovskites, which have sparked a substantial interest due to their excellent photovoltaic properties, have also been synthesized in stable two-dimensional forms. The reduction in dimension promises an exciting opportunity to tune the transport properties of these functional materials. Here, we share findings from first principle calculations of various engineered two-dimensional hybrid organic-inorganic halide perovskite structures. While on one hand, the structures possess excellent transport properties similar to their bulk counterparts, on the other hand, the reduced dimensionality offers the advantage of tuning the band gaps over a broad range. In addition, by employing strain engineering to these two-dimensional materials, we are able to control transport properties including electrical conductivity and Seebeck coefficient. Our efforts are directed towards employing computational sciences for engineering designer perovskites with tailored properties.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Effects of Morphology on the Mechanical Properties of Heterogeneous Polymer-grafted Nanoparticle Networks

Anna Balazs*

*University of Pittsburgh

ABSTRACT

Using computational modeling, we examine how varying the arrangement of binary mixtures of polymer grafted nanoparticles (PGNs) in a network affects the mechanical properties of the composite. The free ends of the grafted chains on the PGNs contain reactive groups that can form labile bonds with reactive ends on nearby PGNs, and thereby form extensive networks. This bond formation is reversible, with the bonds breaking and reforming at a specified rate. The two types of particles in the network differ in the strength of the labile bonds that they form with their neighbors, forming both relatively strong and weak interconnections. We examine the response of this dynamic network to tensile deformation when the binary PGNs are arranged in an alternating, layered structure or a random mixture. We determine the ultimate tensile properties (strength, toughness), the strain recovery and behavior under cyclic loading for samples with the layered and random architectures. We demonstrate that the layered structures display self-healing behavior and exhibit enhanced mechanical properties relative to the random system. Using our model, we can tune both the spatial and temporal characteristics of the hybrid material. Thus, the approach provides a useful tool for determining how to tailor these parameters to achieve superior mechanical behavior in PGN networks.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Beams with Variable Mechanical Properties: Planar Timoshenko-like Model and Numerical Solution via Iso-Geometric Collocation

Giuseppe Balduzzi*, Simone Morganti**, Josef Füssl***, Alessandro Reali****, Ferdinando Auricchio*****

*Institute for Mechanics of Materials and Structures (IMWS), Vienna University of Technology, Vienna, Austria, **Department of Electrical, Computer, and Biomedical Engineering, University of Pavia, Pavia, Italy, ***Institute for Mechanics of Materials and Structures (IMWS), Vienna University of Technology, Vienna, Austria, ****Department of Civil Engineering and Architecture (DICAr), University of Pavia, Pavia, Italy, *****Department of Civil Engineering and Architecture (DICAr), University of Pavia, Pavia, Italy

ABSTRACT

Beams and plates with smooth variations of mechanical properties are frequently used in several engineering fields. As an example, the presence of knots leads to non-uniform distribution of stiffness and grain direction within timber structural elements (e.g., Glued Laminated Timber (GLT) beams and Cross Laminated Timber (CLT) plates) and substantially influences the mechanical response of the structural element. First and foremost, since the structural element under analysis is made of an anisotropic material with principal directions not aligned with the beam axis, shear deformations depend on all stress components. Such a dependency is reasonable and expected considering the 2D constitutive relation of the material, while its influence on the beam 's constitutive relation is less trivial and needs enhanced tools for the evaluation of the stiffness coefficients [1]. Furthermore, [2, 3] highlight that every variation of mechanical properties within the beam body leads axial internal force and bending moment to produce non-vanishing shear stresses and deformations. This contribution discusses a simple and effective Timoshenko-like planar beam that can effectively handle both the so far introduced problematics. The model turns out to be naturally represented by a mixed, explicit system of six ordinary differential equations in which both internal forces and beam 's generalized displacements are the independent variables. Complexity of beam's constitutive relations and variability of its coefficients do not allow for an easy computation of the model 's analytical solution, making the usage of numerical tools mandatory. Unfortunately, classical approaches like mixed finite elements might entail several issues (e.g., shear locking, ill-conditioned matrices, etc.). Conversely, the isogeometric collocation method allows an equal order approximation of all unknown fields, without affecting the stability of the solution. This makes such an approach simple, robust, and particularly suitable for solving the system of ODEs governing the proposed beam model. A rigorous comparison with highly refined 2D FE analysis will demonstrate the effectiveness of the proposed modelling strategy. REFERENCES [1] H Murakami, E Reissner, and J Yamakawa. Anisotropic beam theories with shear deformation. Journal of Applied Mechanics, 63(3):660-668, 1996. [2] Giuseppe Balduzzi, Mehdi Aminbaghai, Ferdinando Auricchio, and Josef Füssl. Planar Timoshenko-like model for multilayer non-prismatic beams. International Journal of Mechanics and Materials in Design, 2017. doi:10.1007/s10999-016-9360-3. [3] Giuseppe Balduzzi, Mehdi Aminbaghai, and Josef Füssl. Linear response of a planar FGM beam with non-linear variation of the mechanical properties. In Alfredo Güemes, Ayech Benjeddou, José Rodellar, and Jinsong Leng, editors, SMART 2017, pages 1285-1294. CIMNE, 2017.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Moving-least-squares Immersed Boundary Method for Thin Rigid Structures

Rahul Bale*, keiji onishi**, Niclas Jansson***, Amneet Pal Singh Bhalla****, Makoto Tsubokura*****

*RIKEN AICS, **RIKEN AICS, ***KTH Royal Institute of Technology, ****Lawrence Berkeley National Lab, *****RIKEN AICS, KOBE University

ABSTRACT

Constraint immersed boundary (CIB) method is a fictitious domain approach for fluid-structure interaction problems in which an immersed body (IB) is represented by volumetric Lagrange multipliers (that impose rigid body constraint) in the combined momentum equation. The incompressible Navier-Stokes equation is solved on a Cartesian mesh, whereas the Lagrange multipliers are defined on a non-conforming Lagrangian mesh. The Eulerian-Lagrangian interactions, i.e., velocity interpolation and force spreading, are mediated by regularized Peskin's delta functions [1]. The CIB approach has been applied successfully to model volumetric bodies at intermediate Reynolds number flow applications in the past [2,3], in which the volumetric treatment of Lagrange multipliers ensure that there is no fluid sloshing inside the IB, and effectively making the fluid inside move with the IB velocity. Representing the IB with only a surface mesh leads to spurious flow inside the body that grows with Reynolds number. For many applications with complex geometries, this is particularly challenging for two reasons. First, in most applications CAD geometry is available in surface mesh format. Second, it may not always be possible to separate the inside region from outside region. In this work, we extend the CIB method to model thin bodies using surface mesh representation. The method requires modifying delta functions using moving-least-squares (MLS) approach by identifying the two sides of the IB surface. The weights of the delta functions are modified such that velocity interpolation and force spreading occur separately on either side of the IB surface, but they still satisfy the original moment conditions which are known to conserve energy, force, and torque during Eulerian-Lagrangian interactions. The MLS approach does not add substantially to the computational cost because the immersed body is an object of codimension-1 in the simulations. We present several cases of flow past bluff bodies showing a dramatic reduction of fluid sloshing using the new approach at intermediate to high Reynolds number. In addition, we also discuss some theoretical properties of the modified delta functions. [1] Peskin CS. The immersed boundary method. Acta numerica. 2002, 11:479-517. [2] Bhalla, A. P. S., Bale, R., Griffith, B. E., & Patankar, N. A. A unified mathematical framework and an adaptive numerical method for fluid-structure interaction with rigid, deforming, and elastic bodies. Journal of Computational Physics, (2013), 250, 446-476. [3] Kallemov B, Bhalla A, Griffith B, Donev A. An immersed boundary method for rigid bodies. Communications in Applied Mathematics and Computational Science. 2016, 11(1):79-141.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Scale-Resolving Simulations of Turbulent Boundary Layers with Flow Separation

Riccardo Balin*, Eric Peters**, John Evans***, Philippe Spalart****, Kenneth Jansen*****

*University of Colorado Boulder, **University of Colorado Boulder, ***University of Colorado Boulder, ****The Boeing Company, *****University of Colorado Boulder

ABSTRACT

Due to the large computational cost associated with DNS and LES, most engineering flows are currently modeled with RANS. During the stages of design, for instance, the large number of simulations required to explore the parameter space dictates the use of the less computationally intensive RANS methods. Moreover, the large Reynolds numbers in which most air and water vehicles operate put DNS and LES completely out of reach. Unfortunately, RANS models perform poorly when dealing with boundary layers affected by strong adverse pressure gradients and flow separation, plaguing the prediction and design of systems exhibiting such characteristics. Therefore, it is of great value to better understand the physics involved in separation of a turbulent boundary layer, and to gather data for such flows with the hope of improving the prediction of RANS models (and other closure models as well) through statistical approaches to turbulence modeling. To accomplish this task, scale-resolving simulations of two turbulent boundary layers affected by adverse pressure gradients and separation are carried out. In one case, the pressure gradient is designed to produce incipient separation of the layer well inside the flow domain, while in the other case full flow separation is studied. DNS, LES, wall-modeled LES, and DES of both separated boundary layers are performed, and comparisons are drawn between the different approaches, as well as with the RANS predictions of the flows. Experimental data is also used to verify the numerical results. Attention is given to the boundary layer in the region leading to and after separation ensues. In particular, the details of the Reynolds stresses, turbulent kinetic energy budget and effective eddy viscosity are reported. The Reynolds number of the boundary layer is close to the upper limit of what is practical for a DNS.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Uncertainty Propagation in a 3D Asymmetrically Pretensioned Guyed Mast

Jorge Sebastian Ballaben*, Marta Beatriz Rosales**, Rubens Sampaio***

*Universidad Nacional del Sur - CONICET, **Universidad Nacional del Sur - CONICET, ***Pontificia Universidade Catolica do Rio de Janeiro

ABSTRACT

The study of the nonlinear dynamic response of a guyed mast considering the uncertainty of the guys pretension is reported in this work. The structure consists in a real life guyed mast of 20 m high and one level of three cables. The mast is represented by an equivalent beam-column with the addition of second order effect due the axial loads of the cables. The three guys behavior is described through cables with an initial pretension and only tensile capacity. The partial differential equations are discretized using the finite element method, considering Hermite elements for the mast (Bernoulli beam theory) and nonlinear cable elements for the guys. A lateral dynamic load is applied on the mast, through a cosine function with its frequency selected to avoid the natural frequencies of the system. An ad hoc software developed by the first author is employed to solve the nonlinear dynamic problem. Once the deterministic problem is stated, an uncertainty quantification is carried out. In this case, the stochastic variable is the pretension. Since the design value can be modified at the construction stage and during the service life, the pretension force is modeled as a random variable with a probability density function (PDF) derived from the Principle of Maximum Entropy (PME). In previous works of the authors, the case in which all the cables have the same pretension (though stochastic) was solved. However, a situation in which the cables do not have the same value of pretension is possible due to eventual discrepancies in the installation. Thus, a small random error is introduced to make the guys tensions different among them. The radial symmetry is thus lost. The model herein presented contributes to attain a more realistic description of the structure, mainly regarding the three-dimensional representation and the sensibility to the variability of the guy pretensions. The obtained results (natural frequencies and modes, dynamic displacements, etc.) and its interpretation through statistic tools, improve the understanding of the real dynamic properties and behavior of slender and flexible guyed structures.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Fully Resolved Cellular-scale Simulation of Blood Flow in Physiologically Realistic Microvascular Networks

Peter Balogh*, Prosenjit Bagchi**

*Rutgers University, **Rutgers University

ABSTRACT

An efficient three-dimensional computational tool [1] for simulating cellular-scale blood flow within highly complex geometries is presented. The motivation behind the development is to provide a framework capable of modeling the diverse range of interface types present in microcirculatory blood flow, thus permitting the study of such complex flows while retaining the cellular-scale details. Simultaneously modeling this diverse range of interface types, however, presents a major challenge numerically. The method must be capable of modeling deformable cell surfaces, such as red blood cells, white blood cells, or circulating tumor cells, highly complex stationary interfaces such as microvascular networks or microfluidic devices, as well as moving rigid interfaces such as inactivated platelets. To accomplish this we use immersed boundary methods (IBMs) integrated into a coupled finite-volume/spectral fluid flow solver. A sharp-interface IBM is used to model the complex stationary interfaces as well as the moving rigid interfaces. A continuous forcing front-tracking method is used in conjunction with the finite element method to model the interfaces of the deformable cells. The overall computational domain resembles a box, discretized in space by a fixed, uniform, rectangular Eulerian grid. The governing fluid flow equations are numerically solved on this grid using a projection method for the time integration, with a staggered arrangement of the flow variables. All interfaces are immersed into this computational domain. With the sharp-interface method constraints are enforced at Eulerian grid points such that a no-slip condition is achieved at the interface. With the front-tracking method, the stresses generated in the membrane due to resistance against shearing, area dilatation, and bending are computed on a Lagrangian grid. They are then coupled to the bulk fluid on the Eulerian grid with a body-force term constructed from a finite-span delta function added to the governing equations. Various validations are presented to establish the accuracy of the simulation tool. The versatility of the tool is then demonstrated by simulations of cells flowing in microfluidic devices as well as in physiologically realistic microvascular networks. The later example was the focus of our recent work [2] in which several unexpected phenomena were revealed. Overall, the methodology presented provides a viable framework for studying the flow of whole blood through highly complex physiological geometries while simultaneously capturing the cellular-scale details. References: [1] Balogh, P. & Bagchi, P., J. Comp. Phys., 2017, 334, 280-307. [2] Balogh, P. & Bagchi, P., Biophys. J., 2017, 113, 2815-2826.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Experimental and Numerical Characterization of Plastic Flow and Ductile Damage in Extruded Aluminium

Sandra Baltic*, René Hammer**, Julien Magnien***, Thomas Antretter****, Werner Ecker*****

*Materials Center Leoben Forschung GmbH, **Materials Center Leoben Forschung GmbH, ***Materials Center Leoben Forschung GmbH, ****Montanuniversität Leoben, *****Materials Center Leoben Forschung GmbH

ABSTRACT

Because of the excellent functional and structural properties, aluminium alloys have many applications: from large lightweight structures, over car bodies to the smallest electronic components. The object of this research is the ductile behaviour of aluminium alloys formed into cans by impact extrusion. The plastic flow and the fracture strain loci of two material grades have been investigated: AW-1050 and AW-6082. To precisely predict the material flow and ductile damage under complex loading, detailed material characterization is required. To this aim, miniature tensile test specimens are optimized by numerical simulations to cover a wide range of stress states for the model calibration. Final sample geometry includes dogbone, notched and shear specimens. We propose a new method, which leads to a biaxial stress state under uniaxial tensile testing. Special attention is paid to the effect of stress triaxiality and Lode angle parameter on the fracture strain under plane stress conditions (Bai and Wierzbicki, 2015). Digital Image Correlation is utilized to track the plastic flow and to identify the initiation and development of localized strain during tensile test. Sample position is planned so that the effect of anisotropy, due to the extrusion process, can be quantified. Three different angles with respect to the extrusion direction are considered: 0°, 45°, 90°. Tensile test results in different orientations allowed to calculate the anisotropy coefficients which determine the shape of the yield function. The tests are accompanied by FEM to identify the damage evolution and strain to fracture for the calibration of the damage model. Tensile testing of miniature samples with non-standard experimental setup and numerical modelling of damage evolution and failure with highly localized strain are the challenges, which have been successfully overcame by this contribution. Complete range of the Lode angle parameter and positive stress triaxialities for plane stress conditions has been covered just by making use of uniaxial tensile experiments. The calibrated model is expected to predict the mechanical response of extruded aluminium cans under complex loading and finds its application in the precise prediction of the opening pressure for safety vent design. References Bai, Y.; Wierzbicki, T.: A comparative study of three groups of ductile fracture loci in the 3D space. In: Engineering Fracture Mechanics 135 (Supplement C), S. 147–167, 2015

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Quantification of the Probability of Failure in Sheet Metal Forming Problems of Advanced High Strength Steel

Daniel Balzani*, Niklas Miska**

*Ruhr-Universitaet-Bochum, Chair of Continuum Mechanics, Germany, **Ruhr-Universitaet-Bochum, Chair of Continuum Mechanics, Germany

ABSTRACT

Numerous production processes and constructions rely on an accurate description of the material behavior and the boundary conditions to the problem. Such input variables may become uncertain and then an accurate calculation of the probability of failure is required. In particular in many modern materials, which make use of heterogeneous microstructures, such as advanced high strength steels, specific challenges arise from a significant variation of microstructure morphology leading to uncertain macroscopic material properties. Here, a new method is proposed to solve this problem. The method is based on the simulation of large sets of microscopic boundary value problems using finite elements and the subsequent homogenization of the microscopic mechanical quantities to obtain the effective macroscopic properties of the material. For each of these simulations a different microstructure is considered, which is selected such that the statistical variation of the computed microstructures is as close as possible to a variation in the real material. To assure this constraint, we exploit the concept of statistically similar representative volume elements (SSRVEs) [1]. This concept is originally formulated as minimization of a statistical least-square functional governed by distances of statistical measures describing the real material 's microstructure and the one of the SSRVE. Thereby, an artificial microstructure is constructed which matches best the morphology of the real microstructure in a statistical sense. Here, we consider the least-square functional as measure for the similarity of microstructure morphology and create a set of statistically similar volume elements (SSVEs) such that the variation of the least-square functional over the SSVEs follows the one of the real material. To ensure an efficient quantification of the associated uncertain macroscopic material parameters, a Multi-Level Monte-Carlo Approach is used. However, the resulting uncertain macroscopic properties may not necessarily follow specific distribution functions. Also other parameters of sheet metal forming problems as e.g. the friction coefficient may pocess uncertainties which can hardly be quantified. This means that only limited data on the uncertain quantities in terms of bounds or moments of reduced order will be available, which prevents a classical uncertainty quantification procedure. In order to overcome this problem, the Optimal Uncertainty Quantification (OUQ) framework [2] can be considered to determine the sharpest bounds possible to the probability of failure in sheet metal forming problems, where the limited data is included as constraint to a global minimization/maximization principle. The proposed method is demonstrated with an example of advanced high strength steels. [1] D. Balzani, L. Scheunemann, D. Brands, and J. Schr\"oder. Construction of two- and three-dimensional statistically similar RVEs for coupled micro-macro simulations. Computational Mechanics, 54(5):1269–1284, 2014. [2] H. Owhadi, T. J. Sullivan, M. McKerns, and M. Ortiz. Optimal Uncertainty Quantification. SIAM Rev., 55(2):271--345, 2013

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Modeling and Validating Conformational and Chemical Pathways in Macromolecular Systems

Nilesh Banavali*

*Wadsworth Center, New York State Department of Health

ABSTRACT

Enhanced Sampling Molecular Dynamics (ES-MD) simulations provide a robust route to overcome the timescale limitations of brute-force MD approaches, and understand the complex free energy landscapes that govern functional behavior of biomolecules. However, novel intermediates identified through ES-MD simulations are frequently considered speculative till experimental validation can be provided for them. Many biological systems also function through a complex combination of conformational and chemical transitions that are difficult to seamlessly model using ES-MD simulations. One underutilized source of validation of conformational transitions is the existing structural data deposited in the RCSB Protein Data Bank (PDB). This presentation will demonstrate how multi-dimensional histograms can be used to mine the structural heterogeneity in the PDB to inexpensively model conformational pathways. Unusual structural intermediates that explain important functional characteristics, and are possibly identifiable only through extensive ES-MD simulations, can be predicted using this approach at minimal computational cost. Specific features of structural intermediates separately identified through enhanced sampling MD simulations can also be validated by easy identification of similar counterparts in the PDB. A strategy called Restrained Geometries and Topology Switching (RGATS) will also be presented that can be used to model chemical reactions in complex environments using any Molecular Mechanics (MM) program, with no additional software implementation. This strategy enables application of any ES-MD method, implemented in any MM program, for elucidating conformational features of biochemical reaction pathways. In particular, this strategy allows rapid prediction of reactant, intermediate, or product state structures for any chemical reaction in any bio-molecular context, when an accurate structural model in any one of these states is available.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Understanding Deformation Capacity Variability in Ductile Fiber-reinforced Cement-based Composite Components through Numerical Simulation

Matthew Bandelt*, Mandeep Pokhrel**

*New Jersey Institute of Technology, **New Jersey Institute of Technology

ABSTRACT

Numerous applications of ductile fiber-reinforced cement-based composites have been proposed to improve the ductility, durability, and damage resistance of structures throughout the world. Experimental findings have shown that the flexural failure of reinforced beams using ductile cementitious materials is often governed by fracture of reinforcement rather than crushing of compression zone, as is commonly observed in traditional reinforced concrete structures. Experimental research has identified how certain factors, such as reinforcement ratio, influence deformation capacity; however, significantly variability in component ductility is still not well understood. This study explores the variability in deformation capacity in ductile fiber-reinforced cement-based composites containing steel reinforcement. Computational finite element models are simulations are carried out to understand the influence of mechanical properties, reinforcement ratio, boundary conditions, and structural geometry on deformation capacity. Two-dimensional continuum models were created and simulated using total strain-based models up to the point of simulated reinforcement fracture. Damage patterns in the fiber-reinforced cementitious material and reinforcement are studied at different deformation levels to identify the spread of plasticity in reinforced components. The results of this study provide a better understanding of how structural members with ductile cement-based composite behave in relation to various material and structural properties. Numerical simulations show how flexure and shear crack progression influences reinforcement strain distribution, rebar fracture, and deformation capacity. Results are compared with experimentally observed damage progression, strain localization, and deformation capacity.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Polycrystal Plasticity Modeling of High Cycle Fatigue Behavior in Ti-6Al-4V and Residual Stresses in Dissimilar Welded Ti Alloys

Ritwik Bandyopadhyay*, Michael Sangid**

*Purdue University, **Purdue University

ABSTRACT

Fatigue is one of the most common modes of failure in engineering components. Despite many studies, the physics of fatigue crack initiation is an open field of research, due to the complexities in evolving micromechanical states and diverse local microstructure in the region of crack initiation. Recently, with the advent of high performance computing, crystal plasticity (CP) models, integrated within the finite element method (FEM), are used to study this issue, by accounting for anisotropic material behavior and slip system activation. These investigations help to identify dominating physical mechanisms, especially strain localization and stress concentration, which are precursors to fatigue crack initiation. Such mechanisms, in general, depend on grain morphology, intergranular misorientation, lattice structure, macroscopic load regime, etc. In the present study, we simulate high R-ratio high cycle fatigue response in Ti-6Al-4V using a CP-FEM framework and analyze several damage indicator parameters in relation to crack initiation observed during a companion experiment. Design against high cycle fatigue crack initiation is strongly influenced by the presence and nature (tensile or compressive) of the residual stress field. In the second part of this talk, we analyze residual stress profiles across the linear friction weld joints of Ti-6Al-4V-to-Ti-6Al-4V and Ti-6Al-4V-to-Ti-5Al-5Mo-5V-3Cr alloys using energy dispersive x-ray diffraction measurements to identify the complete lattice strain tensor in the alpha and beta phases in these materials. These residual stress profiles can be suitably incorporated within polycrystal plasticity finite element framework to study the physics of fatigue crack initiation in an effective way.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Cohesive Zone Modelling on Initiation and Propagation of Fatigue Crack

Anuradha Banerjee*, Nijin I. S**, Shravan Kumar R.***

*Indian Institute of Technology Madras, Chennai, **Indian Institute of Technology Madras, Chennai, ***Indian Institute of Technology Madras, Chennai

ABSTRACT

Fatigue is one of the most critical modes of failure due to the progressive growth of micro-structural damage even under sub-critical loads. Diverse approaches using Cohesive zone law have been adopted for the better prediction of fatigue failure in the recent years [1]. These models were successful in predicting growth data of a pre-existing crack but could not be applied in prediction of initiation of crack from notch tip as there exists significant differences between the state of stress ahead of a notch-tip and a crack-tip. In the present work, a stress-state dependent cohesive model, combined with an irreversible damage parameter has been used in simulation of fatigue crack growth initiation and continued growth in a representative aluminum alloy. For simulation of realistic fatigue crack growth, from its initiation and during its continued growth till final failure, stress-state is incorporated by expressing the traction separation law of cohesive elements as a function of biaxiality ratio (?) and separation [2]. This cohesive law has an associated cohesive strength, ?max, and cohesive energy, ?o. These parameters, however, in the model are dependent on the triaxiality of the stress-state and thus, not material constants. Stress-state with higher ?, corresponds to higher triaxiality, results in higher ?max and lower ?o. Growth of damage, as per the effective stress concept of continuum damage mechanics, results in overall degradation of the process zone [3]. The model is implemented as interface elements and plane strain simulations of crack initiation and growth under cyclic loading are performed for two different load ranges. The stress-state of neighbouring continuum elements is used in the traction-separation behaviour of the cohesive elements. A combination of the fatigue damage model parameters is identified that is able to reproduce the crack growth curves in the high cycle fatigue regime observed experimentally. Further, a discussion is developed on the specific role of the stress-state on the initiation life and crack growth rates under sub-critical cyclic loading. References [1] Kuna M, Roth S. General remarks on cyclic cohesive zone models. Int J Fract 2016:1–21. [2] Banerjee, R. Manivasagam, Triaxiality dependent cohesive zone model, Engineering Fracture Mechanics 76 (12) (2009) 1761–1770. [3] K. Roe, T. Siegmund, An irreversible cohesive zone model for interface fatigue crack growth simulation, Engineering fracture mechanics 70 (2) (2003) 209–232.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Modeling Compressive Fracture of Haversian Bone Using Porosity Based Lattice Model

Anuradha Banerjee*, Ashwij Mayya**, R. Rajesh***

*Indian Institute of Technology Madras, India, **Indian Institute of Technology Madras, India, ***1. The Institute of Mathematical Sciences, Chennai, India 2. Homi Bhabha National Institute, India

ABSTRACT

Cortical bone, found in the central part of long bones like femur, is known to adapt to local mechanical stresses. This adaptation has been linked with Haversian remodeling involving resorption of existing primary bone followed by laying of secondary osteonal systems. As a consequence of remodeling, both, the structure of porosity network as well as the matrix properties can be expected to evolve. Fracture process in complex heterogeneous quasi-brittle materials like bone involves multiple porosities and dissipative micro-fracture events leading to progressive loss in load bearing capacity prior to failure. Modeling such complex fracture process is vital for assessment of bone health, to design mechanically compatible implants and porous scaffolds. Also, similar models may be applicable in understanding the fracture behavior of other brittle porous materials like wood, rock etc. Here, we characterize the three dimensional porosity network of bovine Haversian bone and examine the role of the overall porosity, structure of the porosity network and the matrix properties in its vulnerability against compressive failure. Using micro-Computed Tomography, the detailed structure of porosity network is obtained pre- and post-compression testing. Based on the periodicity in the features of porosity along tangential direction, we develop a two dimensional porosity-based random spring network model (RSNM) for Haversian bone. The load bearing capacity in compression predicted using RSNM simulations is shown to be significantly lower than experiments of Haversian bone as a result of changes in structure of the porosity network and increase in mean porosity while considering matrix properties as those of primary/plexiform samples obtained from same cross-section [1]. Using EDS line scans, however, the Haversian bone matrix is shown to be less stiff than that of plexiform samples. The failure properties of Haversian bone matrix that are iteratively determined to reproduce the experimental response are shown to be consistently higher than corresponding primary/plexiform bone matrix properties. The predictions, thus, suggest that Haversian bone due to remodeling has a bone matrix that is less stiff but significantly tougher than primary/plexiform microstructure of same cross-section. The findings are consistent with the variations in properties due to differences in levels of structural hierarchy of the microstructures [2]. References 1. Mayya, A., Banerjee, A., Rajesh, R., 2017. Phys. Rev. E 96 (5), 053001. 2. Zhang, Z., Zhang, Y.-W., Gao, H., 2011. Proc. R. Soc. Lond., B, Biol. Sci. 278 (1705), 519–525.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Probabilistic Thermomechanical Material Modeling of Ductile Metals from Uncertain Test Data

Aakash Bangalore Satish*, Michael D. Shields**

*Johns Hopkins University, **Johns Hopkins University

ABSTRACT

The mechanical response of ductile metals in simulations is represented using viscoplastic material models that are calibrated using experimental data. Calibration is usually performed deterministically from a small number of test data, often from one test, and therefore does not account for natural variability in the material properties. We present a Bayesian framework for probabilistic calibration of a viscoplastic damage model for ductile metals from an ensemble of test data under differing boundary conditions (uniaxial tension to plane strain) possessing variability in its temperature dependent mechanical response. The influence of the material variability on the response of structural components is then illustrated in comparison with the response of structural components whose material model is calibrated using traditional deterministic methods. The method is specifically applied to modeling the response of aluminum 6061-T6 components, where the material is calibrated using a series of over 150 mechanical tests under two different stress states at six temperatures. A brief description of the testing program and the resulting material variability will also be presented.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Stable and Accurate Partitioned FSI Algorithm for Incompressible Flow and Rigid Bodies

Jeffrey Banks*, William Henshaw**, Donald Schwendeman***, Qi Tang****

*Rensselaer, **Rensselaer, ***Rensselaer, ****Rensselaer

ABSTRACT

This talk discusses our continuing study of fluid-structure interaction (FSI) problems involving incompressible fluids and rigid bodies. Such FSI problems arise in many applications of science and engineering, such as particulate flows and mechanical heart valves. We discuss the development of the an added-mass partitioned (AMP) algorithm that remains stable, without sub-iterations, for light and even zero mass rigid bodies when added-mass and viscous added-damping effects are large. The scheme is based on a generalized Robin interface condition for the fluid pressure that includes terms involving the linear and angular acceleration of the rigid body. Added mass effects are handled in the Robin condition by inclusion of a boundary integral term that depends on the pressure. Added-damping effects are treated with approximate added-damping tensors that are defined by certain integrals over the surface of the body. We begin by discussing the development and analysis of the AMP scheme for simple model geometry in two spatial dimensions. Extension of the scheme to general geometry and three dimensions is then performed using finite difference methods and overlapping grids. For our parallel implementation we employ parallel sparse linear solvers for the pressure Poisson equation, including the non-standard AMP interface condition. Stability for light solids, and second-order accuracy are demonstrated for a series of challenging benchmark problems

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Multiscale Data Assimilation via Multivariate Gaussian Process Regression

David Barajas-Solano*, Alexandre Tartakovsky**

*Pacific Northwest National Laboratory, **Pacific Northwest National Laboratory

ABSTRACT

We present a spatial interpolation approach for parameter fields incorporating measurements with two different support volumes, a point support or fine scale, and a finite support or coarse scale. The proposed approach treats the fine and coarse fields as components of a bivariate Gaussian process with a parameterized multiscale covariance model. We employ a full bivariate Matérn kernel as multiscale covariance model, with shape and smoothness hyperparameters that account for the coarsening relation between fine and coarse fields. In contrast to similar multiscale kriging approaches that assume a known coarsening relation between scales, the hyperparameters of the multiscale covariance model are estimated directly from data via pseudo-likelihood maximization. We illustrate the proposed approach with a predictive simulation application for PDEs with heterogeneous parameters. Multiscale Gaussian process regression is employed to estimate the two-dimensional parameter distribution from synthetic multiscale measurements. The resulting stochastic model for coarse saturated conductivity is employed to quantify uncertainty in pore pressure predictions.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Reduced Order Modeling via PGD for Highly Transient Thermal Evolutions in Additive Manufacturing

Andrea Barbarulo*, Bruna Favoretto**, Charles-Andre De Hilllerin***, Victor Oancea****, Omar Bettinotti*****

*CentraleSupélec Université Paris-Saclay, **CentraleSupélec Université Paris-Saclay / Dassault Systèmes SIMULIA Corp, ***Dassault Systèmes SIMULIA Corp, ****Dassault Systèmes SIMULIA Corp, *****Dassault Systèmes SIMULIA Corp

ABSTRACT

Since their inception, Selective Laser Melting (SLM) and Electron Beam Melting (EBM) Powder Bed Fabrication (PBF), as prime examples in additive manufacturing (AM), proved to be a paradigm shift for manufacturing processes. They consist in selective melting of superposed layers of metal powder thanks to a machine-controlled moving high energy source. Due to their nature, these processes allow for unprecedented freedom in designing, personalizing and optimizing mechanical parts. Moreover, they are particularly suited for software-hardware integration when the desired geometry is conceived with a Computer Assisted Design (CAD) tool and directly produced by an automated process, removing all intermediate steps between designers ' vision and the physical world. Nevertheless, due to the young age of AM and to the lack of a complete mastering of the process by either experimental or numerical means, the mechanical properties of the produced parts are often unpredictable, severely constraining its use in high end applications. For this reason, numerical methods capable to predict final characteristics of the part, to spot critical points during the process and to help the design process itself, seem a necessity. Unfortunately, SLM and EBM encompass complex multiphysics (thermal, mechanical, electromagnetic, metallurgic, phase change) and pose a gigantic multi-scale problem in both space and time, which requires special consideration in numerical analysis. This work focuses on highly nonlinear thermal phenomena occurring in the immediate proximity of the fast moving heat source where temperature evolution rates, phase changes and thermal gradients are the most intense, all happening on a very small scale. The idea is to provide a low-cost / high accuracy simulation of this important zone. To provide this solution, a Reduction Order Model (ROM) technique called Proper Generalized Decomposition (PGD) has been adapted for this problem to consider highly temperature dependent material properties, phase change, latent heat, a laser that moves rapidly along the path and rapidly evolving Neumann boundary conditions. This model order reduction technique allows computing a reduced base for each variable without solving the full eigenvalue problem. Thanks to this technique, computational cost is significantly reduced and variable separation is achieved enabling to deal with highly meaningful reduced bases. This work also contains an in-depth study on PGD controls (number of modes, number of iterations, etc.) and on how they can be best selected for efficient computations. This work is part of an ongoing collaboration between Dassault Systèmes and MSSMat, CentraleSupelec University.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

An Active Set Type Method for 2D Hyperelastic Problems with Unilateral Contact and Coulomb's Friction

Mikaël Barboteu*, David Danan**

*University of Perpignan, France, **INSERM Rennes, France

ABSTRACT

In this work a Primal Dual Active Set (PDAS) type method is considered to solve mathematical problems which describe the frictional contact between hyperelastic bodies and a perfectly rigid obstacle. The Primal Dual Active Set type method is based on two points: first, the reformulation of frictional contact conditions as equivalent nonlinear complementarity functions and, next the use of a semismooth Newton method for the solution of the nonlinear complementarity equations, see [2,3]. This iterative method leads to consider specific boundary conditions on the contact boundary nodes belonging to active or inactive sets directly related to the status of contact and friction. Therefore, at each Newton iteration, we have to consider the solutions of problems with simple boundary conditions, such as Dirichlet, Neumann or Robin boundary condition as mentioned in [1,2,3]. This kind of method, as the well-known Stabilized or Nitsche's methods, allows more flexibility for finite element discretization (no discrete inf-sup condition, non-conforming meshes, etc.). The main trait of such method is that it does not require the use of the Lagrange multipliers both for the enforcement of the frictional contact conditions and the determination of the contact and friction stresses. As a consequence the implementation of the algorithm is facilitated, the condition number of the systems is better and the resolution is faster. Our aim is to present in detail the theoretical formulation and numerical algorithm of the PDAS method for three-dimensional problems with unilateral constraints and Tresca or Coulomb friction law. Then we derive a specific and simplified form of the frictional contact active set conditions in the case of 2D problems. In particular, we analyze this active set method and carry out qualitative theoretical and numerical comparisons with the well-known augmented Lagrangian method by considering representative contact problems for quasi-static and dynamic processes. [1] S. Abide, M. Barboteu and D. Danan, Analysis of two active set type methods for unilateral contact problems, Appl. Math. and Comput., 284 Issue C, 2016, 286-307. [2] M. Hintermuller, V. Kovtunenko, and K. Kunish, Semismooth Newton methods for a class of unilaterally constrained variational problems, Adv. In Math. Sci. and Appl., 147, 2004, 513-535. [3] S. Hueber, G.Stadler and B.I. Wohlmuth, A primal dual active set algorithm for three-dimensional contact problems with coulomb friction, SIAM J. Sci. Comput., 30(2), 2008, 572-596.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Robust Inside-Outside Segmentation Using Generalized Winding Numbers

Gavin Barill*, Neil G. Dickson**, Ryan Schmidt***, David Levin****, Alec Jacobson*****

*University of Toronto, **Side Effects Software, Inc., ***Gradientspace, ****University of Toronto, *****University of Toronto

ABSTRACT

Solid shapes in computer graphics are often represented with boundary descriptions, e.g. triangle meshes, but animation, physically-based simulation, and geometry processing are more realistic and accurate when explicit volume representations are available. Tetrahedral meshes which exactly contain (interpolate) the input boundary description are desirable but difficult to construct for a large class of input meshes. Character meshes and CAD models are often composed of many connected components with numerous self-intersections, non-manifold pieces, and open boundaries, precluding existing meshing algorithms. We propose an automatic algorithm handling all of these issues, resulting in a compact discretization of the input's inner volume. We only require reasonably consistent orientation of the input triangle mesh. By generalizing the winding number for arbitrary triangle meshes, we define a function that is a perfect segmentation for watertight input and is well-behaved otherwise. This function guides a graphcut segmentation of a constrained Delaunay tessellation (CDT), providing a minimal description that meets the boundary exactly and may be fed as input to existing tools to achieve element quality. We highlight our robustness on a number of examples and show applications of solving PDEs, volumetric texturing and elastic simulation. Furthermore, we express the generalized winding number as a boundary integral common to electrostatics. This allows us to employ the fast multipole method to expand our algorithm to a wider variety of geometries and applications.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Joule Heating Effect of Electroosmotic Flow through Soft Nanochannel

Sirsendu Sekhar Barman*, Somnath Bhattacharyya**

*Indian Institute of Technology, Kharagpur, **Indian Institute of Technology, Kharagpur

ABSTRACT

The present study deals with thermal transport characteristics of an electrolyte solution flowing through a slit nanochannel with polyelectrolyte walls, known as soft nanochannel. The sources of the fluid flow are the electrokinetic effects that trigger an electroosmotic flow (EOF) under the impact of a uniformly applied electric field. The direction and flow rate of EOF is governed by strength of the electric field, concentration of electrolytes, temperature, pressure, viscosity etc. The thermal transport characteristics is mainly dependent on Joule heating which is generated when an electric field is applied across conductive liquids. Such Joule heating not only causes increase in temperature but also creates a temperature gradient. The change of liquid temperature and the presence of temperature gradient would have an impact on the EOF. Ion and liquid transport in polyelectrolyte-grafted soft nanochannels have been employed for various applications such as biological analysis, chemical process, developing nanofluidic and much more. The present study includes the coupling Poisson-Boltzmann equation, the modified Navier-Stokes equations, the modified Nernst-Planck equation and the modified energy equation. Governing equations along with proper boundary conditions are solved numerically through a control volume approach over a staggered grid arrangement. Discretized equations are solved through the pressure correction based iterative SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) algorithm. The results are expressed in form of the average velocity, average entropy generation ((Savg)) for both step-like PEl and diffuse PEL. Solutions are obtained with a good agreement with the corresponding linear solutions of Matin, Ohshima et al.(2016) [1] for both the velocity field and temperature field. Extensive studies are carried out showing how the average velocity changes with the change of surface temperature. The average entropy generation is estimated with the solutions of Zhao et al.(2010) [2]. The average entropy generation is presented to analyse its dependency on softness parameter, bulk electrolyte concentration, PEL concentration, PEL thickness, surface charge density. The average entropy diminishes with the increase of surface temperature and it also increases with the increase of Joule heating. The average entropy decreases with the increase of decay length for diffuse PEL.
References [1] M. Matin, H. Ohshima, Thermal transport characteristics of combined electroosmotic and pressure driven flow in soft nanofluidics, Journal of colloid and interface science 476 (2016) 167–176. [2] L. Zhao, L. Liu, Entropy generation analysis of electro-osmotic flow in open-end and closed-end micro-channels, International Journal of Thermal Sciences 49 (2) (2010) 418–427.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Shock Waves Produced by the Interaction of Dynamic Crack with Heterogeneities

Fabian Barras*, Philippe H. Geubelle**, Jean-François Molinari***

*École Polytechnique Fédérale de Lausanne, **University of Illinois at Urbana-Champaign, ***École Polytechnique Fédérale de Lausanne

ABSTRACT

Recent experiments reveal how dynamic fracture is characterized by the interplay of the crack front with microscopic material heterogeneities (see for example [1]). Heterogeneous dynamic fracture remains a current challenge both for numerical modeling and experiments because of the associated fine time and length scales. In this work, we rely on a spectral boundary integral formulation of the elastodynamic wave equations derived in [2]. The numerical discretization focuses only along the rupture plane bounding two semi-infinite solids and allows a very fine description of the fracture process which is modeled following a cohesive approach. This work study the perturbation of dynamic crack front in presence of tougher inclusions along the rupture plane. We show numerically how shock waves are radiated from cusp emerging after large distortion of the crack front. We detail how these short-lived bursts persist far from the heterogeneity location and impact the overall rupture dynamics. Since any material presents heterogeneities at a certain scale, we further investigate how the heterogeneous interface properties (heterogeneity size, toughness contrast, crack speed) control the transition from quasi-homogeneous to heterogeneous dynamics. We finally measure the size of the fracture process zone and discuss the role of this critical length scale for heterogeneous dynamic fracture. REFERENCES [1] Guerra, C. and Scheibert, J. and Bonamy, D. and Dalmas, D. Understanding fast macroscale fracture from microcrack post mortem patterns. Proceedings of the National Academy of Sciences, Vol. 109, 390–394, 2012. [2] M. S. Breitenfeld and P. H. Geubelle. Numerical analysis of dynamic debonding under 2D in-plane and 3D loading. International Journal of Fracture, Vol. 93, 13–38, 1998. [3] F. Barras, P. H. Geubelle and J.-F. Molinari. Interplay between Process Zone and Material Heterogeneities for Dynamic Cracks. Physical Review Letters, Vol. 119, 2017.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Level-Set XFEM Sensitivity Analysis and Topology Optimization of Elastomeric Gels

Jorge Luis Barrera Cruz*, Kurt Maute**

*University of Colorado, Boulder, **University of Colorado, Boulder

ABSTRACT

Research on soft, active materials has flourished in recent years driven by a broad range of applications including actuation systems, tissue engineering, and soft robotics. These applications benefit from unique material properties such as large deformations, wide range of stimulants, and high motion complexities. Elastomeric gels are among the dominant members of this group of materials. The computational design of components/devices using these materials require not only mathematical models that accurately predict their response, but also robust optimization methods capable of handling model intricacies. This paper introduces a topology optimization approach for finding the spatial arrangement of stimuli-responsive elastomeric gels that swell upon contact with water, namely, hydrogels. The optimization approach combines a level set method for describing the material layout and a generalized version of the extended finite element method (XFEM) for predicting the response. This combination of methods yields optimization results that can be directly printed without the need for additional post-processing techniques. The highly nonlinear chemo-mechanical transient behavior of hydrogels is described by partial differential equations that advance in time through an internal state variable that represents the swelling state of the gel. A formulation for the computation of the sensitivities using the adjoint method for transient models captures the internal state variable dependencies. Computational aspects of the implementation of this approach into the level-set XFEM framework are discussed. The effect of the internal state variable on the sensitivities of problems subjected to various objectives is examined with numerical examples. Furthermore, the ability of the proposed optimization method to yield a highly resolved description of the optimized material layout is demonstrated by design studies in which initial simple configurations transform into target shapes. As the complexity of the target shape increases, the optimal spatial arrangement of the material phases becomes less intuitive, highlighting the advantages of the proposed optimization method.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Uncertainty Quantification of a Damage and Fatigue Phase Field Model

Eduardo Augusto Barros de Moraes*, Mohsen Zayernouri**, Mark Meerschaert***

*Michigan State University, **Michigan State University, ***Michigan State University

ABSTRACT

In this talk we present the uncertainty quantification of the structural damage and fatigue phase field model presented in [1]. In the non-isothermal, thermodynamically consistent model, the damage phase field is a continuous dynamical variable, and fatigue is treated as a continuous internal variable. The underlying assumptions and hypotheses involved in the modeling process may lead to gaps in the physical intuition, and uncertainties in the results from the choice of parameter values. In order to develop better models that can accurately predict failure in materials, we need to understand and identify the sources of uncertainty presented in current models. In this analysis, we consider an isothermal isotropic linear elastic material with viscous dissipation under the hypothesis of small deformations. We use the Monte Carlo and the Probabilistic Colocation methods to evaluate the expectation of the quantities of interest and measure the uncertainty with respect to the variation of several parameters. [1] JL Boldrini, EA Barros de Moraes, LR Chiarelli, FG Fumes, and ML Bittencourt. A non-isothermal thermodynamically consistent phase field framework for structural damage and fatigue. Computer Methods and Applied Mechanics and Engineering, 312:395-427, 2016.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Two-scale Homogenization Approach for Fluid Saturated Porous Media Based on TPM and FE²-Method

Florian Bartel*, Tim Ricken**, Jörg Schröder***, Joachim Bluhm****

*TU Dortmund University, **Stuttgart University, ***Duisburg -Essen University, ****Duisburg -Essen University

ABSTRACT

Thinking about the description of porous materials, e.g. metal foam, human tissue, plants or soils, we always have to take into account a global design composed of various substructures with different characteristics on a lower level. Examples of such substructures are pores which can be saturated with fluids or gases, fibers with different orientations or cells which can be influenced by chemical reactions. For the theoretical description of the behavior, enhanced continuum mechanical models give promising approaches. Up to now, due to the high complexity, it has not been possible to simulate these systems with only one design model. Hence, it is necessary to think about techniques which simplify the model but still consider the essential characteristics. It is clear, future applications will consider the discrete microstructure of materials. For example the topology can be received by CT-scanning and therefrom Representative Volume Elements (RVEs) can be designed. Therefore, we are preparing the Theory of Porous Media (TPM), see [1], for the usage in combination with the FE2?Method, cf. [2] and [3]. This contribution will present a two-scale homogenization approach for fluid saturated porous media with a reduced two-phase material model, which covers the behavior of large poro-elastic deformation. The main aspects of theoretical derivation for the weak form, the lower level boundary conditions under consideration of the Hill-Mandel homogeneity condition and the averaged macroscopic tangent moduli will be pointed out and a numerical example will be shown. Still, solving a coupled problem in FE² environment is extremely time consuming. Therefore, a parallel solution strategy is absolutely essential. Remarks on the investigation of High Performance Computation in this context will be given. Besides, model order reduction techniques lead to an impressive improvement of runtime. Hereby one has to accept approximation inaccuracy, however errors are small for engineering problems. Hence, we investigate in modified Proper Orthogonal Decomposition (POD) methods. Conceptional ideas will be discussed. References [1] R. de Boer and W. Ehlers, Theorie der Mehrkomponentenkontinua mit Anwendung auf bodenmechanische Probleme, Technical report, Teil I, Forschungsberichte aus dem Fachbereich Bauwesen, Heft 40, UniversitätGH-Essen, 1986. [2] C. Miehe, Computational micro-to-macro transitions for discretised micro-structures of heterogeneous materials at finite strains based on the minimization of averaged incremental energy, Computer Methods in Applied Mechanics and Engineering, 2002. [3] J. Schröder, A numerical two-scale homogenization scheme: the FE2-method, in J. Schröder, K. Hackl (editors), CISM course 550, Plasticity and Beyond, Springer, 1-64, 2014.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Gaussian Quadrature for C1 Cubic Clough-Tocher Macro-triangles

Michael Barton*, Jiri Kosinka**

*BCAM - Basque Center for Applied Mathematics, **University of Groningen

ABSTRACT

A numerical integration rule for multivariate cubic polynomials over n-dimensional simplices was designed by Hammer and Stroud [12]. The quadrature rule requires n + 2 quadrature points: the barycentre of the simplex and n + 1 points that lie on the connecting lines between the barycentre and the vertices of the simplex. In the planar case, this particular rule belongs to a two-parameter family of quadrature rules that admit exact integration of bivariate polynomials of total degree three over triangles. We prove that this rule is exact for a larger space, namely the C1 cubic Clough-Tocher spline space over macro-triangles if and only if the split-point is the barycentre. P. C. Hammer and A. H. Stroud. Numerical integration over simplexes. Mathematical tables and other aids to computation, 10(55):137-139, 1956.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Modeling Microstructural Heterogeneity During Failure Using Coupled Porosity and Crystal Mechanics

Nathan Barton*, John Moore**

*Lawrence Livermore National Laboratory, **Lawrence Livermore National Laboratory

ABSTRACT

Porosity (i.e., microscale void fraction) is a mechanism of ductile failure that is of ongoing concern, with recent interest spurred by new additive manufactured materials where initial voids and defects occur during component fabrication. Voids are often modeled explicitly at the crystal scale or implicitly—based on homogenized porosity models—at the component scale. This work couples crystal mechanics with these homogenized porosity models to alleviating the need for mesh resolution of sub-scale voids in crystal-scale modeling. This approach allows for the study of void families of varying potency, size, and distribution and their interaction with heterogeneous microstructures. This work shows examples from both quasi-static and dynamic loading scenarios and explores the connections among porosity kinetics, microstructural realism, and materials strength. This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 (LLNL-ABS- 743444).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Phase Field Microcracking Description Coupled with Viscoelastic Concrete Behavior

Benoit Bary*, Thomas Helfer**, Olivier Fandeur***, Julien Yvonnet****, Qi-Chang He*****, Daicong Da******

*CEA, Service d'Etude du Comportement des Radionucléides, France., **CEA, Service d'Etude et de Simulation du comportement des Combustibles, France., ***CEA, Service d'Etudes Mécaniques et Thermiques, France., ****Université de Paris-Est Marne-La-Vallée, France., *****Université de Paris-Est Marne-La-Vallée, France., ******Université de Paris-Est Marne-La-Vallée, France.

ABSTRACT

Concrete is an important constitutive material of nuclear power plants and waste storage structures whose main role is to ensure high level of performance regarding the required middle to long-term containment function. As such, creep and microcracking are known significant factors affecting the mechanical properties and the long term behavior of concrete, and may call into question the safety of nuclear facilities. The accurate modelling of these phenomena including their coupled effects have then to receive a special attention. We propose in this study to apply the relatively recent method making use of a phase field approach to reproduce the initiation and propagation of microcracking in concrete. This method rests on a diffuse description of the microcrack surfaces by one scalar variable whose values result from a specific balance equation. As a main contribution, it is extended here and coupled to a linear viscoelastic behavior to mimic the creep (and possibly shrinkage) of the material. A classical generalized Maxwell model is retained for modelling this viscoelastic behavior. At first, an energy-based formulation is developed to express the equations governing both viscoelastic mechanical and phase field problems. In this first attempt, only cracking due to extensions is considered. Different simple fracture criteria based on positive stresses or strains with and without threshold are applied and tested. The resulting approach is next implemented in the FE code Cast3M so as to solve both systems of equations. Applications to a homogeneous material subject to loading with various durations and intensity are then analyzed and discussed with regard to the different crack driving state functions. In a second stage, 3D simulations of heterogeneous concrete samples made up of elastic aggregates dispersed in a mortar matrix concentrating the viscoelastic behavior are performed. These numerical specimens are generated with polyhedral aggregates having various size and shapes, and which are randomly distributed in a box. The effects of the aggregate shape on the microcracking development and the macroscopic behavior of samples subject to creep loading are investigated. To this aim, different specimens are created with elongated and flattened polyhedral aggregates with given aspect ratio, and the obtained results are analyzed and confronted in particular in terms of microcrack patterns.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Multivariant Martensitic Transformations at Finite Strains and with Interfacial Stresses, and Interaction between Inclusion and Martensitic Transformations: A Phase Field Study

Anup Basak*, Valery Levitas**

*Iowa State University, **Iowa State University

ABSTRACT

A thermodynamically consistent novel multiphase phase field approach for temperature- and stress-induced martensitic transformations with N variants is developed at finite strain and taking the interfacial stresses into account. The model considers N+1 order parameters, where one of them describes austenite <->martensite transformations and the others describe the variant. The free energy of the system consists of the strain energy, thermal energy for austenite <->martensite transformations, barrier energy for all possible transformations, penalization energy for derivation of the variant-variant transformation path from a straight line and also for coexistance of three or more phases at a single material point, and penalization for the interfacial energy. Considering that N order parameters related to the variants are constrained to a plane in the order parameter space, the coupled system of Ginzburg-Landau equations are derived, the thermodynamic equilibrium conditions for homogeneous phases are obtained, and the instability criteria for homogeneous phase transformations are established. The present model resolves all the shortcomings existing in the models available in the literature. Three kinematic models (KMs) for the transformation deformation gradient are assumed: in KM-I it is a linear combination of the Bain tensors for the variants; in KM-II it is exponential of the linear combination of the natural logarithm of the Bain tensors; in KM-III it is derived using the twinning equation from crystallographic theory. Based on this model a finite element code has been developed. Several problems yielding complex microstructures are studied: (i) Evolution of microstructures with two variants in a sample under biaxial strains, and also the effect of sample size. (ii) Twinning using the generalized plane strain method, and also the sample size effect. (iii) Microstructure in a two-variant system under nanoindentation. (iv) Microstructure evolution in samples with nontransforming inclusion, where the energy of the interface between the inclusion and the surrounding phases is consistently taken into account. The influence of the ratio between the widths of the inclusion-martensite interfaces, austenite-martensite interface, and variant-variant interfaces are studied. Reference A. Basak, V.I. Levitas, Interfacial stresses within boundary between martensitic variants: Analytical and numerical finite strain solutions for three phase field models, 139 (2017) Acta Materialia, 174-187

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Damage Mechanics Theory with No Curve Fitting: Unification of Newtonian Mechanics & Thermodynamics

Cemal Basaran*

*University at Buffalo

ABSTRACT

Abstract The field of classical mechanics is based on Sir Isaac Newton's work in "The Principia," published in 1687. In this work, Newton introduced the world to three universal laws of motion, which describe the relationships of any object, the forces acting upon it and the object's resulting motion. It is these three laws that make up the foundation for classical mechanics, and all subsequent theories of mechanics are derived from them. But Newtonian mechanics still cannot account for the past, present or future of any aspect of a physical body or its governing equations. Around 1850, Rudolf Clausius and William Thomson (Kelvin) formulated both the First and Second Laws of Thermodynamics. Because the field of thermodynamics governs the past, present and future of all physical bodies, the aging process and life span of any physical body can be modeled in accordance with the thermodynamics laws. Still, thermodynamics alone cannot convey the response of a physical body under an external force at any given moment – something classical mechanics equations are able to achieve. Being able to accurately predict the life span of physical bodies, both living and non-living, has been one of humankind's eternal endeavors. Over the last 150 years, many unsuccessful attempts were made to unify the fields of classical mechanics and thermodynamics, in order to create a generalized and consistent theory of evolution of life-span of inorganic and organic systems. The objective has been to map out the aging process of a physical body using classical mechanics equilibrium equations while also predicting its life span. Most past attempts were based solely on the use of physical experiments, which would reveal the aging rate and life span of any physical body first. The experimental data is later be used to create a life-span expectancy model by curve fitting, like in the damage mechanics theory proposed by L. M. Kachanov. Authors, will report a new unified mechanics theory that can now predict the aging and life span of any physical body based purely on mathematical calculations and without the need for any prior life-span degradation testing or curve fitting phenomenological damage mechanics models.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Computational Approach to Additive Manufacturability of Low and High Gamma Volume Fraction Nickel-Based Superalloys

Hector C. Basoalto*, Chinnapat Panwisawas**, Richard Turner***, M. J. Anderson****, B. Saunders*****, J. W. Brooks******

*University of Birmingham, **University of Birmingham, ***University of Birmingham, ****University of Birmingham, *****Rolls-Royce, PLC, ******University of Birmingham

ABSTRACT

The manufacture of engineering components for aerospace applications through the selective laser melting (SLM) process is challenging. High volume fraction nickel-based superalloys are prone to cracking during the SLM process or subsequently in hot isostatic pressing (HIP) of the SLM part. This paper presents a numerical study on the evolution of microvoid dispersions and precipitate distributions for two nickel-based superalloys representing a low (IN718) and high (CM247LC) volume fraction alloys. The proposed modelling framework explicitly takes into account chemical compositions and commercially representative powder size distributions for each alloy. Simulations of single layer depositions indicate that CM247LC has a higher propensity to form lack-of-fusion and melt-flow induced micro-voids than IN718. It is shown numerically that, for the conditions investigated and thermodynamic parameters used, these differences are largely governed by the powder size distribution and not by the thermophysical parameters of these alloys for the conditions investigated. Composition dependent properties are shown to influence the thermal gradients during solidification, with CM247LC predicted to cool at a faster rate than IN718. These differences are expected to influence the residual stress development during SLM. A coupled mean field/finite element approach has been used to predict the global precipitate evolution within a simple rectangular build as well as a subsequent HIP cycle. Unimodal and multimodal particle distributions are predicted for IN718 and CM247LC at the end of SLM, respectively. A higher volume fraction of is predicted for CM247LC at the end of the SLM process. During HIP, simulations indicate a dramatic increase in the volume fraction in CM247LC, which can result in a reduction in stress relaxation and consequently large tensile residual stress states.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Calving Glaciers and Ice Shelves: New Insight from Old Theories

Jeremy Bassis*, Morgan Whitcomb**, Lizz Ultee***

*University of Michigan, **University of Michigan, ***University of Michigan

ABSTRACT

Projections of the growth and demise of ice sheets and glaciers require physical models of the processes governing flow and fracture of ice. The flow of glacier ice has been treated using increasingly sophisticated dynamical models. In contrast, fracture, the process ultimately responsible for half of the mass lost from ice sheets through iceberg calving, is often included using ad hoc parameterizations. Here we seek bridge this gap by introducing a model where ice obeys a power-law rheology appropriate for intact ice only up to a yield strength. Above the yield strength, we introduce a separate, weaker rheology that represents quasi-brittle failure along pre-existing faults and fractures—similar to Nye's unfortunately abandoned plastic approximation of glacier ice. Assuming glacier ice is unyielded allows us to bound the long term average rate of terminus advance of grounded glaciers, providing a first principles estimate of rates of retreat associated with the so-called marine ice cliff instability. Application of the model to idealized ice shelves, in contrast, shows that in the absence of strong ocean forcing, the yield strength is exceeded along the shear margins of ice shelves. If we allow the yield strength to decrease with increasing plastic strain of yielded ice, then rifts localize along the margins, in a pattern remarkably similar observations. These rifts decrease the coupling with the margin decreasing the buttressing capacity of the ice shelves, but also can extend across portions of the ice shelf, becoming the detachment boundary of ice bergs. Our approach to simulating failure of glacier ice provides a promising method of simulating the large-scale failure of glaciers and ice shelves that includes not only marine-ice-cliff instability failure, but also rifting and failure of ice shelves yet is computationally tractable enough to be included in continental ice sheet models.

13th World Congress on Computational Mechanics (WCCM XIII) and 2nd Pan American Congress on Computational Mechanics (PANACM II), July 22-27, 2018, New York City, NY, USA

STABILITY MODELING UNCERTAINTY WHEN DRILLING VERTICAL AND INCLINED WELLBORES THROUGH HETEROGENEOUS FIELD

NATHALIA A. BATALHA[1], OMAR Y. DURÁN[1], PHILIPPE R. B. DEVLOO[1], LUIZ C. M. VIEIRA JR.[1]

[1]University of Campinas Av. Albert Einstein,
951 Campinas, SP – BR, 13083-852
nathalia_batalha@hotmail.com,
omaryesiduran@gmail.com,
phil@fec.unicamp.br, vieira@fec.unicamp.br.

Key words: Vertical and Inclined Wellbore, Wellbore Stability, Stochastic Field, Numerical Modeling.

Abstract. A stochastic two-dimensional geomechanical model developed by the authors and presented herein is used to predict wellbore stability in heterogeneous formations. It consists of a finite element model and assumes linear elastic and isotropic material behavior under plane strain state. The model simulates the stress state around vertical and inclined wellbores when a formation is submitted to internal drilling fluid pressure. This new state of stress may lead to rock failure, which is analyzed through a failure criteria. Since the exact variation of formation mechanical properties is not known, a spatially correlated field is used to evaluate the variability of the rock material properties. In the present model, the random variable is the formation elastic modulus. The correlation between each pair of finite elements is determined by a covariance function. A two-dimensional spatially correlated field is used to verify the correlation between the elements of a vertical wellbore. A different approach, however, is necessary to model inclined wellbores. Once the direction and inclination of a wellbore are defined, a three-dimensional spatially correlated field becomes necessary to best simulate the formation field. Simulations using the stochastic model proposed herein and considering constant elastic modulus have been compared. It is observed that when considering a constant elastic modulus, the area of the plastic zone is symmetric at the borehole wall; when using the stochastic model, however, the plastic zone area surrounding the well is not symmetric. Stochastic simulations have been carried out with different heterogeneous fields for vertical and inclined wells, and distributions of the plastic zone areas were obtained for each case. Based on the stochastic field probabilistic analysis, a distribution function is presented, which aims to best assist a decision making process to determine if a mud pressure is operationally acceptable or not.

1 INTRODUCTION

Numerical models have been developed to simulate the stress state around wellbores, in order to predict the formation behavior in drilling operations. Those models intend to define the best drilling fluid density (or mud weight) to be used. The mud weight must be designed to keep the well stable and not cause rock failure. Most models, however, assume that the mechanical properties of the rocks are constant in all the simulated domain. In fact, it is known that the formation elastic properties are not the same in all drilled layer. Thus, a heterogeneous field must be considered to obtain a more realistic analysis. Since the variation of rock mechanics is not known due to challenging wellbore locations and sample procedures, a randomic but correlated field can be assumed in order to carry out a probabilistic analysis.

The present work aims to introduce a geomechanical modeling coupled to a geostatistics model to predict heterogeneous formation behavior in drilling operations. The geomechanical model assumes linear elastic and isotropic rock material behavior with plane strain condition. An yield criterion was selected to identify the formation's failure area/plastic region around borehole wall. The geostatistics analysis was developed based on a stochastic field model. The stochastic field is based on a covariance function, which specifies the correlation between the mechanical characteristics of neighboring elements of a domain.

This stochastic analysis approach enables a more realistic evaluation of the wellbore failure. A mud weight believed to be safe, may not be indicated to a well once a stochastic analysis is carried out. The geostatistical model can help on decison-making over these issues. The model can be used for vertical, horizontal and inclined wellbores.

2 ROCK AND DRILLING FLUID: A MECHANICAL INTERACTION

A stable and well designed wellbore guarantees operation safety and prevents several issues such as stuck pipe, cavity enlargement, formation fracturing, time loss and substantial expenditures. The stability of a well depends on: the equilibrium of the rock stresses (in-situ stresses), its material properties, and the drilling fluid's density or also called, mud weight.

In-situ stresses are natural developed during a rock formation and they are a consequence of gravity interactions, tectonic process, and others. These stresses are composed by the overburden pressure σ_{ov}, defined by the weight of all rock layers over a rock element. In a response to the overburden stress (or vertical stress $\sigma_{ov} = \sigma_V$), there are the horizontal stresses, which avoid the lateral deformation induced by vertical loading. In-situ stresses are subjected to the static equilibrium equation:

$$\mathrm{div}(\boldsymbol{\sigma}) + \mathbf{b} = 0 \tag{1}$$

The drilling process, however, changes the state of stress around the borehole wall. The drilling fluid is used in the drilling operation to avoid the borehole closure and fill the open space once occupied by the rock. The drilling fluid temporarily supports the borehole wall while drilling. The drilling fluid's density must be high enough to prevent kicks (pore pressure - PP) and wellbore

closure, but low enough to prevent hydraulic fracture, formation failure and circulation loss, [6]. Thus, the mud weight (or drilling fluid density) is responsible for keeping the wellbore walls stable.

The formation around the borehole wall experiences deformation due to the relief of stresses, once the rock is removed, and then, replaced by the drilling fluid. It is possible that the stress state change is significant, which leads to operational problems. In order to minimize these risks, geomechanical models have been used in the project and development stage of wells. Understanding the new stress state of vertical, inclined and horizontal wellbores is essential to ensure a safe operation. The stress state simulation allows the definition of the optimal drilling fluid density to be used in a certain formation.

3 METHODOLOGY

A geomechanical model was developed in order to simulate the formation behavior when mud pressure is applied to the borehole wall. The numerical model presented herein was developed using finite element method (FEM), and assumes linear elastic and isotropic material behavior under plane-strain state. The method was implemented in NeoPZ, which is an open-source library for the development of finite element simulations, [2]. An yield criterion was selected to describe the formation's plastic region at the borehole wall. The geostatistics analysis was developed based on a stochastic field model. The methodology used to implement this model is presented in this section.

3.1 The geomechanical model

Once the wellbore lenght is very long (kilometers long sometimes) compared to the selected domain x and y, it is assumed a plane-strain state model, considering null displacement in the z direction. The simulation is, therefore, two-dimensional, which significantly reduces computational time. As depicted in Figure 1, the finite element mesh is selected as a cross section of the wellbore. The hole cavity is the central circumference and the remaining area, refers to the original formation being drilled.

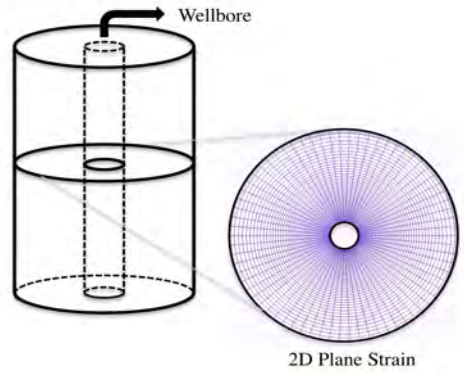


Figure 1: Two-dimensional mesh surrounding the wellbore

The FEM algorithm starts at finding the displacement $\mathbf{u}(x,y)$ from the equilibrium equation,

$$\begin{cases} \text{div}(\sigma) + \mathbf{b} = 0 \\ \mathbf{u} = \mathbf{u_D} \; on \; \delta\Omega_D \\ \sigma \cdot n = g \; on \; \delta\Omega_N \end{cases} \tag{2}$$

Where,
- σ is the stress tensor;
- $\mathbf{b}$ is the body force vector;
- $\mathbf{u}$ is the displacement vector;
- u_D and g are known functions;
- $\sigma \cdot n$ is the normal flux on the boundary $\delta\Omega_N$;
- Ω is the domain;
- $\delta\Omega_D$ and $\delta\Omega_N$ are the boundary conditions, Dirichlet and Neumann respectively.

The space of testing functions is defined by:

$$V(\Omega) = \{\mathbf{v} \in H^1(\Omega); \mathbf{v} = 0 \text{ on } \delta\Omega_D\} \tag{3}$$

Where,

$$H^1(\Omega) = \{\mathbf{v} \in \mathbf{L^2}(\Omega); \nabla \mathbf{v} \in \mathbf{L^2}(\Omega)\} \tag{4}$$

By multiplying the equilibrium equation by the testing function $\mathbf{v}$, integrating over the domain Ω, and using the divergence theorem, we have that:

$$-\int_{\Omega} \nabla \mathbf{v} \cdot \sigma \, d\Omega + \int_{\delta\Omega} \mathbf{v} \cdot \sigma n \, ds + \int_{\Omega} \mathbf{v} \cdot \mathbf{b} \, d\Omega = 0 \tag{5}$$

Assuming that between the elements,

$$\int_{\Gamma} [\![\mathbf{v} \cdot \sigma \cdot n]\!] \approx 0 \tag{6}$$

and applying,

$$\sigma \cdot n = g \text{ on } \delta\Omega_N \tag{7}$$

$$\mathbf{v} = 0 \text{ on } \delta\Omega_D \tag{8}$$

The forming function can be stated as:

$$\text{a}(\mathbf{u}, \mathbf{v}) = \text{f}(\mathbf{v}) \;\; \forall \mathbf{v} \in V(\Omega) \tag{9}$$

Given that:

$$\text{a}(\mathbf{u}, \mathbf{v}) = \sum \int_{\Omega} \nabla \mathbf{v} \cdot \sigma \, \mathbf{d}\Omega \tag{10}$$

$$\mathrm{f}(\mathbf{v}) = \sum \int_{\Omega} \mathbf{v} \cdot \mathbf{b}\, d\Omega + \int_{\delta\Omega_N} \mathbf{v} \cdot g\, ds \tag{11}$$

And by the stress-strain relation for linear elastic condition, we find the stress tensor

$$\sigma = \mathbf{C}\,\varepsilon + \sigma_0 \tag{12}$$

With $\mathbf{C}$ being the elastic constant matrix, σ_0 the initial stress tensor and ε the strain tensor as follows:

$$\varepsilon(\mathrm{x}, y) = \begin{pmatrix} \frac{\partial u_x}{\partial x} & \frac{1}{2}\left(\frac{\partial u_y}{\partial x} + \frac{\partial u_x}{\partial y}\right) \\ \frac{1}{2}\left(\frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x}\right) & \frac{\partial u_y}{\partial y} \end{pmatrix} \tag{13}$$

DiMaggio-Sandler yield criterion was selected and implemented in the geomechanical model in order to describe the failure area/plastic region surrounding the wellbore. This failure criteria was chosen once it well describes the constitutive behavior of rocks, [1]. The failure criteria yield function Φ is composed of two functions. In the present analysis, however, only the failure surface envelope function is considered. Therefore, the envelope which limits the elastic deformation under confinement is disregarded. Failure occurs when $\Phi > 0$.

3.2 Spatially correlated field for heterogeneous formation

Heterogeneous rock mechanics properties may significantly influence the formation behavior, and as a consequence, also influence the mud weight to be used in the operation. A probabilistic evaluation of a given field allow a more realistic analysis of the rock stress state, and help, with better accuracy, selecting the best density for the drilling fluid. The pore pressure and fracture gradients are very narrow and a small change can affect wellbore stability. Therefore, this stochastic field modeling represents an important issue to be addressed in wellbore stability analysis.

Since the model is a plane model, the simulation is set for a specific layer or rock formation. In other words, it assumes one average mechanical property for the whole field. Therefore, the stochastic model is built with one layer at a time.

The finite elements mesh is built using a geometric progression, which leads to a greater mesh refinement close to the wellbore wall, where the greatest change in stress state is found. The stochastic grid follows the same geometry as the finite element mesh. Thus, each element receives a random but correlated value of Young's modulus. Following the geometric progression, there is more variation closer to the wellbore wall and less changes over the remaining domain. Nevertheless, it is also possible to not use the geometric progression and then the elements would be equally distributed and the Young's modulus would also be uniformly defined in the mesh.

A spatially correlated field is used to evaluate the variability of the formation material properties. The correlation between each pair of elements is defined by a covariance function. In this model, the random variable is the formation elastic modulus (Young's modulus). The Squared Exponential

covariance function was chosen for this model. The covariance function, also known as kernel, is as follows:

$$k = \exp^{-\gamma r^2} \tag{14}$$

The selected kernel allows the user to control the distance for which the correlation between the elastic modulus of two elements is not relevant. The control is set by the constant γ, which is associated to the spatial frequency in the field, [4]. Therefore, the scale γ defines the smoothness of the stochastic field.

The covariation function also depends on the distance between the elements centroids, defined by r. A matrix $R_{m,m}$ holds all distances between each pair of elements, calculated by their elements centroids coordinates (X) :

$$R_{ij} = \begin{pmatrix} \sqrt{(X_1 - X_1)^2} & \sqrt{(X_1 - X_2)^2} & \cdots & \sqrt{(X_1 - X_m)^2} \\ \sqrt{(X_2 - X_1)^2} & \sqrt{(X_2 - X_2)^2} & \cdots & \sqrt{(X_2 - X_m)^2} \\ \vdots & \vdots & \ddots & \vdots \\ \sqrt{(X_m - X_1)^2} & \sqrt{(X_m - X_2)^2} & \cdots & \sqrt{(X_m - X_m)^2} \end{pmatrix} \tag{15}$$

The correlation matrix $K_{m,m}$, holds the correlation between all pair of elements, and it is a function of the matrix R and the scale γ:

$$K(\gamma, R)_{ij} = \begin{pmatrix} k_{1,1} & k_{1,2} & \cdots & k_{1,m} \\ k_{2,1} & k_{2,2} & \cdots & k_{2,m} \\ \cdots & \cdots & \ddots & \vdots \\ k_{m,1} & k_{m,1} & \cdots & k_{m,m} \end{pmatrix} \tag{16}$$

Matrix K is then decomposed by the singular value decomposition method, such that $K = USV^T$. The product of the left singular vector U and the square root of the diagonal matrix S, multiplies a Gaussian random and uncorrelated vector $\mathbf{d_{rand}}$, generating a correlated vector $\mathbf{d_{corr}}$.

The random but correlated vector $\mathbf{d_{corr}}$ is then scaled multiplying it by a standard deviation (std_E) and summed to an average Young's Modulus (E_{avg}).

$$\text{E}_{\text{StochasticField}} = \mathbf{d_{corr}} * std_E + E_{\text{avg}} \tag{17}$$

$\text{E}_{\text{StochasticField}}$ refers to a stochastic but correlated field of Young's modulus. The variable std_E is the standard deviation of the Young's modulus, and E_{avg} is the Young's modulus, both given as input.

3.3 A 3D spatially correlated field for inclined wellbores

A new approach must be considered for inclined wellbores. Inclined wellbores are obtained from drilling in a given direction and inclination angle. Inclination angle is the angle between the

wellbore axis tangent and the local gravitational vector. Therefore, a vertical wellbore has inclination angle of 0 degrees and a horizontal wellbore has inclination angle of 90 degrees. Direction angle consists of the angle between the horizontal wellbore projection and the true geographic north. This angle is commonly referred as "wellbore azimuth". It varies from 0 degrees to 360 degrees, and is measured in the clockwise direction starting at the geographic north, [5].

Fjar et al (2008) [3] presented in his work that a transformation of the in-situ stresses to the local stress tensor of a inclined wellbore can be obtained from a rotation between the z and y axes. This operation can be represented in matrix notation as follows:

$$[\sigma^o] = [Q][\sigma_{InSitu}][Q]^T \tag{18}$$

Where,

$$Q = \begin{pmatrix} cos[\alpha]cos[\beta] & sin[\alpha]cos[\beta] & -sin[\beta] \\ -sin[\alpha] & cos[\alpha] & 0 \\ cos[\alpha]sin[\beta] & sin[\alpha]sin[\beta] & cos[\beta] \end{pmatrix} \quad \text{and,} \quad \sigma_{InSitu} = \begin{pmatrix} \sigma_H & 0 & 0 \\ 0 & \sigma_h & 0 \\ 0 & 0 & \sigma_V \end{pmatrix}$$

σ_{InSitu}: In-situ stresses
α: wellbore direction/azimuth
β: wellbore inclination
Q: rotation matrix, composed by the rotation between the z and y axis.

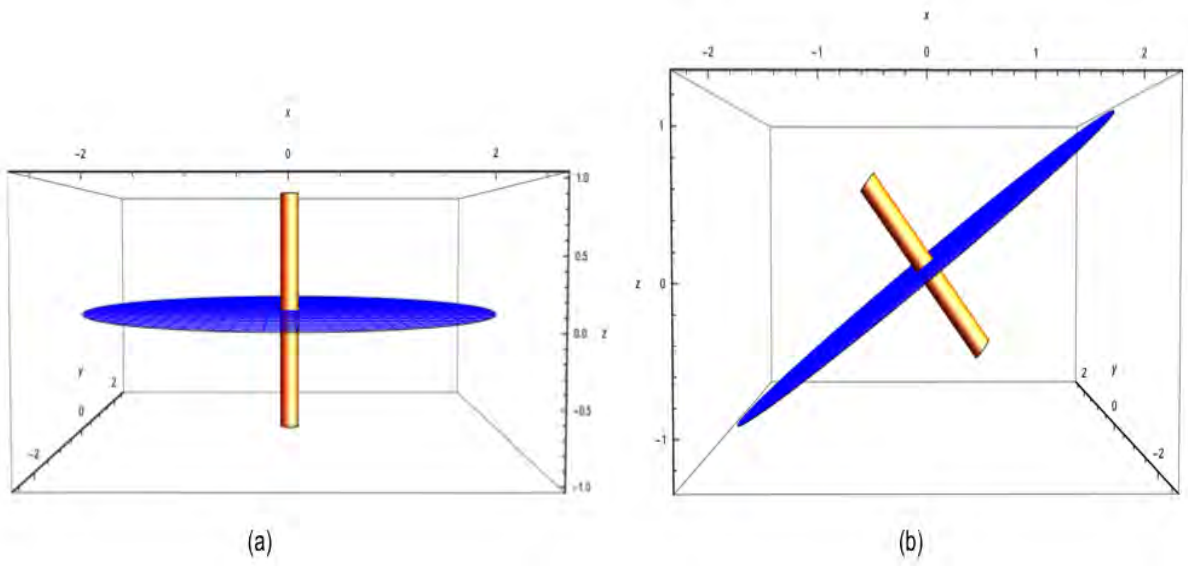


Figure 2: a) Vertical wellbore mesh (b) Inclined wellbore mesh

A two-dimensional correlated field is considered for vertical wellbores since the mesh is perpendicular to the well. Inclined wellbores' mesh is also perpendicular to the well orientation, but

embedded in the layer that the geomechanical model is being analyzed. Figure 2 illustrates the difference between the two cases.

The geomechanical model also assumes a two-dimensional approach for inclined wellbores. The simplification is possible due to the local stress tensor transformation previously described. For the stochastic analysis, however, the mesh is inclined compared to the horizontal formation layer; according to the wellbore inclination and direction. In order to evaluate the heterogeneous field of a drilled layer and determine the correlation between elements, a three-dimensional correlated field was developed.

The three-dimensional approach follows five steps: (1) definition of the height and radius of a cylindrical layer, (2) selection of two-dimensional mesh as if it had been in the vertical model, (3) selection of number of cross sections inside the cylindrical layer using the same two-dimensional mesh, (4) rotation of an extra two-dimensional mesh inside the cylindrical layer following the wellbore direction and inclination, and (5) definition of the coordinates of all elements centroids. All the steps can be seen in Figure 3. All meshes are discretized in the same way, as well as the inclined mesh.

The correlation matrix $K_{m,m}$ is therefore, calculated for all pair of elements centroids. The stochastic field over the inclined mesh (in red) is correlated with inclined neighboring elements, which allows the use of the two-dimensional geomechanical model. The methodology described herein to create three-dimensional correlated layers, allows the user to expeditiously generate drilling fields.

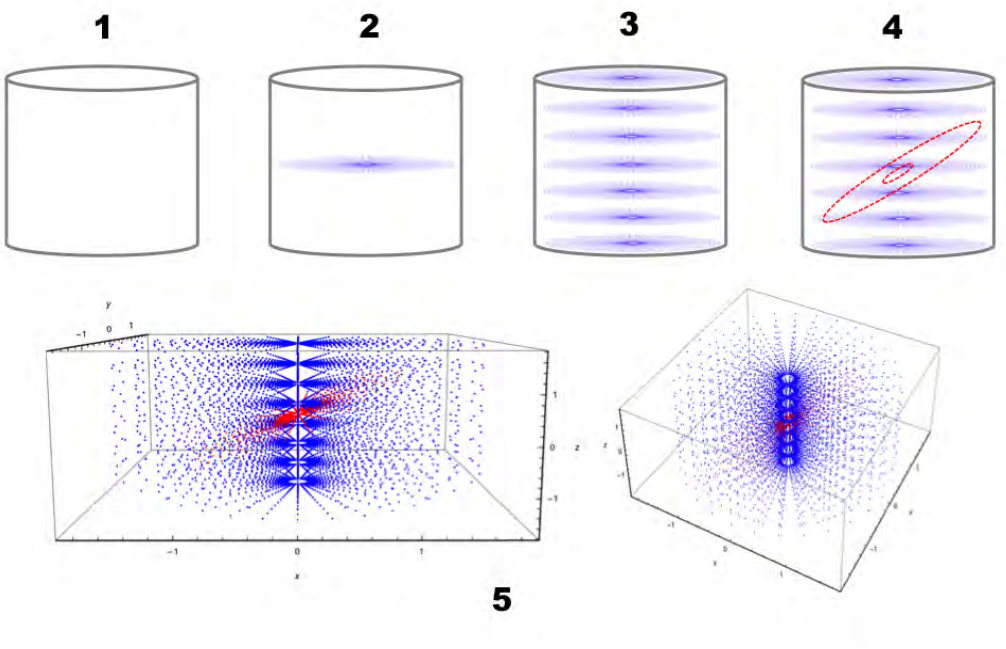


Figure 3: Five steps of the 3D spatially correlated field methodology

4 RESULTS AND DISCUSSIONS

This section presents the results of a case study carried out using the numerical model and analysis method proposed herein. The wellbore in question was a carbonatic rock, and it was already known that the selected drilling fluid pressure would induce a plastic zone at the wellbore wall. The wellbore parameters were reported in [1] as well as, the material parameters for the yield criterion. The input values used in the simulations are summarized in Table 1; the same values were used in vertical and inclined wellbores. The carbonatic material parameters for DiMaggio-Sandler criterion are A : 152.52; B : 0.0015489, and C : 146.29.

Wellbore Radius	0.10795	Meters
External Radius	3	Meters
Young's Modulus	29269	MPa
Poisson's ratio	0.203	-
Wellbore Pressure (Pw)	19.5	MPa
Vertical In-situ Stress (σ_V)	-48.2	MPa
Minor Horizontal Stress (σ_h)	-45.9	MPa
Major Horizontal Stress (σ_H)	-62.1	MPa
$\mathbf{b}(\mathrm{x},\mathrm{y})$	0	Body forces neglected

Table 1: Geomechanical model input data

4.1 Vertical wellbore homogeneous and heterogeneous field

Heterogeneous field cases were compared to a homogeneous field simulation. All models assumed the same input parameters, except for Young's modulus. Note that an homogeneous field simulation - single value of Young's modulus for the entire dominion - is common practice by petroleum engineers. The same Young's modulus value used in the homogeneous case became the mean of the stochastic field. The standard deviation considered in this study was based on a coefficient of variation of 10%. Figure 4 depicts for a homogeneous field model and for a single model of heterogeneous field simulation: Young's modulus fields, plastic zone at the borehole wall (where $F_1 = \Phi$) based on the yield criterion, and the plastic region areas plot.

The total area of the plastic zone for the homogeneous field was $13.9cm^2$, and $12cm^2$ for the heterogeneous field example case depicted in Figure 4. It can be noted that the plastic region around the wellbore for a homogeneous field was symmetric. For the heterogeneous case, however, the plastic zone surrounding the wellbore was not symmetric, presenting 56% of the total area on the top side and 44% of the total plastic zone area on the down side in Figure 4. The scale factor used in this heterogeneous case analysis was $\gamma = 4.318$, which is forty times the wellbore radius.

This asymmetry commented above may lead to operational problems while drilling. Thus, a drilling fluid density believed to be safe considering a homogeneous formation, may present higher and asymmetric plastic zone in a heterogeneous analysis. Note that, the mud properties are designed to stabilize the most vulnerable side of the well.

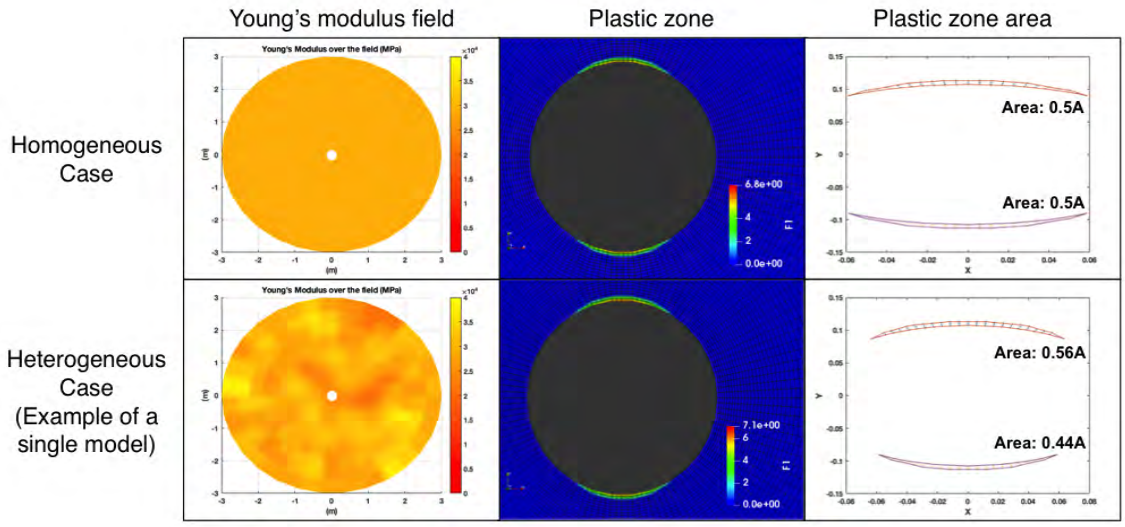


Figure 4: Plastic zone for the homogeneous and a heterogeneous case - Vertical wellbore

4.2 Inclined wellbore

An inclined wellbore analysis was carried out. The analysis assumed the same input parameters as the vertical analysis, but for this inclined study the three-dimensional stochastic field generation method was used. Therefore, a cylinder was built for the stochastic analysis. For the present case, the cylinder had eight equal cross sections and each section includes a two-dimensional and horizontal mesh, while the inclined mesh was embedded within the cylinder.

In order to reduce computational processing time, the mesh was changed to 2 meters of external radius. The number of elements and the wellbore radius were kept the same as in the vertical analysis. The space between each mesh in the cylinder was 0.5 meters and the cylinder's total height was 4 meters. The borehole had 45 degrees of inclination and azimuth/direction of 30 degrees. The scale factor used in the heterogeneous analysis for the inclined wellbore was also $\gamma = 4.318$. Similar to the vertical wellbore, the inclined wellbore heterogeneous analysis also presented asymmetric plastic regions.

4.3 Probabilistic analysis

Ten thousand simulations were carried out with different stochastic fields for vertical and inclined wellbores. The total plastic zone area distributions were obtained for both cases. Figure 5 depicts the simulations histograms. The vertical analysis presented standard deviation of $0.92cm^2$ and the total plastic region area ranged from $9.9cm^2$ to $17cm^2$ approximately. For the inclined case, the analysis presented standard deviation of $1.04cm^2$ and the total plastic region ranged from $0.57cm^2$ to $8.72cm^2$.

The mean and the total plastic zone area of the homogeneous cases are also depicted in the histograms. The histogram depicts that the total area of the plastic region for the inclined wellbore was significantly smaller than for the vertical case.

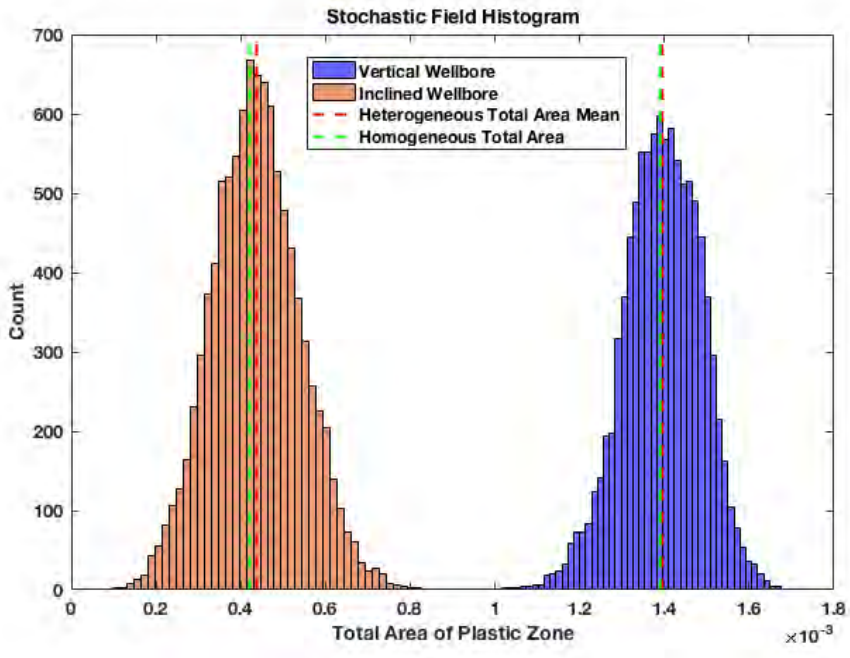


Figure 5: Stochastic Field histograms

The probabilistic analysis allows the user to verify the failure probability based on a maximum value of plastic zone area, using the simulated drilling fluid's density. If the maximum allowed area (A_y) of the plastic region at the borehole wall were a percentage of the well cavity area (A_w), the failure probability of reaching the maximum failure area could be verified by:

$$P_f = P(A_T > A_y) \tag{19}$$

Where, $A_y = p\%$ of A_w, and A_T is the total area of plastic region.

A_y	P_f - Vertical Wellbore	P_f - Inclined Wellbore
$0.1A_w$	1.8426e-134	9.4579e-210
$0.05A_w$	1.0743e-06	6.2867e-41
$0.03A_w$	0.9993	1.1642e-10
$0.01A_w$	0.9999	0.75141

Table 2: Failure Probability based on Monte-Carlo simulation of the plastic zone area

As an example, Table 2 presents the failure probability (P_f) of the vertical and inclined stochastic cases for 10%, 5%, 3%, and 1% of A_w. It was assumed normal distribution for both cases, and the probability density function was integrated from A_y to $+\infty$.

It can be noted that, for the present study, the mud pressure at the borehole wall may be safer for inclined wells than vertical wells.

5 CONCLUSIONS

A stochastic geomechanical model was developed to predict the formation behavior in drilling operations considering heterogeneous fields. The simulation method proposed herein predicted the total area of plastic region surrounding the wellbore once it is submitted to a mud/drilling fluid's pressure. The results showed that, when considering a heterogeneous field, a non-symmetric plastic region may occur. This lack of symmetry may lead to future operational problems.

A new procedure was proposed to evaluate stochastic fields of inclined wellbores; this procedure allows the modeling of thick formation layers based on two-dimensional geomechanical models.

The distributions of the total plastic zone areas determined in the stochastic analysis leads to an evaluation of the probabilistic failure and if it is still operationally accepted or not, using the considered mud pressure. The present model also allowed to assess the failure probability by setting a maximum acceptable plastic region area at the borehole wall. A mud pressure believed to be safe may not be indicated for the operation after a probabilistic analysis is carried out.

The present study intends to prevent operational issues while drilling and help on decision making process.

References

[1] Diogo Lira Cecílio. *Modelagem Elastoplástica Aplicada à Simulação Numérica da Estabilidade de Poços de Petróleo*. PhD thesis, State University of Campinas, December 2014.

[2] Philippe Remy Bernard Devloo. Pz: An object environment for scientific programming. *Comput. Methods Appl. Mech. Engrg.*, 150:133–153, 1997.

[3] E. Fjar, R. M. Holt, A.M. Raaen, R. Risnes, and P. Horsrud. *Petroleum Related Rock Mechanics*. Number 978-0-444-50260-5. Elsevier, 2nd edition, 2008.

[4] P. Graham Cranston; Mathew C.Richie; Luiz C.M. Vieira Jr. Effects of soil support on the stability of corrugated metal pipe. *Structural Stability Research Council*, March 2017.

[5] L. A. S. Rocha, D. Aruaga, R. Andrade, J. L. B. Vieira, and O. L. A. Santos. *Perfuração Direcional*. Interciência, 2008.

[6] Luiz Alberto Santos Rocha and Cecilia Toledo de Azevedo. *Projetos de Poços de Petróleo*. Interciência, 2nd edition, 2007.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

An Isogeometric Approach to the Forward Problem of Optical Tomography: An Efficiency Comparison in Solving Radiative Transfer Equation

Vahid Bateni*, Robert West**

*Virginia Tech, **Virginia Tech

ABSTRACT

Optical Tomography (OT) is a powerful imaging modality for medical diagnosis as well as biological tissue observations. OT is a sensitive and relatively inexpensive method of medical imaging which uses Near-Infra-Red (NIR) Light as the source, hence it is a non-invasive and non-ionizing modality compared with other x-ray based Computed Tomography (CT)-Scans. The NIR light is applied to the tissue and the output photon intensity is measure at the boundaries. OT Reconstruction is achieved through solution of an Inverse problem of object identification based on the measured photon intensity. The Inverse solution is usually performed in the form of an optimization scheme with iterative steps based on solving the forward scattering problem in the medium. The forward problem is solved in a number of methods, the most accurate of which is through numerical solution to the Radiative Transfer Equation (RTE). A simpler solution for RTE is performed through application of Diffusion Approximation (DA), and numerically solving the result, e.g. using Finite Elements Method (FEM). Recently we applied the Isogeometric Analysis (IGA) to solve this problem. However for many novel applications of OT encompassing small volumes, shallow depth or early photon scattering patterns (first few femtoseconds) the DA is not applicable. Hence more solutions are required. Previously Discontinuous Galerkin Finite Element Method (DG FEM) has been applied in parallel with the Discrete Ordinate Method (DOM) to solve the non-diffuse RTE. Also a “streamline diffusion modified Continuous Galerkin (CG) method” has also been suggested. Recently, a Blended Isogeometric Discontinuous Galerkin (BIDG) Method has also been introduced. In this paper, we apply the BIDG method in parallel with DOM to solve non-diffuse RTE. Initial results are generated and evaluated with previous methods.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

CFD Simulation of Breathing in the Upper Airway of Patients with Obstructive Sleep Apnea Using Prescribed Motion from Cine MRI

Alister Bates*, Andreas Schuh**, Keith McConnell***, Robert Fleck****, Jason Woods*****, Raouf Amin******, Charles Dumoulin*******

*Cincinnati Children's Hospital Medical Center, **Imperial College London, ***Cincinnati Children's Hospital Medical Center, ****Cincinnati Children's Hospital Medical Center, *****Cincinnati Children's Hospital Medical Center, ******Cincinnati Children's Hospital Medical Center, *******Cincinnati Children's Hospital Medical Center

ABSTRACT

Introduction Previous methods for computational fluid dynamics (CFD) simulation of airflow in the upper airways have been based either on static geometries, which do not account for changes in airway shape, or on fluid-structure interaction, which only predicts pressure-induced motion. Obstructive sleep apnea (OSA) is a condition where the upper airway collapses during breathing, causing the patient to wake, and long-term, leads to cardiovascular complications and, in pediatrics, developmental delay. CFD has the potential to provide regionalized diagnostic information about the causes of airway collapse and the effect this has on patients' breathing effort[1,2]. Therefore, a need exists for CFD to assess the causes of airway collapse in OSA, incorporating airway movement due internal air pressure or neuromuscular motion. Methods Magnetic resonance imaging (MRI) generated 3D images of the airway. This non-ionizing technique allows patients to be scanned for long periods covering many breaths, meaning breaths in which the airway collapses can be identified and analyzed. A static high-spatial-resolution scan (0.35×0.35×0.8mm) was segmented to create an accurate airway surface (ITK-snap 3.6.0). High-temporal-resolution cine-MRI then captured the airway motion through 3D images captured every 0.32s throughout breathing. Inlet breathing flowrates were captured synchronously with imaging via MRI-compatible spirometry. Airway motion was calculated from image and surface registration of the cine-MR images (MIRTK 1.1)[1]. This motion field was applied to the high-spatial-resolution airway surface, resulting in a moving airway wall throughout breathing. Large-eddy simulation CFD was performed in STAR-CCM+ 12.0.4 using the moving wall boundary condition and recorded breathing flowrates (CFD timestep=0.1ms). Meshing resulted in approximately 3 million polyhedral and prismatic cells. Control points on the airway surface moved following recorded airway motion, causing the interior mesh to morph. The work done by the airway wall on the internal flow (neuromuscular motion) and vice versa (pressure-driven motion) were calculated from the dot product of the pressure-force and airway-wall motion vectors. Results In a healthy volunteer and OSA patient, respectively, the airway anatomy did 25% and 37% more work on the internal airflow than the flow did on the wall. Conclusions In both a healthy volunteer and sedated pediatric sleep apnea patient, the majority of motion was not correlated with the pressure force on the airway wall, meaning most of the motion was neuromuscular, rather than pressure-driven and therefore fluid-structure-interaction modelling is not appropriate in OSA. References 1 Bates, A.J. et al. Clin. Biomech. (2017) 2 Bates, A.J. et al. J. Biomech. (2016)

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Numerical Simulation of Spheres Immersed in Viscous One- and Two-fluid Flows

Laura Battaglia*, Esteban A. Zamora Ramírez**, Mario A. Storti***, Marcela A. Cruchaga****, Roberto Ortega Aguilera*****

*Centro de Investigación de Métodos Computacionales (CIMEC), UNL-CONICET, Predio CONICET Santa Fe "Dr. Alberto Cassano", Colectora Ruta Nac. Nro 168, Km 0, Paraje El Pozo, Santa Fe, Argentina, **Centro de Investigación de Métodos Computacionales (CIMEC), UNL-CONICET, Predio CONICET Santa Fe "Dr. Alberto Cassano", Colectora Ruta Nac. Nro 168, Km 0, Paraje El Pozo, Santa Fe, Argentina, ***Centro de Investigación de Métodos Computacionales (CIMEC), UNL-CONICET, Predio CONICET Santa Fe "Dr. Alberto Cassano", Colectora Ruta Nac. Nro 168, Km 0, Paraje El Pozo, Santa Fe, Argentina, ****Departamento de Ingeniería Mecánica, Universidad de Santiago de Chile (USACH). Av. Bdo. O'Higgins 3363, Santiago de Chile, Chile, *****Departamento de Ingeniería Mecánica, Universidad de Santiago de Chile (USACH). Av. Bdo. O'Higgins 3363, Santiago de Chile, Chile

ABSTRACT

The behaviour of immersed spheres moving in one and two-fluid systems is determined by the solution of two main problems, which are the fluid dynamics and the rigid body dynamics. The fluid problem is solved with a stabilized finite element method, with an interface capturing technique for the two-fluid flow cases. The body dynamics is followed with a Newton scheme, that require velocities and pressures from the flow field in order to determine the external forces over the sphere and, then, the corresponding displacements inside the domain. This multiphysics coupling strategy is applied to different analytical and experimental cases, with special emphasis on a sloshing case in a tank with a baffle.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Simulating the Effects of Microscale Heterogeneities on the Mechanical Response of Tantalum during High-Rate Loading

Corbett Battaile*, Michael Prime**, Damian Swift***, Nathan Moore****, Matthew Lane*****

*Sandia National Laboratories, **Los Alamos National Laboratory, ***Lawrence Livermore National Laboratory, ****Sandia National Laboratories, *****Sandia National Laboratories

ABSTRACT

Nearly all engineering materials contain internal heterogeneities that exist on one or more length scales, e.g. dislocations from thermomechanical processing, grains in a polycrystalline metal, voids in a pressed or additively manufactured material, or second phases in an alloy. These internal microstructures can have a strong effect on a material's properties, and are often used advantageously for just that purpose. In this paper we will focus on two types of microscale heterogeneities in tantalum: internal voids in thermally sprayed coatings, and engineered surface ripples. In the former case, voids are an unavoidable consequence of thermal spraying, but they can be used to achieve advantageous properties in certain applications. In the latter case, the Rayleigh-Taylor instability that occurs when the rippled surface is subjected to dynamic conditions can be used to study the strength of the material. We will describe micromechanics simulations using Sandia 's Alegra software [1] to model "flyer plate" impact of thermally sprayed tantalum, and Rayleigh-Taylor experiments conducted on both the University of Rochester 's Omega Laser [2] and Lawrence Livermore National Laboratory 's National Ignition Facility (NIF) [3]. We will also discuss how we use these results to establish microstructure-properties relationships for Tantalum under high-rate loading. 1) <http://www.cs.sandia.gov/ALEGRA/Alegra_Home.html> 2) <http://www.lle.rochester.edu/omega_facility/> 3) <http://lasers.llnl.gov/about/what-is-nif>

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Coupled, Two-Phase Fluid-Sediment Material Model and Mixture Theory Implemented Using the Material Point Method

Aaron Baumgarten*, Ken Kamrin**

*Massachusetts Institute of Technology, **Massachusetts Institute of Technology

ABSTRACT

Dynamic fluid-sediment interactions present a challenge to traditional numerical modelling techniques. These flows can involve bulk motion of millions of sediment particles (e.g. riverbed and shoreline erosion) and therefore require intensive computational resources for modeling using discrete element methods (DEM). Other flows of interest have highly turbulent regions (e.g. the head of submerged slope avalanches) and are therefore difficult to capture in finite element methods (FEM). Recent work on modeling granular materials as continuum using the material point method (MPM) has shown promise for capturing such complex material dynamics. A numerical implementation of a new fluid-grain coupled material model in MPM is presented. Qualitative results show the breadth of problems which this model can address. Quantitative results demonstrate the accuracy of this model as compared with analytical models, results of other numerical techniques, and empirical observations.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Data-driven Computational Modeling to Link Diagnostics with Prognostics

Konstantinos Baxevanakis*, Brian Wisner**, Krzysztof Mazur***, Vignesh Perumal****, Antonios Kontsos*****

*1) Theoretical and Applied Mechanics Group, Department of Mechanical Engineering & Mechanics, Drexel University, USA and 2) Wolfson School of Mechanical, Electrical and Manufacturing Engineering, Loughborough University, LE11 3TU, UK, **Theoretical and Applied Mechanics Group, Department of Mechanical Engineering & Mechanics, Drexel University, USA, ***Theoretical and Applied Mechanics Group, Department of Mechanical Engineering & Mechanics, Drexel University, USA, ****Theoretical and Applied Mechanics Group, Department of Mechanical Engineering & Mechanics, Drexel University, USA, *****Theoretical and Applied Mechanics Group, Department of Mechanical Engineering & Mechanics, Drexel University, USA

ABSTRACT

Current damage identification in materials under operational conditions is accomplished using experimental characterization and testing methods as well as Nondestructive Testing and Evaluation (NDE&T) techniques. Despite the progress in instrumentation and measuring, the estimation of the evolving material state and the reliable prediction of remaining useful life at the component and structural levels remain challenging tasks. In this context, a computational damage approach which is driven by material and NDE data is presented in this talk. The material investigated is an aerospace grade precipitate-hardened aluminum alloy. In this class of metals, damage nucleation is known to be linked with second phase particles that are inherent in the material and result from the alloying process. In this work, subsized specimens were mechanically loaded inside a Scanning Electron Microscope (SEM), while acoustic and optical methods were used to track the damage process. The experimental studies revealed a connection between the particle crystallography and stoichiometry with the location of particle fracture relative to soft and hard grains. In addition, the pronounced mismatch in stiffness between particles and neighboring grains caused strain localizations and led to fracture of these particles or crack propagation into the surrounding matrix, depending on the local microstructural features which was confirmed with both in situ and ex situ X-ray computer microtomography. To form the data-driven computational damage model, first the experimental information was used in a crystal plasticity finite element model (FEM) that predicted the location of strain localizations near the particles. This information was transferred into a continuum plasticity FEM in which the extended FEM approach coupled with specific fracture initiation criteria was used to study the particle fracture and the associated wave propagation that relates to Acoustic Emission. Then, the recorded data was post-processed using a novel machine-learning approach that combines outlier analysis with clustering to form custom damage evolution curves appropriate for both monotonic and cyclic loading cases. The derived curves were subsequently implemented in the FEM as custom damage laws. To simulate the effect of evolving damage state the plasticity FEM was coupled with a stiffness degradation approach dictated by custom subroutines that implemented the previously defined damage laws. The results highlight the effect of the data-driven damage model on the macroscopic mechanical response using different specimen and component geometries.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Hydraulic Crack Branching, Gas Permeability and Creep of Shale: Comprehensive Computational Model

Zdenek P. Bazant*, Gowri Srinivasan**, Hari S. Viswanathan***, William Carey****, Viet Tuan Chau*****, Saeed Rahimi-Aghdam******, Hyunjin Lee*******, Hoang Nguyen********, Cunbao Li*********

*Northwestern University, **Los Alamos National Laboratory, ***Los Alamos National Laboratory, ****Los Alamos National Laboratory, *****Northwestern University, ******Northwestern University, *******Northwestern University, ********Northwestern University, *********Northwestern University

ABSTRACT

The talk will summarize extensive recent results at Northwestern University and Los Alamos Scientific Laboratory on the mathematical and computational modeling of hydraulic fracturing of gas shale and the problem of its preexisting permeability. Presented will be: 1) A three-phase medium model for cracking of anisotropic shale, flow of fracking fluid in cracks and diffusion of water into shale pores, 2) its computational implementation, 3) analysis of creep closing of cracks over geologic time span and 4) the problem of preexisting gas permeability of deep shale strata. Results of extensive computational simulations will be provided.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

IGA: From Early Results to Recent Developments

Yuri Bazilevs*

*Brown University

ABSTRACT

This presentation honoring Prof. T.J.R. Hughes will cover the early days of IGA development, and will summarize progress made in the last decade on this subject. Achievements in several areas of computational mechanics - solids, structures, fluids, and FSI - will be highlighted, focusing on the uses of IGA that are pushing the boundaries of there disciplines. Integration with engineering design, which to this day remains the main goal of IGA, will be highlighted in the advanced applications shown.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Computational Verification of Extreme Value Probability of Fishnet Strength Model for Imbricated Lamellar Nacre-like Biomimetic Materials

Zdenek Bažant*, Wen Luo**

*Northwestern University, **Northwestern University

ABSTRACT

Similar to nacre or brick-and-mortar structures, imbricated lamellar structures can be widely found in natural and man-made materials and are of interest for biomimetics. These lamellar structures are known to be rather insensitive to defects and have a high fracture toughness. Their deterministic behavior has been intensely studied, but statistical studies have been rare and no undisputed theoretical basis exists for its probability distribution (pdf and cdf) of strength. This paper presents a numerical and theoretical study of the probability distribution of strength and of the corresponding statistical size effect of the brick-and-mortar structure. After reasonable simplifications of the shear bonds, a lamellar axially loaded lamellar shell is statistically modelled as a fishnet pulled diagonally. A finite element model with stochastic element strength is developed and used in Monte Carlo simulations of fishnet failure for over 1 million (10^6) numerical realizations. An analytical model for failure probability of the fishnet is developed and matched to the computed statistical histograms of strength for various sizes and different link strength distributions. Finally, the statistical size effect of fishnet is studied numerically and analytically.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Numerical Investigation on Damage and Breakage of Ore Particles under Impact Loading

Lawrence Bbosa*, Temitope Oladele**, Dion Weatherley***

*Centre for Minerals Research, University of Cape Town, South Africa, **Centre for Minerals Research, University of Cape Town, South Africa, ***Sustainable Minerals Institute, Julius Kruttschnitt Mineral Research Centre, The University of Queensland

ABSTRACT

Abstract Comminution is a critical stage of mineral processing, in which size reduction of mined ore is achieved by crushing and grinding in order to increase the likelihood of mineral liberation in subsequent stages. The process is well known to be energy intensive, often accounting for the highest operating cost, while also frequently being reported to be highly inefficient. Fundamental research in the area of ore fracture is the most promising means of improving or optimizing current industrial practices. In this regard, computational modelling has emerged as a valuable tool to glean new insights into the design and operation of a wide range of devices. The impact breakage of ore by grinding media falling under gravity is a common size reduction mechanism in many comminution devices. In the present work, laboratory experiments are conducted with a Short Impact Load Cell (SILC), with which a steel ball of known mass is released by a pneumatic mechanism and descends in freefall onto a particle from a fixed height. The impact response is measured with a load cell and is used to derive quantities such as force to fracture and absorbed strain energy. Numerical simulations of these tests are conducted using the Discrete Element Method (DEM). Particles are modelled as assemblies of indivisible spheres with adjacent spheres connected by cylindrical linear elastic beams. These cohesive bonds are broken when the inter-particle stress exceeds a specified limit. The results highlight the good agreement between numerical simulations and experiments, demonstrating the ability of the simulations to capture realistic physical behavior. The paper also highlights the unique insights that such simulations provide on understanding the breakage of ore particles in comminution. References [1] Bourgeois, F.S. & Banini, G.A., 2002. A portable load cell for in-situ ore impact breakage testing. International Journal of Mineral Processing. 65(1):31-54 [2] Napier Munn, A., Morrell, S., & Kojovic, T., 1999. Mineral Comminution Circuits (their Operation and Optimization). The University of Queensland: JKMRC Monograph Series in Mining and Mineral Processing, 2 . [3] Weatherley, D., Boros, V., & Hancock, W., 2011. ESyS-particle tutorial and user's guide Version 2.1. Earth Systems Science Computational Centre, The University of Queensland.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Direction Fields Based on Ginzburg-Landau Functional: Computing Cross and 3D Frame Fields

Pierre-Alexandre Beaufort*, Alexandre Chemin**, Christophe Geuzaine***, François Henrotte****, Jean-François Remacle*****

*Université catholique de Louvain, **Université catholique de Louvain, ***Université de Liège, ****Université catholique de Louvain, *****Université catholique de Louvain

ABSTRACT

Tensorial elements such as quadrangles and hexahedra are considered to be superior to simplices (triangles, tetrahedra). For a given number of vertices, there are much less tensorial elements than simplices: in the case of quadrangles versus triangles, it is about a factor two. Hexahedra are preferred among mechanical engineering community since they avoid the shear locking problem which tetrahedra suffer. However, meshing quadrangles or hexahedra is not a trivial task. The quality of tensorial elements is strongly related to vertex location. Indeed, the vertices have to be consistent with a grid, i.e. to be connected each other in an orthogonal way with adequate valence. This connectivity scheme may be described by a direction field: for quadrangles (hexahedra), a cross (3D frame) field (respectively). Those direction fields should be smooth, and **unit normed**. Actually, the direction field should give the mean orientation of the boundaries (if any) within the domain. However, it is not always possible to build a full unit normed (and smooth) direction field on a domain: some critical/singular points (lines) arise. In the case of direction field on closed surfaces, it is due to the topology according to the Poincaré-Hopf theorem. We propose here a PDE approach to compute those directions. The PDEs express the minimum of the Ginzburg-Landau functional. This functional has two terms: a smoothing term and a penalty term. The latter term fosters directions which are unit normed. The representation of a direction depends on its dimension: a cross field is represented by a vector field (which corresponds to a complex valued function), while a 3D frame field is modelled by a 4th order tensor field. The full consistence of using Ginzburg-Landau functional lays in its penalty factor which is parametrized by the coherence length, i.e. the characteristic length of the domain. The coherence length affects the critical points (lines) of the direction fields. In 2D, Bethuel et al. has deeply detailed its effects: the Ginzburg-Landau energy is mostly due to the squares of indices of critical points, and the logarithm distances between them. In 3D, it becomes interesting: the Dirichlet energy of singularities becomes finite. [Bethuel et al.] F. Bethuel, H. Brezis, F. Hélein, Ginzburg-Landau Vortices, volume 13, Springer Science & Business Media, 2012. [Beaufort et al.] P.-A. Beaufort, J. Lambrechts, F. Henrotte, C. Geuzaine, J. Remacle, Computing cross fields: a PDE approach based on Ginzburg-Landau theory

13th World Congress on Computational Mechanics (WCCM XIII) and 2nd Pan American Congress on Computational Mechanics (PANACM II), July 22-27, 2018, New York City, NY, USA

OPTIMUM DESIGN OF ROBUST COMPLIANT MECHANISMS WITH UNCERTAINTIES IN OUTPUT STIFFNESS

GUSTAVO A. DA SILVA†, EDUARDO. L. CARDOSO*, AND ANDRÉ T. BECK†

†Structural Engineering Department, University of São Paulo
Av. Trabalhador São-Carlense, 400, 13566-590, São Carlos, SP, Brazil
gustavoassisdasilva@gmail.com (G. A. DA SILVA), atbeck@sc.usp.br (A. T. BECK)

*Mechanical Engineering Department, State University of Santa Catarina
89219-710, Joinville, Santa Catarina, SC, Brazil
eduardo.cardoso@udesc.br (E. L. CARDOSO)

Key words: Topology Optimization, Robust Optimization, Compliant Mechanism, Uncertain Stiffness.

Abstract. It is nowadays widely acknowledged that optimal structural design should be robust w.r.t. the uncertainties in operational parameters. Compliant mechanisms must operate under a variety of conditions; hence, the uncertainty in output stiffness is large and also determinant for the optimal design. In this paper, optimal topology of compliant mechanisms is addressed. Two approaches are considered to formulate the objective function of the robust optimization problem: a probabilistic approach, where the objective function combines the expected value and the standard deviation of the output displacement, and a possibilistic approach, where both the crisp value and the width of the uncertainty interval of the output displacement are considered. The probabilistic solutions are computed by Monte Carlo Simulation; the possibilistic solutions are computed by smart interval propagation. It is shown that both formulations lead to designs where the output displacement is less sensitive to the variations in output stiffness. The possibilistic and probabilistic solutions are compared in terms of resulting topologies and computational efficiency. As an additional benefit, it is observed that large variations in output stiffness can hinder the appearance of one-node connected hinges, usually found in the deterministic approach to compliant mechanism design.

1 INTRODUCTION

Topology optimization is an important tool widely employed in structural design. It has been employed to solve several kinds of engineering problems, from academic to industrial applications[1]. Among its variety of applications, it is found the compliant mechanism design under uncertainty, main subject of this research.

A literature review revealed several papers addressing the topology design of compliant mechanisms under uncertainty. In Maute and Frangopol[2], reliability-based design optimization is employed to achieve optimized compliant mechanisms under boundary conditions and material property uncertainties. In Kogiso et al[3], robust design is employed for solving continuum mechanisms problems under load uncertainty. In Chen et al[4], a robust approach is proposed to take load and material property uncertainties into account in the design of compliant mechanisms. In Sigmund[5] and Wang et al[6], the robust approach based on erosion, intermediate and dilation operators is proposed and employed to the design of manufacturing tolerant compliant mechanisms. This approach is latter improved to take non-uniform boundary uncertainties into account[7].

The classical topology optimization problem of compliant mechanisms consists in the maximization of the geometrical advantage given an output stiffness[8]. It is well known, that the output stiffness has a great impact over the topology of the optimized compliant mechanism. A compliant mechanism, optimized for actuating over a specific output, may not be suitable for actuating over an output with slightly different stiffness. This matter would not be an issue when working with outputs whose stiffness is certainly known. However, if there is uncertainty in the output stiffness, one has to employ an alternative technique to the traditional formulation of compliant mechanisms design, in order to properly handle this uncertainty during the optimization process.

This work aims at proposing two robust formulations to solve the problem of compliant mechanisms design considering an uncertain output stiffness, depending on how the uncertain stiffness is addressed: 1) probabilistic; and 2) possibilistic. When the uncertain output stiffness is modelled as a random variable, one can employ the probabilistic formulation, where the traditional objective function (output displacement) is replaced by a weighted sum between its expected value and standard deviation. On the other hand, when there is no sufficient information about the uncertain output stiffness, and only its maximum and minimum values are available, one can employ the possibilistic approach, where the objective function is replaced by a weighted sum between the mean value of the interval and a measure of its width.

In order to demonstrate applicability of proposed approaches (probabilistic and possibilistic), the classical inverter mechanism problem is solved. Obtained results are compared with the traditional (deterministic) result from the literature, clearly demonstrating the importance of employing such formulations when addressing topology design problems of compliant mechanisms under uncertain output stiffness.

2 TOPOLOGY OPTIMIZATION OF COMPLIANT MECHANISMS

In this work, the traditional density-based approach[9] is employed. It consists in a layout optimization procedure of a fixed reference domain: 1) the topology optimization problem of compliant mechanisms is formulated; 2) the design domain is discretized with finite elements; 3) each finite element is associated with a relative density ρ_e (design variables of the optimization problem), that can assume values from 0 (which mimics void material) to 1 (which mimics solid material); 4) the topology optimization problem is solved by employing well established mathematical programming approaches.

In this paper, all formulations are developed based on the displacement-based Finite Element Method (FEM) under the hypotheses of linear elasticity subjected to static loads. The resulting

topology optimization problems are solved by employing the Sequential Linear Programming (SLP) approach. Sensitivities are obtained with the adjoint procedure.

The traditional linear density filter[10] is employed to avoid checkerboard patterns and mesh dependency.

2.1 Deterministic formulation

In this work, we formulate the topology optimization problem of compliant mechanisms for one output only, as illustrated in Figure 1.

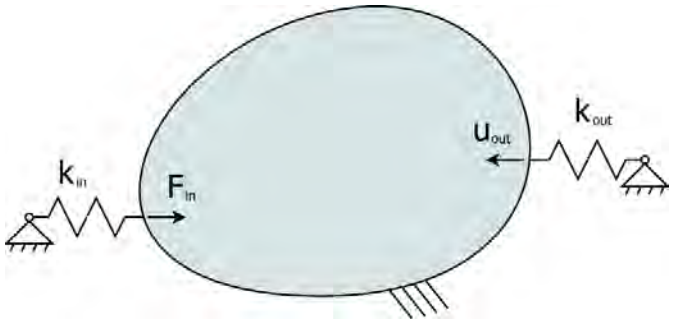


Figure 1 – Illustration of design with input stiffness k_{in}, output stiffness k_{out}, input force F_{in} and output displacement u_{out}.

The objective is the maximization of the displacement at the output port, while constraining the amount of material (volume fraction). The output displacement acts on a linear spring with stiffness k_{out}, representing the stiffness of the output medium. The mechanism is actuated by a given load coupled to a linear spring with stiffness k_{in}, in order to simulate a force transducer.

The optimization problem is written as:

$$\begin{aligned} Max. \quad & u_{out}(\boldsymbol{\rho}) \\ & V(\boldsymbol{\rho}) \leq V_{max} \\ s.t. \quad & \mathbf{K}(\boldsymbol{\rho})\mathbf{U}(\boldsymbol{\rho}) = \mathbf{F} \\ & 0 \leq \rho_{min} \leq \rho_e \leq 1 \qquad\qquad e = 1..N_e \end{aligned} \tag{1}$$

where the objective function, $u_{out}(\boldsymbol{\rho})$, is the displacement at the output port, $V(\boldsymbol{\rho})$ is the volume of the structure, V_{max} is the maximum admissible volume (volume constraint) defined by the designer, $\mathbf{K}(\boldsymbol{\rho})$ is the global stiffness matrix, $\mathbf{U}(\boldsymbol{\rho})$ is the global displacement vector, $\mathbf{F}$ is the global load vector and N_e is the number of elements in the mesh. The global stiffness matrix is obtained by assembling, in the global level, all the local element stiffness matrices, $\mathbf{k}_e(\rho_e) = \mathbf{k}_e^b \rho_e^p$ (SIMP – Solid Isotropic Material with Penalization[1]), and, in addition, the stiffness of input k_{in} and output k_{out} ports. We can denote this assembly symbolically as:

$$\mathbf{K}(\boldsymbol{\rho}) \leftarrow \cup_{e=1}^{N_e} \mathbf{k}_e(\rho_e) \,, \cup\, k_{in} \,, \cup\, k_{out}, \tag{2}$$

where the minimum value of ρ_{min} is assumed for the relative densities to avoid a singular FEM problem.

The structural volume of the structure is computed as

$$V(\boldsymbol{\rho}) = \sum_{e=1}^{N_e} V_e \rho_e, \tag{3}$$

where V_e is the volume of finite element e.

The traditional formulation, Equation (1), is suitable for designing compliant mechanisms when there is no source of uncertainty related to any parameter utilized during optimization. Next subsections aim at proposing two distinct formulations for solving the compliant mechanisms problems when there is uncertainty in the output stiffness k_{out}.

2.2 Probabilistic formulation

When there is uncertainty in the output stiffness, i.e., when its value is not certainly known, formulation described in Equation (1) is no longer appropriate, since it can lead to non-optimal solutions. Considering that magnitude of the output stiffness is represented by a random variable X, as $k_{out}(X) = (1 + X)\, k_{out}^0$, where k_{out}^0 is the mean value of the output stiffness, one can rewrite optimization problem described in Equation (1) to take the aleatory uncertainty into account, under a robust framework, such that:

$$\begin{aligned} Max. \quad & \mathrm{E}[u_{out}(\boldsymbol{\rho}, X)] + \beta\, \mathrm{Std}[u_{out}(\boldsymbol{\rho}, X)] \\ & V(\boldsymbol{\rho}) \leq V_{max} \\ s.t. \quad & \mathbf{K}(\boldsymbol{\rho}, X)\mathbf{U}(\boldsymbol{\rho}, X) = \mathbf{F} \\ & 0 \leq \rho_{min} \leq \rho_e \leq 1 \qquad\qquad e = 1..N_e \end{aligned} \tag{4}$$

where $\mathrm{E}[u_{out}(\boldsymbol{\rho}, X)]$ is the expectation and $\mathrm{Std}[u_{out}(\boldsymbol{\rho}, X)]$ the standard deviation of the displacement at the output port.

The main difference between the probabilistic formulation, Equation (4), and the deterministic formulation, Equation (1), is in the consideration of an additional term in the objective function, related to the standard deviation of the output displacement.

The inclusion of the standard deviation in the objective function has a great impact over the optimized designs. It works at reducing the sensitivity of the optimized result with respect to variations in the output stiffness, i.e., we can achieve robust designs which are not affected from slight variations in the output stiffness, unlike the deterministic unstable solution.

Of course it becomes a compromise relation when one has to choose the number of standard deviations, β, to be considered during optimization. For small values of β we basically recover the original deterministic formulation, Equation (1); whereas for large values of β we focus at reducing design sensitivity with respect to the uncertain output stiffness. Hence, the number of standard deviations β has an important role over the optimization problem and must be carefully chosen by the designer, depending on the application of the compliant mechanism.

In this work, evaluation of $\mathrm{E}[u_{out}(\boldsymbol{\rho}, X)]$ and $\mathrm{Std}[u_{out}(\boldsymbol{\rho}, X)]$ are performed through Monte Carlo Simulation[11].

2.3 Possibilistic formulation

When there is uncertainty in the output stiffness, but it cannot be reasonably represented through a random variable, one may employ a possibilistic approach to address the problem. In this subsection, we assume the only available information regarding the output stiffness are its minimum and maximum values, i.e., the output stiffness is represented by an unknown variable Z, as $k_{out}(Z) = (1 + Z)\, k_{out}^0$, with $Z \in [\underline{Z}, \overline{Z}]$.

The possibilistic version of the optimization problem is written as:

$$\begin{aligned} Max. \quad & \frac{\max(u) + \min(u)}{2} + \gamma\sqrt{(\max(u) - \min(u))^2} \\ & V(\boldsymbol{\rho}) \leq V_{max} \\ s.t. \quad & \mathbf{K}(\boldsymbol{\rho}, Z)\mathbf{U}(\boldsymbol{\rho}, Z) = \mathbf{F} \\ & 0 \leq \rho_{min} \leq \rho_e \leq 1 \qquad\qquad e = 1..N_e \end{aligned} \tag{5}$$

where $u = u_{out}(\boldsymbol{\rho}, Z)$. Purpose of formulation presented in Equation (5) is remarkably similar to the purpose of formulation in Equation (4). Despite presenting distinct numerical behaviors, parameter γ has the same purpose of parameter β and the term $\sqrt{(\max(u) - \min(u))^2}$, related to the width of the interval of the output displacement, has the same purpose of the standard deviation in the probabilistic approach.

Since linear analysis is employed when solving for equilibrium, minimum and maximum values of output displacement are easily obtained by evaluating for $\overline{Z}$ and $\underline{Z}$, associated with maximum and minimum values of output stiffness, respectively, such that: $\min(u_{out}(\boldsymbol{\rho}, Z)) = u_{out}(\boldsymbol{\rho}, \overline{Z})$ and $\max(u_{out}(\boldsymbol{\rho}, Z)) = u_{out}(\boldsymbol{\rho}, \underline{Z})$.

3 NUMERICAL RESULTS

In this section, the inverter mechanism problem is addressed, Figure 2. Hypotheses of plane stress are adopted. Input data are: Young's Modulus of 3 GPa, Poisson's coefficient of 0.4, input force of $F_{in} = 200$ N, input stiffness of $k_{in} = 1 \times 10^5$ N/m, admissible structural volume of $V_{max} = 20\%\, V_{domain}$, stiffness penalization factor of $p = 3$ (SIMP), thickness of 5 mm and filter's radius of 1.5 mm. The problem is discretized with $N_e = 2000$ four-node bilinear isoparametric elements with additional deformation modes[12]. The optimization problem is solved with a SLP algorithm with fixed moving limits of 5%.

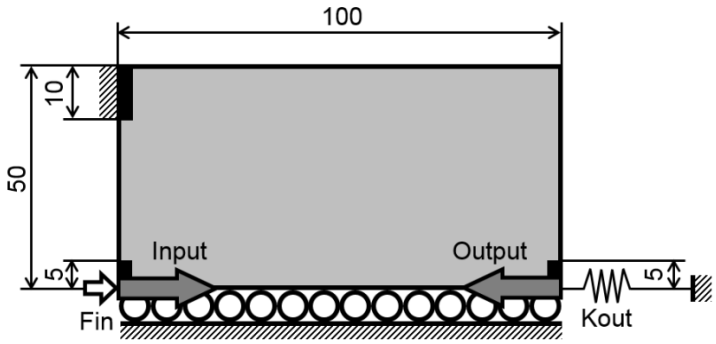


Figure 2 - Design domain for the inverter compliant mechanism. All the dimensions are in mm.

The optimization problem is solved by the three approaches presented in this work:

1) the traditional deterministic approach, with $k_{out} = 1 \times 10^3$ N/m;

2) the proposed probabilistic approach, with $k_{out}^0 = 1 \times 10^3$ N/m and $X \sim U(-0.5,0.5)$, i.e., the output stiffness follows an uniform distribution as $k_{out}(X) \sim U(0.5 \times 10^3, 1.5 \times 10^3)$ N/m;

3) the proposed possibilistic approach, with $k_{out}^0 = 1 \times 10^3$ N/m and $Z \in [-0.5,0.5]$, i.e., the output stiffness may assume any value in range $k_{out}(Z) \in [0.5 \times 10^3, 1.5 \times 10^3]$ N/m;

An important choice when solving the optimization problem under uncertain output stiffness is regarding the parameters β and γ, that governs the weight of standard deviations or width of intervals, for probabilistic and possibilistic approaches, respectively. For this study, we choose $\beta = \gamma = 20$.

Figure 3 shows optimized topologies for the three problems analyzed herein. One can clearly see the differences between deterministic solution (leftmost topology) and robust solutions (middle and rightmost topologies). The deterministic solution presents a larger number of structural members when compared with the robust solutions.

Deterministic Probabilistic Possibilistic

Figure 3 – Topologies optimized for the three presented approaches.

Regarding the performance of the mechanisms, one can also verify large differences between deterministic and robust solutions. In order to demonstrate the unstable behavior of the deterministic solution and, on the other hand, demonstrate the extremely small sensitivity of robust solutions with respect to changes in the output stiffness, all solutions are post-processed for minimum and maximum output stiffness considered during optimization, Figure 4.

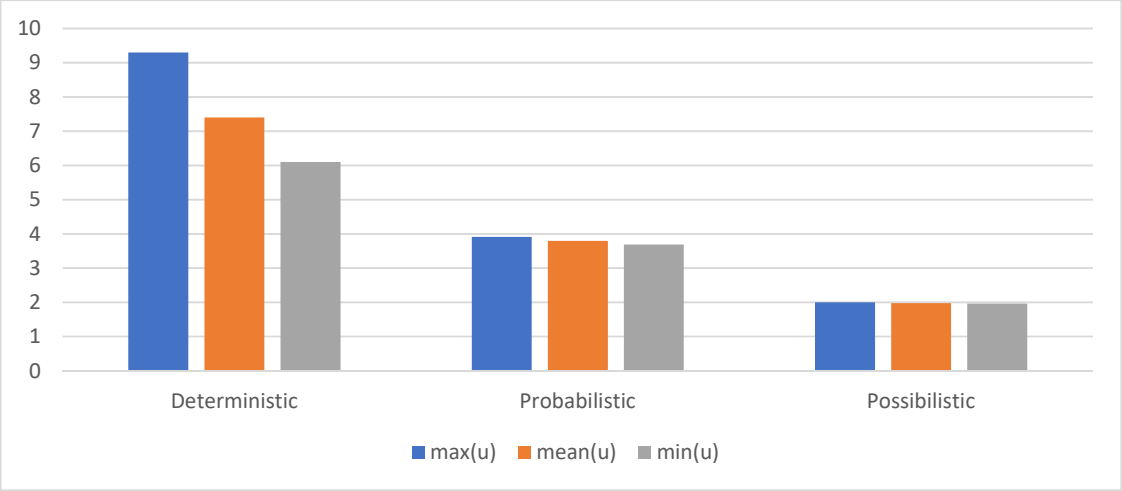


Figure 4 – Output displacements evaluated for the mean output stiffness and its extreme values. All the dimensions are in mm.

Although a larger output displacement is obtained when the deterministic design is employed, its variation with respect to a variation in the output stiffness is extremely large. Both probabilistic and possibilistic approaches work at reducing this large variation of the output displacement, however, its magnitude is also reduced. It is a compromise relation between performance and robustness, that should be taken into account by the designer, depending on the application of the compliant mechanism.

Both probabilistic and possibilistic approaches lead to robust results, but different mean performances are observed, due to different mathematical behavior of the formulation for same parameters β and γ (a smaller value of γ is necessary if the goal is obtaining equivalent result to the probabilistic approach). Both approaches are suitable if the goal is achieving a robust solution, with smaller performance sensitivity with respect to change in the output stiffness. The choice between both approaches should be done depending on how the uncertainty in the output stiffness is described. If there is sufficient information to describe the output stiffness as a random variable, the probabilistic formulation is suitable, otherwise, one can employ the possibilistic formulation.

4 CONCLUSIONS

Topology design of compliant mechanisms under uncertainty in the output stiffness was addressed. Two distinct robust formulations were proposed to handle the uncertainty in the stiffness of the output medium, depending on how the uncertain variable is described: 1) a probabilistic approach, if the output stiffness is described by a random variable; 2) a possibilistic approach, if one has only the bounds of the output stiffness.

Both approaches were employed to solve the inverter problem and compared with the traditional deterministic design. Post-processing demonstrates that the deterministic design is extremely sensitive with respect to changes in the output stiffness. It was also demonstrated that both robust approaches are suitable at greatly reducing the sensitivity of the output displacement with respect to variations in the output stiffness.

REFERENCES

[1] Bendsøe, M.P. and Sigmund, O. Topology Optimization: Theory, Methods and Applications, Springer, 2003.

[2] Maute, K. and Frangopol, D.M. (2003) Reliability-based design of mems mechanisms by topology optimization. Comput Struct 81(8–11):813–824. https://doi.org/10.1016/S0045-7949(03)00008-7

[3] Kogiso, N., Ahn, W., Nishiwaki, S., Izui, K. and Yoshimura, M. Robust topology optimization for compliant mechanisms considering uncertainty of applied loads. Journal of Advanced Mechanical Design, Systems, and Manufacturing, 2(1):96–107, 2008.

[4] Chen, S., Chen, W. and Lee, S. Struct Multidisc Optim (2010) 41: 507. https://doi.org/10.1007/s00158-009-0449-2.

[5] Sigmund, O. Manufacturing tolerant topology optimization, Acta Mechanica Sinica 25 (2) (2009) 227–239. doi:10.1007/s10409-009-0240-z.

[6] Wang, F., Lazarov, B.S. and Sigmund, O. On projection methods, convergence and robust formulations in topology optimization, Structural and Multidisciplinary Optimization 43 (6) (2011) 767–784. doi:10.1007/s00158-010-0602-y.

[7] Schevenels, M., Lazarov, B.S. and Sigmund, O. Robust topology optimization accounting for spatially varying manufacturing errors. Comput Meth Appl Mech Eng. 2011;200(4952):3613-3627. https://dx.doi.org/10.1016/j.cma.2011.08.006

[8] Sigmund, O. (2007) On the Design of Compliant Mechanisms Using Topology Optimization, Mechanics of Structures and Machines, 25:4, 493-524, doi: 10.1080/08905459708945415

[9] Sigmund, O. and Maute, K. Topology optimization approaches, Structural and Multidisciplinary Optimization 48 (6) (2013) 1031–1055. doi:10.1007/s00158-013-0978-6.

[10] Sigmund, O. Morphology-based black and white filters for topology optimization. Struct Multidiscipl Optim. 2007;33(4–5):401-424. https://doi.org/10.1007/s00158-006-0087-x

[11] Melchers, R.E. and Beck, A.T. (2017) Structural reliability analysis and prediction, 3rd edn. Wiley, New York

[12] Jiao, Z.-P., Pian, T.H.H. and Yong, S. A new formulation of isoparametric finite elements and the relationship between hybrid stress element and incompatible element. International Journal for Numerical Methods in Engineering, pages 15–27, 1997.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

An Immersed Reproducing Kernel Particle Method for Modeling Inhomogeneous Media Using Nitsche's Method

Frank Beckwith*, J. S. Chen**

*University of California, San Diego, **University of California, San Diego

ABSTRACT

Many structures are constructed using reinforced concrete. The modeling of reinforced concrete at the rib-scale is difficult with conventional methods such as the finite element method (FEM) due to the conforming requirements with respect to the material interface. An immersed Reproducing Kernel Particle Method (RKPM) is proposed to model the complex reinforcement geometry using an immersed domain approach. The compatibility conditions on the material interfaces are enforced via Nitsche 's method with embedded equilibrium. This approach allows independent approximations and discretizations for the background matrix and the foreground inclusion, and naturally yields strain jumps across the material interfaces. The reproducing kernel (RK) approximations and discretizations of both foreground and background domains are considered in this work due to their high continuity [1], but other approximations such as the finite element method can also be employed under this framework. Several numerical examples with application to reinforced concrete are presented to examine the effectiveness of the proposed method. The modeling of mechanical interlock and bar debonding phenomena in the reinforced concrete pull-out test by the proposed is also demonstrated. References [1] J. S. Chen, M. Hillman, and S.-W. Chi. Meshfree methods: Progress made after 20 years. Journal of Engineering Mechanics, 143(4):04017001, 2017.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Molecular Dynamics Simulation of Nanosize Effects in Nanoreinforced Polymers; From Interface to Macroscopic Mechanical Properties

Fahmi Bedoui*, Andres Jaramillo-Botero**, William A. Goddard III***

*Sorbonne Universités - Université de Technologie de Compiègne, **Materials and Process Simulation Center, CalTech, ***Materials and Process Simulation Center, CalTech

ABSTRACT

The process-structure-property relationships are far less well understood in nanoreinforced polymers than in other materials; to the point that these are rarely of any practical or commercial utility. In addition to the microstructural complexity, nanoreinforced polymer behavior seems to be dependent on the size of the reinforcing nano structures (e.g. nanoparticles, nanowires, nanotubes, etc.) Here, we report on recent efforts to quantify and model such nanosize effects on the elastic and thermal properties of a Poly(methyl methacrylate) -PMMA polymer reinforced with spherical silica nanoparticles ranging in diameter, from 15 nm to 500 nm. Our results, confirm the nanosize effect and mechanisms that alter the experimentally observed macroscopic elastic modulus of the nanocomposite (see Blivi et al., 2016 [1]). This data allowed us to calibrate the interface characteristics that enter into an extended version of the linear homogenization model proposed by Brisard et al. [2] and Duan et al [3]. In order to provide cross quantitative validation and to tailor the experimental work, we adopted an atomistic modeling approach to help answer the main question that needs to be answered: • Do particles act through interface, interphase or both, to convey the polymer with enhanced mechanical properties (origin of size effect) at nanometric particle size? This work will present preliminary results from molecular dynamics simulations that confirm the effect of particle size on the macroscopic materials properties of silica-PMMA nanoreinforced composites made with constant volume fraction but different silica particles. We used the two-phase thermodynamic model [4] to derive the entropy distribution in the various polymer layers from the interface to the bulk. This provides new insights into the local mechanical and physical properties, that otherwise are inaccessible. References [1] A.S.Blivi, F.Benhui, J.Baib, D.Kondoc, F.Bedoui. Polymer Testing 2016;56:337. [2] Brisard S, Dormieux L, Kondo D. Computational Materials Science 2010;48 589. [3] H.L.Duan, J.Wang, Z.P.Huang, Z.Y.Luo. Mechanics of Materials 2005;37 723. [4] Lin S-T, Maiti PK, Goddard WA. The Journal of Physical Chemistry B 2010;114:8191.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Simplified Formulation for Avaliating Displacements in Beams with Moving Boundary Conditions

Thomás Bedusque Verderesi*, Marco André Argenta**

*Universidade Federal do Paraná, **Universidade Federal do Paraná

ABSTRACT

The corotational method is a powerful approach for solving non-linear finite beam elements, mostly utilized to investigate its dynamics. However, where most papers present studies in the shape functions and its derivations (to obtain mass and stiffness matrices), this work takes advantage of the cubic interpolations for solving the inertia terms, combining it to moving boundary conditions with constant velocity and acceleration. We simulated the beam as an overcomplicated n-arms pendulum. ,The first problem is that with more arms the less stiff it becomes. The solution is to embed nonlinear longitudinal springs for the axial stiffness and with rotational springs for its rotational and shear stiffness , containing one of each for connecting pendulum arms,. then, simulating as a moving pendulum. Once described its law of motion correctly, the elements match the displacements of one another at springs with multifreedom constraints (MFC), where one displacement, velocity, and acceleration has to be constrained to another, eliminating the chaotic nature of the multi-pendular motion. We used the master-slave method, which eliminates the slaves degrees of freedom and makes the otherwise singular stiffness matrix solvable again. We simulated the beam with a concentrated force and different positions and moving boundary conditions with constant velocity at first and then with constant acceleration, in order to study the stresses and strains variations within it. The other parameter is the number of elements used to build the beam model, analyzing if the number of elements makes an analysis more accurate. We compared the model to an accepted one such as the corotational Timoshenko's beam theory, in a stationary situation, validating it for the displacements caused by an applied force and for the rigid body movement.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Solving the Linearized Stationary Quasi-Geostrophic Equations of the Ocean Using the Particle Difference Method

Andrew Beel*, Tae Yeon Kim**, Jeong-Hoon Song***

*University of Colorado Boulder, **Khalifa University of Science, Technology and Research, ***University of Colorado Boulder

ABSTRACT

The development of accurate and robust numerical methods for solving higher order partial differential equations is crucial for both theoretical model validation and practical applications in many areas of science and engineering. This study explores the capability of the recently developed strong form collocation method, i.e. the particle difference method (PDM) [1] in solving the linear Stommel (the second-order PDE) and Stommel-Munk (the fourth-order PDE) models, linearized versions of the stationary quasi-geostrophic equations (SQGE) of the ocean [2]. The PDM is based on a Taylor polynomial approximation of the solution field with moving least squares approach. Numerical examples considered herein include: i) the Stommel equation on a square domain with a strong Western boundary layer, ii) the Stommel-Munk equation on a rectangular domain with and without a strong Western boundary layer, and iii) the Stommel-Munk equation on an irregular polygon representing the Mediterranean Sea. In the first example, numerical solutions from the PDM are compared with exact solutions, producing near-optimal empirical convergence results for both a quadratic and quartic polynomial approximation. In the second example, for both uniform tensor product grid and meshing software-generated random arrangements of collocation points, the PDM exhibits excellent convergence properties in both the discrete relative L¬2 norm error and relative infinity norm error. For the third example, the analytical solution is unavailable, so a contour plot and qualitative comparison to numerical results from another numerical method, presented originally in [3], are presented. References [1] Y.C. Yoon and J.H. Song, “Extended particle difference method for weak and strong discontinuity problems: Part I. Derivation of the extended particle derivative approximation for the representation of weak and strong discontinuities”, Computational Mechanics, 53 (2014), 1087-1103 (2014). [2] Tae-Yeon Kim, Traian Iliescu, Eliot Fried, “B-spline based finite-element method for the stationary quasi-geostrophic equations of the ocean”, Computer Methods in Applied Mechanics and Engineering, 286 (2015) 168-191. [3] T.Y. Kim, E.J. Park and D.W. Shin, “A C0-discontinuous Galerkin method for the stationary quasi-geostrophic equations of the ocean”, Computer Methods in Applied Mechanics and Engineering, 300 (2016) 225-244.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Estimating Material Parameter Distributions of Fibers with Extremely Limited Experimental Efforts

Lars Beex*, Hussein Rappel**, Stephane Bordas***

*University of Luxembourg, **University of Luxembourg, ***University of Luxembourg

ABSTRACT

Numerous materials are essentially discrete networks of fibers, yarns or struts at length scales substantially smaller than the application scale. Some examples of these materials are foams, paper materials, printed lattices and textiles. Besides the possible geometrical randomness, many of these materials are characterized by the fact that each fiber, yarn or strut has its own set of material parameters. Incorporating this randomness in discrete mechanical models can substantially influence the predictions, compared to those of mechanical models in which no randomness of material parameters is included. If we assume that the material parameters of each discrete constituent are realisations from a distribution, the parameters of this probability density function (PDF) must be identified. The most conventional manner of identifying the parameters of such a PDF is to experimentally identify the material parameters of hundreds of fibers, yarns or struts and subsequently, use these material parameters to identify the parameters of the distribution. This entails an enormous amount of experimental efforts, which is the reason that hardly anybody has gone and will go through these efforts. As an alternative to testing hundreds of fibers, yarns of struts, we will present an approach that requires the testing only a few fibers. We will use Bayes' theorem for this purpose, which entails the proposition of the shape of PDF, as well as a proposition of the possible values of this PDF (albeit as distributions as well). For each set of material parameters, we then assess how likely it is that it comes from the proposed PDF including its proposed parameters and we update the PDF's proposed parameters such that the likelihood that the set is a realisation of this PDF increases. In order to explain the approach as gently as possible, we will not directly deal with the PDF's parameters as parameters that also originate from a PDF. Instead, we will first focus the PDF's parameters as deterministic variables [1]. Since our study does not deal with actual experimental results and we artificially generate our experimental data instead, we know the actual parameters we try to recover and hence, we can accurately and consistently assess the accuracy of the approach. [1] Rappel H, Beex LAA, Bordas SPA, 'Bayesian inference to identify parameters in viscoelasticity', Mechanics of Time-Dependent Materials, 2017, In press.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Unstructured Space-Time Meshes in the Context of Stabilized Finite Element Methods and Moving Boundary Problems

Marek Behr*, Violeta Karyofylli**

*Chair for Computational Analysis of Technical Systems, RWTH Aachen University, **Chair for Computational Analysis of Technical Systems, RWTH Aachen University

ABSTRACT

Moving-boundary flow simulations are an important design and analysis tool in many areas of engineering, including civil and biomedical engineering, as well as production engineering. Interface-capturing offers unmatched flexibility for complex free-surface motion, while interface-tracking approach is very attractive due to its better mass conservation properties at low resolution. We focus on these alternative approaches in the context of flow simulations based on stabilized finite element discretizations of Navier-Stokes equations, including space-time formulations that allow extra flexibility concerning grid design at the interface. Space-time approaches offer some not-yet-fully-exploited advantages when compared to standard discretizations; among them, the potential to allow some degree of unstructured space-time meshing. A method for generating simplex space-time meshes has been developed, allowing arbitrary temporal refinement in selected portions of space-time slabs. The method increases the flexibility of space-time discretizations, even in the absence of dedicated space-time mesh generation tools. The resulting tetrahedral (for 2D problems) and pentatope (for 3D problems) meshes are being used in the context of cavity filling flow simulations, such as those necessary to design injection molding processes.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Dynamic Fracture Modeling of Ductile Materials with Peridynamics

Masoud Behzadinasab*, John Foster**

*University of Texas at Austin, **University of Texas at Austin

ABSTRACT

Prediction of crack initiation, propagation, and ductile fracture can be very challenging in metallic materials with complex geometries. Damage accumulation along the plastic loading path governs the fracture initiation in ductile materials. Over the past two decades, the peridynamic theory has been exploited for modeling dynamic problems involving fracture. Peridynamics has, however, mostly applied in modeling fracture in brittle materials, and its robustness in ductile fracture modeling has not been fully explored. Recently Foster et al. (2017) proposed a new framework to incorporate classical finite deformation material models in peridynamics. Tupek et al. (2013) has also introduced a constitutive damage modeling approach for peridyanmics to take advantage of the well-established classical damage models. A material model corresponding to the finite strain elastoplasticity theory of Simo (1988) and a damage model corresponding to Johnson-Cook model (1985) have been implemented in Peridigm, an open-source massively-parallel computational peridynamics code. This framework has been applied to the Sandia Fracture Challenge 3. The model was first calibrated by the data provided by Sandia National Laboratories. Following that, a blind prediction was performed on the challenge geometry and results were compared. We demonstrate the capabilities of the new correspondence framework and possible factors behind the discrepancy between the simulation results and the experiments.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Contact of Higher-Order Elements for Explicit Dynamics

Stephen Beissel*

*Southwest Research Institute

ABSTRACT

In recent years, higher-order elements have been used to great advantage in various fields of scientific computing, but not in the dynamics of solids. There are likely multiple reasons for this. However, one of the primary reasons is probably the difficulty of accurately enforcing contact boundary conditions between the curved surfaces of higher-order elements. This difficulty is magnified by the essential role of contact in problems of practical significance. Recently, higher-order elements have been introduced for the dynamics of solids with explicit time integration. These elements have been shown to provide much greater accuracy to the analysis of wave propagation than standard first-order elements on the bases of equal mesh refinement, equal computing time, and equal allocated memory. In the first part of this presentation, a typical legacy contact algorithm is adapted to contact of the new higher-order elements. This algorithm was derived from the preservation of nodal momenta and has been used successfully for years with first-order elements. It is evaluated for higher-order elements by examining the transmission of a compressive planar wave through a flat interface. The wave is correctly transmitted across the interface only under special conditions, but not for all alignments of the elements on the opposing surfaces, and not when the elements are of differing orders. In the next part of the presentation, a new formulation of contact is derived for the higher-order elements to avoid these shortcomings, and to accommodate curved surfaces. The new formulation is derived from the weak form of the equations of motion, in a manner consistent with the derivation of the higher-order elements. As a result, the new formulation correctly transmits a compressive planar wave across a contact interface for any alignment of the opposing elements, and any combination of element orders. In the last part of the presentation, comparisons of numerical examples demonstrate the importance of modeling the curved surfaces of the elements by their nth-order polynomials, rather than decomposing them into multiple first-order facets for the legacy algorithm. The examples include sliding of surfaces with initial curvature, and contact between surfaces with deformation-induced curvature resulting from large plastic flows.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Optimisation Methods for the Design of Tall Buildings Based on Sustainability and Efficiency Factors

Laura Bellamy*, Theodoros Mourtis**, Andrew Phillips***

*Imperial College London, **Robert Bird Group, ***Imperial College London

ABSTRACT

Sustainability is an increasingly important factor in global decision-making, and provision of infrastructure is responsible for a large part of global greenhouse gas emissions [1]. Whilst efforts are made to reduce the operational carbon in the construction industry, work is still necessary to lower embodied carbon [2]. Currently, in many cases when designing a tall building, the optimisation process is largely based on engineers' experience. Whilst this experience is extremely valuable and will often reach good results, making use of the parametric tools that are now available could reach improved results and save time in the design process. This can lead to efficient designs and savings on material quantities, lowering the embodied carbon of structures. Tools are being developed, in collaboration between industry and academia, for the optimisation of tall buildings to work towards these objectives. They include slab, column and core optimisation. Rhinoceros 3D and its parametric design tool Grasshopper are used to conduct the optimisation. They allow to analyse thousands of designs in a short time, easily implement design changes and compare optimisation goals. The plug-in Karamba and the genetic algorithm component Galapagos are used for finite element analysis and optimisation. For the slab, the variables are the column locations and the number of columns on the plate; the column dimensions can be computed in the analysis, based on ultimate load capacity and axial shortening criteria. Multiple objective functions, such as net moment in the slab, strain energy or deflections, are used for the optimisation. For core optimisation, the variables include wall thicknesses both in plan and with height, lintel properties, shear wall lengths, as well as different geometrical arrangements. Possible objective functions include overall deflections, inter-storey drifts and lintel and wall stresses. The dynamic response of the structure is considered. These tools are versatile and can be used at different design stages. They can be used for the conceptual design where the outputs are trends that the engineers can use, allied to their experience, to achieve optimised, efficient designs. They can also be used later in a project when there are more constraints and the results confirm or improve the decisions made. The tools are being tested on theoretical examples and case studies and are used by industry for real projects. [1] UNEP SBCI, 2009, Buildings and Climate Change: Summary for Decision-Makers. [2] De Wolf, C., Pomponi, F., Moncaster, A., 2017, Energy and Buildings, 140, 68-80.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

An Application of a Constitutive Model with Damage to a Foundation with Fiber Reinforced Soil

Juan Pablo Bellassai*, Ruben Lopez**, Antonio Aquino***, Nilo Consoli****

*National University of Asuncion, **National University of Asuncion, Faculty of Engineering, ***National University of Asuncion, Faculty of Engineering, ****Federal University of Rio Grande do Sul

ABSTRACT

The addition of fibers in the soil improves several of its mechanical properties and modify the mechanism of failure of the same. On the other hand, the Continuous Damage Mechanics can conveniently describe the beginning of microcracks to coalescence and the subsequent formation of macrocracks, to make this can be used a homogenization techniques defining the representative volume to evaluate the evolution of the damage of the material. In geotechnical engineering, the first proposals of constitutive models with continuous damages for granular soils and for cohesive soils were published. This work consists in the presentation of the numerical results of the application of an elastoplastic constitutive law with continuous damage developed recently. This developed model is based on the hypothesis of equivalent deformation and consists of a constitutive law of the type Drucker-Prager modified by introducing the damage of the material. For the integration of the model an algorithm with an implicit integration scheme was used. Even if the damage model developed was anisotropic, the model implementation was performed considering isotropic damage, predicting the necessary tests for the characterization of the material in our laboratory. The model was coded in the FORTRAN programming language and later inserted as the UMAT subroutine of ABAQUS software. To obtain the parameters and to make the calibration of the model, experimental data obtained in the CML were used, by means of a triaxial equipment under cyclic loading and unloading tests. For the validation of the model, several samples of soil with fibers were simulated and the results compared with the experimental values available in our laboratory. Subsequently, a study of a foundation was carried out in a fiber reinforced soil, submitted to a tear test. The results show the regions where it presents the highest concentration of damage and its evolution during the application of the load. Based on the results obtained it is possible to conclude that: (a) The Continuous Damage Mechanics is applicable in the study of the behavior in the elastoplastic state with damage of the fiber reinforced soils, (b) The measurement of the damage of the material based on the variation of the elastic modulus and in an elastoplastic constitutive law with damage developed based on the hypothesis of equivalent deformation between damaged and effective configurations, is adequate to model the phenomena associated with geotechnical projects

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Goal-Oriented Adaptive Error Control of Stochastic Compressible System Approximations

Anca Belme*, Frédéric Alauzet**, Didier Lucor***, Jan Van Langenhove****

*University Pierre and Marie Curie, Institut Jean le Rond d'Alembert, **INRIA Saclay, ***LIMSI, CNRS, University Paris-Saclay, ****University Pierre and Marie Curie, Institut Jean le Rond d'Alembert

ABSTRACT

The simulation of complex nonlinear engineering systems such as compressible fluid flows may be targeted to make more efficient and accurate the approximation of a specific (scalar) quantity of interest of the system. Putting aside modeling error and parametric uncertainty, this may be achieved by combining goal-oriented error estimates and adaptive anisotropic spatial mesh refinements. To this end, an elegant and efficient framework is the one of (Riemannian) metric-based adaptation where a goal-based a priori error estimation is used as indicator for adaptivity (see for example [1]). Indeed, goal-based methods have the advantage of focusing resolution where is needed, reducing thus the computational cost in computing the targeted quantity of interest. This work proposes a novel extension of the aforementioned approach based on a Riemannian metric computation to the case of systems approximations bearing a stochastic component. The adaptive approach is indeed necessary in the stochastic space since we are interested in accurately capturing singularities such as shocks known to propagate from the deterministic (spatial) to the uncertain parameters domain ([2,3]). To this end, an optimisation problem leading to the best control of the distinct sources of errors is formulated in the continuous framework of the Riemannian metric space [4]. Algorithmic developments are also presented in order to quantify and adaptively adjust the error components in the deterministic and stochastic approximation spaces. The capability of the proposed method is tested on various compressible, steady problems, including on a HyShot II scramjet configuration subjected to geometrical and operational parametric uncertainties. It is demonstrated to accurately capture discontinuous features of stochastic compressible flows impacting some quantities of interest, while balancing computational budget and refinements in both spaces. References: [1] A. Loseille, A. Dervieux, and F. Alauzet. Fully anisotropic goal-oriented mesh adaptation for 3D steady Euler equations. J. Comp. Phys., 229:2866–2897, 2010. [2] C.M. Bryant, S. Prudhomme, and T. Wildey. Error decomposition and adaptivity for response surface approximations from PDEs with parametric uncertainty. SIAM/ASA Journal on Uncertainty Quantification, 3(1):1020–1045, 2015. [3] L. Mathelin and O. Le Maˆ?tre. Dual-based a posteriori error estimate for stochastic finite element methods. Communications in Appl. Math. and Comput. Science, 2(1):83–115, 2007. [4] J.W. Van Langenhove. Adaptive control of deterministic and stochastic approximation errors in simulations of compressible flow. PhD thesis, University Pierre and Marie Curie (Paris VI), Paris, France, 2017.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Computational Model for the Finite Element Analysis of Coupled Hygro-thermo-elasto-visco Plastic Behaviours: Application to Timber Structures

Salim Belouettar*, Ahmed Makradi**, Marc OUDJENE***

*Luxembourg Institute of Science and Technology, Luxembourg, **Luxembourg Institute of Science and Technology, ***University of Lorraine, France

ABSTRACT

A 3-D rheological model that accounts for elastic, plastic, hygro-expansion, viscoelastic and mechano-sorption is developed. A coupled hygro-mechanical multiscale modelling is developed and implemented in a finite element commercial software via user subroutine material. The modelling considers instantaneous and time-dependent responses of material wood that include elastic, plastic, hygro-expansion, viscoelastic and Mechano-sorption deformations. The partial differential equations governing heat transfer and thermo-elasticity are solved in the three-dimensional space whereas the partial differential equation for moisture diffusion in the two dimensional domains. The model is used to analyze the response of wood structures when subjected to coupled loading such as moisture, heat and mechanical loading.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Dassault Systèmes 3DEXPERIENCE High Performance Modelling-meshing, Visualization and New SIMULIA AMG-based Iterative Solving Technology to Solve Real-world Industrial Problems of 200+ Million Degrees of Freedom

Vladimir Belsky*

*Dassault Systemes, R&D; SIMULIA

ABSTRACT

For a long time, many of our customers are looking for ways to solve super large problems but have little success due to many constraints: difficulty creating such models, inability to solve those models that could be created, and the inability to display the results of those problems that could be solved. We currently observe an “explosion” of model sizes from many customers from very different industries all over the world. 100M Degrees of Freedom implicit finite element models are becoming the reality these days. In this presentation we discuss both our experience with the state-of-art AMG-based iterative solving technology and its performance using real world industrial examples for solving ultra-big models which size can be up to 200M Degree of Freedom. During the last decade, almost all the commercial vendors of finite element software started offering both iterative and direct solver technology for solving large sparse systems of linear equations arising from finite element discretization of structural mechanical problems using an implicit time integration approach. Typically, when working with large problems, a majority of the wall clock time is spent in the linear equation solver. For blocky models the time spent in the direct sparse solver is more than 2/3 of the entire analysis time and all other processing steps are much faster. From our experience the number of floating point operations (FLOPS) required by a direct sparse solver to factorize the matrices has a quadratic grow rate with the number of degrees of freedom; and sometimes the growth rate could be even higher! This means that the direct solver technology has limitations when it comes to solving really “large” scale problems. However, “large” scale problem means not only the number of equations, but mainly the number of FLOPS required for factorization. In other words, the applicability of the direct- solution technique depends largely on how “bulky” the problem is (the power in the exponent in the relation between the number of FLOPS and the number of degrees of freedom). Alternatively, iterative solvers provide a scalable and fast solution for “large” problems. They are scalable in the problem size sense as well as parallel scaling. They provide dramatic performance improvements for suitable applications. Moreover, in many cases they act as enabling technology rather than a solver alternative. Particularly, this is true for cases where the direct solver factorization cost is prohibitively expensive. Unfortunately, iterative solver technology has inherent limitations and robustness issues. Very often in real-world industrial applications, iterative solvers fail to converge because of various modeling issues that are present in a model. The direct solver technology is much more forgiving in this aspect. There are many reasons for traditional iterative solvers having convergence problems (unphysical behavior of gasket elements, insufficient amount of contact constraints to keep all of the parts in the model from rigid body movements, highly heterogeneous materials, etc. A new AMG-based technology was recently developed and implemented in Abaqus/Standard which allows for dramatic robustness improvement of the AMG iterative procedure applied to real world industrial problems which routinely include advanced modelling features such as multipoint constraints, gaskets with highly nonlinear material properties, contact constraints, kinematic couplings, pretension sections, periodicity boundary conditions, etc. Our extensive experiments with the most complex customer models demonstrated robustness of the new equation solver which was absolutely impossible to observe with the traditional AMG procedures. We will demonstrate this claim using some of these results.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Conservative Extension of the MAC Scheme to Polyhedral Meshes

René Beltman*, Martijn Anthonissen**, Barry Koren***

*Eindhoven University of Technology, **Eindhoven University of Technology, ***Eindhoven University of Technology

ABSTRACT

The MAC scheme introduced by Harlow and Welch [1] is one of the most popular methods for simulating viscous incompressible flow. The MAC scheme is a staggered Cartesian mesh method in which the incompressible Navier-Stokes equations are discretized in terms of the normal velocity components at the cell faces and the pressure variables in the cell centers. The staggered positioning of the velocity variables allows for an efficient discretization of the continuity equation that leads to exact conservation of mass and avoids pressure oscillations. Moreover, it can be shown that the method also conserves momentum, and, secondary quantities like kinetic energy (in the inviscid limit) and vorticity. In recent years, many advances have been made in the field of polytopal discretization methods. These advances allow for an extension of the MAC scheme to polytopal meshes. For the incompressible Stokes equations these extensions have been introduced in recent years (see for example [2]). However, a fully conservative extension of the discrete convective term to polytopal meshes has not been found yet. In this paper we study different extensions of the MAC scheme to polytopal meshes. We show that these extensions have many of the favorable properties of the Cartesian-mesh MAC scheme. Moreover, we focus on the convective term and discretize different formulations (conservative, rotational) of this term. We analyze them and compare their numerical efficiency. References [1] F.H. Harlow, J.E. Welch, Numerical calculation of time-dependent viscous incompressible flow of fluid with free surface, Physics of Fluids 8, 2182-2189, 1965. [2] J. Bonelle, A. Ern, Analysis of compatible discrete operator schemes for the Stokes equations on polyhedral meshes, IMA Journal of Numerical Analysis 35, 1672-1697, 2014.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Comparative Responses of the Q6 and PIPER 6YO Human Body Model in Simulated Frontal Impacts

Aditya Belwadi*, Jalaj Maheshwari**, Nhat Duong***

*The Children's Hospital of Philadelphia, **The Children's Hospital of Philadelphia, ***The Children's Hospital of Philadelphia

ABSTRACT

There has been ample evidence from real world crashes that belt-positioning booster seats reduce injury risk for children 4 through 7 years of age. Newer booster seat designs have been moving the lap-belt anterior of the anterior superior iliac spine (ASIS) potentially causing them to load the pelvis at a later time in the crash sequence. The objective of this project was to gain insight into causation of injuries sustained by children seated in newer booster seat designs in simulated frontal impacts utilizing pediatric human body finite element models. The PIPER 6-year-old human body finite element (FE) model along with a Q6 FE model was utilized. The test environment was modeled as per FMVSS 213 test conditions. Booster seat models were developed by scanning physical seats and converting them FE mesh with elastic/plastic material properties. The sled test condition was validated against physical test conditions of the instrumented Q6 restrained using a 3-point lap-shoulder belt (without a retractor/pretensioner). HIC36, head and chest resultant accelerations were matched to within (plus/minus 8% of maximum along with phase matching). The PIPER HBM was then positioned as per the test condition on four different booster conditions (No booster, Highback, lowback and portable) on the 213-test bench. A frontal crash pulse of 24G (Max at 80ms over 120ms) was utilized. A total of 16 simulations were carried out with the Q6 and PIPER FE models. Kinetic and kinematic measures were extracted and processed as per SAEJ211. The kinetic measures (HIC36, head and chest resultant acceleration) of the Q6 were well within FMVSS 213 IARV limits. For the newer seat designs with anterior lap-belt routing, the response of the Q6 was similar to the test condition – increased neck force (Fy) and delayed engagement with the pelvis causing the torso to arch forward. The PIPER HBM submarined as expected for the condition with a booster seat. In both the no-booster and portable seat condition the shoulder belt engaged the neck (ie; medial motion) causing excessive strain (21%) in the neck musculature. The torso arching caused higher lumbar Booster seats are in general shown to be effective measures for restraining children safely. Newer seat designs have proved to be innovative while providing solutions to changes in mobility. The human body model provides a good measures of injury assessment for children restrained in these seats. Additional testing is needed to address other crash modes.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Extended-adpative Computational Methodology for the Solution of Adhesive Contact Problems

Hachmi Ben Dhia*, Shuimiao Du**

*CentraleSupélec-Université Paris-Saclay, **CentraleSupélec-Université Paris-Saclay

ABSTRACT

Adhesive contact between solids is important to many areas of applied science and technology, paticularly nowadays for the design of micro and and nano electronic devices. This is one of the reasons for which an important range body of reseach works is still devoted to adhesive contact problems (ACP) at different scales. This work is an investigation on some mathematical and computational aspects of theoretical formulations and numerical approximation methods in this topic. We present and test some new ideas that contribute to the enhancement of the reliability and efficiency of the resolution of ACP, based on the Lennard-Jones (LJ) surface potential, in the continuum framework. More precisely, to address mathematical and numerical pitfalls of the phenomenological stiff repulsive part of the LJ model, a sequence of partitions of contact models is adaptively constructed to both extend and approximate the LJ model. It 's formed by a combination of the LJ model with a sequence of shifted-Signorini (or, alternatively, -Linearized-LJ) models, indexed by a shift parameter field, defined on the potential contact surface. For each model of this sequence, a weak (hybrid mixed or primal) formulation of the associated local ACP is developed. To track the critical localized areas of adhesive contact, a two-step strategy is developed: Independently of the iterations, a macroscopic contact problem, based on a macro contact model (no adhesion), is first formulated, approximated and solved once to detect contact-noncontact separation zones. In the second step and at each shift-adaptive iteration, a micro-macro ACP, based on a given shifted partition of micro-macro adhesive contact model is re-formulated within the multiscale Arlequin framewok [1]-[3]; the micro-Arlequin patches being defined in the critical areas detected in the first step. This problem is consistently approximated and solved to compute accurately the solution in the adhesive contact zones, while reducing significantly the computation costs. Numerical results for classical adhesive contact tests are given. The adaptive shift-algorithm proves to be remarkably performant and the comparaison of our results with available analytical and numerical results, obtained with other approaches, shows the effectiveness of our global strategy. [1] H. Ben Dhia, Multiscale mechanical problems: the Arlequin method, Comptes Rendus Acad Sci, Paris, 326(12), 1998, 899-904 [2] H. Ben Dhia, C. Zammali, Level-Sets fields, placement and velocity based formulations of contact-impact problems, IJNME, 69, 13, 2007, 2711-2735 [3] H. Ben Dhia, Further Insights by Theoretical investigations of the Multiscale Arlequin Method, IJMCE, 6(3), 2008, 215-232 2008

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Multidisciplinary Design Optimization of Transport Aircraft Wing Using High Fidelity Modeling Process

Abdelkader Benaouali*, Stanislaw Kachel**

*Military University of Technology, **Military University of Technology

ABSTRACT

Because of its role as the primary lifting surface of an aircraft, a special attention must be drawn to the wing design by considering both structural mechanics and aerodynamics as well as the strong dependency between them. The design is no longer a trial-and–error procedure due to the introduction of numerical optimization, resulting in what is currently designated as multidisciplinary design optimization MDO in the case where several disciplines are involved. The aim to accurately model the complex wing behavior necessitates the use of high fidelity modeling techniques, namely finite element method (FEM) and computational fluid dynamics (CFD). The objective of this work is to construct an MDO framework, proposed for the design of transport aircraft wing, based on an automated environment which integrates a set of most popular and commonly used commercial modeling and simulation software. It goes through geometric modeling in SIEMENS NX, Aerodynamic meshing in ICEM CFD, flow solution using ANSYS FLUENT, Structural modeling and analysis in MSC.PATRAN/NASTRAN. The integration is made possible by means of data exchange translators available in most of computer aided tools, while the design automation is realized via respective software scripting capabilities as well as the possibility to run in batch mode. Because of the simulation cost required for evaluating the high fidelity models, especially for CFD calculations, a single run of the design framework may be very time consuming making a direct optimization on the design framework highly impractical. Therefore, an optimization strategy based on meta-modeling techniques is adopted. The improved Latin Hypercube Sampling (IHS) is used for the Design of Experiments (DoE) and the radial basis function (RBF) method is used as the surrogate model. The reliability of the proposed approach is investigated through its application for design of a transport aircraft wing considering shape and structural design variables. In order to perform an optimization that considers both structural and aerodynamic performance, the objective function must combine the wing aerodynamic and structural properties. In this work, aircraft range is chosen as it is a function of the lift-to-drag, which represents the wing aerodynamic performance, and the ratio of the initial and final cruise aircraft weights which represents the structural optimization term.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A First--Principles Approach to the Derivation of a Reduced Order Model for Vortex--Induced Structural Oscillations

H. Benaroya*, S. Mottaghi**

*Rutgers University, **William J. Hughes Technical Center, FAA

ABSTRACT

While variational methods have proven to be very effective tools in modeling the dynamics of solid systems, there have been many challenges faced in applying them to fluid systems and fluid-structure interaction (FSI) problems. As evident from the literature, the efforts to apply Hamilton's principle and Lagrange's equations to the problems of fluid dynamics have had relative success in certain cases, mainly ideal fluids. There exist no general variational approaches for fluid-structure interactions, or for viscous fluid dynamics problems. One main challenge arises from relating the variational principles in the Lagrangian frame to the Eulerian frame. Therefore, we start by considering the Eulerian and the Lagrangian reference frames and review the relations between dynamic properties as described in these reference frames for a general control volume. Then, these relations are used to identify the difficulties faced in applying variational principles in an Eulerian frame of reference. Having identified the challenges above, Jourdain's principle (JP) is proposed as an effective tool to overcome some of those difficulties. Then, JP is extended so as to become applicable to control volumes containing Newtonian incompressible viscous fluids. In this way we derive the Navier-Stokes equations. Subsequently, JP is used to derive the energy rate equation for a general control volume containing Newtonian incompressible viscous fluids, suggesting that a correction term may need to be added to the classical energy equation. Moreover, the limitations of the classical energy equation are explored by deriving it from Hamilton 's principle. This lays the theoretical foundation for utilizing JP for modeling both fluids and structures as FSI systems. The general formulation is extended so that the reduced-order modeling of FSI and VIV systems can be performed using the extended JP. By using this very general framework, we can add assumptions in order to derive well-known “flow-oscillator” models. These flow-oscillator models are generally presented following an examination of experimental results, with semi-empirical equations of motion that generally represent similar global dynamic behavior stipulated. By being able to simplify the more general equations to these flow-oscillator equations, we are able to discover some of the implicit assumptions they represent.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Modeling of Failure Propagation in High Explosive Using Dominant Crack Approach

Bart Benedikt*, Partha Rangaswamy**

*Los Alamos National Laboratory, **Los Alamos National Laboratory

ABSTRACT

Numerical simulations of systems composed of High Explosives (HE) capable of accurately predicting the state of stress and deformation during various dynamic loading scenarios require high-fidelity constitutive models of HE. In this research, a strain rate-dependent model for propagating damage under dynamic loading is presented. The constitutive model is based on the concepts of Statistical CRAck Mechanics (SCRAM) and strain rate dependent visco-elasticity. The damage evolution in HE is modelled by simulating the rate of growth also called the critical crack. Critical crack is defined as a crack that becomes unstable for a given loading conditions. In the formulation presented here the critical crack propagation is assumed to depend on the rate and history of loading rate. The numerical implementation of the constitutive model into ABAQUS/Standard implicit finite element code through a user subroutine is also presented. The developed finite element code is used to numerically simulate several tests performed on HE materials available to the authors. The results of the simulations and the comparison with the experimental work are presented and discussed. The method to calibrate the model parameters based on the testing results is discussed. In general, the numerical simulation was able to correctly predict the material regions, which were most likely to initiate the failure. In conclusion, we argue that the present approach is a considerable improvement over existing models used to simulate HE behavior [1-2] and it can be successfully used to predict the bulk response and the initiation and propagation of failure in the studied HE materials. References 1. Addessio, F. L., Johnson, J. N., 1990. A constitutive model for the dynamic response of brittle materials. Journal of Applied Physics 67, 3275-3286 2. Bennett, J. K., Haberman, K. S., Johnson, J. N., Assay, B. W., Henson, B. F., 1998. A constitutive model for the non-shock ignition and mechanical response of high explosives. Journal of the Mechanics and Physics of Solids 46, 2303-2322. LA-UR-17-31482

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Improvement and Verification of Moving Particle Semi-Implicit Method for Multi-Physics Simulation of High Viscosity Fluids

Nicolas Benkemoun*, Seiichi Koshizuka**, Kazuya Shibata***

*The University of Tokyo, **The University of Tokyo, ***The University of Tokyo

ABSTRACT

The MPS method was originally proposed for use for purely Newtonian fluids and is mainly used with water or oils, or fluids of similar viscosities. However, issues arise when using increasingly higher viscosities. Using the higher order terms proposed by Khayyer and Gotoh [1], we analyze the flow of highly viscous polymers. We also implement a Cross viscosity model to check the behavior of shear dependent fluids, which allows the study of more realistic behaviors. Comparison with an improved SPH scheme [2] is done to evaluate this improvement of the MPS method. A qualitative thermal analysis is also carried out for future applications to a Thermoplastic Injection Process. [1] A. Khayyer and H. Gotoh, “Enhancement of stability and accuracy of the moving particle semi-implicit method”, J. Comput. Phys., 230, pp. 3093-3118, (2011) [2] J. Ren et al., “Simulation of complex filling process based on the generalized Newtonian fluid model using a corrected SPH scheme”, Comput. Mech., 46, pp. 643-665, (2012)

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

On the Role of Structure Tensors in Large Strain Anisotropic Hyper-Elastoplasticity of Geomaterials and Drucker-Prager/Cap Plasticity

Kane Bennett*, Richard Regueiro**, Darby Luscher***

*Los Alamos National Laboratory, **University of Colorado Boulder, ***Los Alamos National Laboratory

ABSTRACT

Describing anisotropic mechanical behavior of a material requires identifying preferential directions of the material, giving rise to second order structure tensors (also called fabric tensors in the context of geomechanics). Structure tensors allow the scalar valued tensor functions of hyper-elastoplasticity, namely the free-energy, plastic potential, and yield function, to be expressed as isotropic functions representing an anisotropic material response. Ensuring thermodynamic consistency of elastoplastic constitutive models for geomaterials further requires accounting for inelastic volume changes and appropriately discriminating between elastic and plastic contributions to the deformation field. The precise way that these two basic requirements are fulfilled (i.e., formulating anisotropic hyper-elastoplastic models for geomaterials) necessitates making certain assumptions and material specific constitutive choices. In this talk, large strain anisotropic hyper-elastoplasticity of geomaterials is examined, with emphasis on the role of structure tensors in formulating thermodynamically consistent constitutive equations. Formulation is carried out in terms of Mandel and Eshelby-Mandel stresses within the intermediate configuration associated with the multiplicative split of the deformation gradient. Necessary material assumptions and particular constitutive choices are identified for the development of a novel anisotropic Drucker-Prager/Cap material model. The ability of the model to capture anisotropic elastoplastic behavior is exemplified through numerical experiments and nonlinear finite element modeling of existing measurements.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Recent Developments in Isogeometric Analysis for LS-DYNA

David Benson*, Liping Li**, Attila Nagy***, Stefan Hartmann****

*LSTC, **LSTC, ***LSTC, ****Dynamore GmbH

ABSTRACT

LS-DYNA is the first commercial code to support IGA through the implementation of generalized elements, and then through key word descriptions of patches of B-spline and NURBS elements. Three shell formulations and a solid element formulation are currently available. Additional capabilities have been recently added, including improved contact, anisotropic material modeling, spotweld modeling and support for unstructured spline capabilities through the specification of their Bezier extraction. These and other recent additions are described and demonstrated. In addition, some of the difficulties industry has encountered in moving to this new technology are discussed.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Extended Virtual Element Method for Problems with Singularities

Elena Benvenuti*, Andrea Chiozzi**, N. Sukumar***, Gianmarco Manzini****

*Engineering Department, University of Ferrara, Italy, **Engineering Department, University of Ferrara, Italy, ***UC Davis, USA, ****Los Alamos National Laboratory, New Mexico, USA

ABSTRACT

Extended Virtual Element Method for Problems with Singularities E. Benvenuti1*, A. Chiozzi1, N. Sukumar2, G. Manzini3 1 University of Ferrara, Ferrara, Italy 2 University of California, Davis, USA 3 Los Alamos National Laboratory, New Mexico, USA E-mail: andrea.chiozzi@unife.it, elena.benvenuti@unife.it, n.sukumar@ucdavis.edu, gmanzini@lanl.gov Keywords: virtual element method; extended finite element method; singularities. The eXtended Finite Element Method (XFEM) was first proposed by Belytschko 's group [1] as an innovative computational technology for dealing with discontinuities and singularities without tailored meshes. This goal is achieved by enriching the approximation space by means of additional shape functions that reproduce the non-smooth features of the expected solution. Owing to its great flexibility, XFEM has become one of the most exploited methodology for crack simulation in mechanical and structural engineering. More recently [2], an eXtended Finite Element Method exploiting polygonal basis functions has been proposed for polytopal meshes, that can be especially useful when meshing complex domains, such as those occurring in bodies with cracks and inclusions. The Virtual Element Method (VEM) is a generalization of the Finite Element Method capable of dealing with very general polytopal meshes without using polygonal basis functions[3]. The key feature of VEM relies on the introduction of a suitable projector operator to approximate the bilinear form arising in the weak formulation of the continuous problem, so that the explicit construction of the elemental basis functions can be avoided. Based on illustrative numerical examples, the presentation to be delivered at the conference aims to discuss how to extend the XFEM to polytopal meshes by exploitation of the VEM methodology in problems with singular unknown fields. References [1] Moës, N., Dolbow, J. and Belytschko, T., “A finite element method for crack growth without remeshing”, International Journal for Numerical Methods in Engineering, 46, 131-150, 1999. [2] Tabarraei, A. and Sukumar, N., “Extended finite element method on polygonal and quadtree meshes”, Computer Methods in Applied Mechanics and Engineering, 197, 425-438, 2008. [3] Beirao da Veiga, L., Brezzi, F., Cangiani, A., Manzini, G., Marini, L.D. and Russo, A., “Basic Principles of Virtual Element Methods”, Mathematical Models and Methods in Applied Sciences, 23, 119-214, 2013.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Towards Optimal Design of Engineering Systems

Viktor Berbyuk*, Seyed Milad Mousavi Bideleh**

*Chalmers University of Technology, Gothenburg, Sweden, **VETEC AB, Mölndal, Sweden

ABSTRACT

This paper presents a review on methods, algorithms and tools available for robust optimal design of engineering systems. The focus primarily is put on methods and algorithms for global sensitivity analysis (GSA) and solution of Pareto optimization problems (POP) for multidimensional nonlinear mechanical systems. The computer code SAMO, developed at Chalmers University of Technology, is presented as an efficient toolbox for optimal design of engineering systems with different applications. At this stage, the toolbox SAMO includes two modules: SAMO-GSA and SAMO-POP. The module SAMO-GSA is developed based on the multiplicative version of the dimensional reduction method (M-DRM) [1]. In the SAMO-GSA an efficient approximation is employed to simplify the computation of variance-based sensitivity indices associated with a general function of n-random variables. The GSA results of the engineering system in question are then presented as a mapping of the design parameters and total sensitivity indices of the objective functions. These results might be used as an input to the SAMO-POP for multi-objective optimization. The module SAMO-POP works based on genetic algorithm (GA). The GA settings include lower and upper bounds for variation of the design parameters, population size, number of generations, elite count, and Pareto fraction settings. The results of SAMO-POP are presented in terms of Pareto fronts and corresponding Pareto sets for further analysis and decision making by the user. The efficiency of the proposed algorithms and developed toolbox is illustrated, first on scholar applications (thermally induced stress intensity factor and quarter car vehicle model), and second by GSA and solutions of several multi-objective optimization problems for a nonlinear multidimensional mechanical system which represents bogie suspension components of a high-speed train [2-3]. Finally, based on the literature review and the results obtained the paper presents the outlook of the future research in developing of computationally efficient algorithms for extension of the toolbox SAMO for robust optimal design of engineering systems. References 1. Zhang, X. and M. D. Pandey, (2014), An effective approximation for variance-based global sensitivity analysis, Reliability Engineering and System Safety, 121, 164-174. 2. Mousavi Bideleh, M.S. and V. Berbyuk, (2016), Global sensitivity analysis of bogie dynamics with respect to suspension components, Multibody System Dynamics, 37, No. 2, 145-174, DOI: 10.1007/s11044-015-9497-0, http://dx.doi.org/10.1007/s11044-015-9497-0 3. Mousavi-Bideleh, M.S., and V. Berbyuk, (2016), Multiobjective optimisation of bogie suspension to boost speed on curves, Vehicle System Dynamics, 54, No 1, 58-85, DOI: 10.1080/00423114.2015.1114655 http://dx.doi.org/10.1080/00423114.2015.1114655

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Finite Element Method for Modeling Surface Growth and Resorption of Deformable Solids

Guy Bergel*, Panayiotis Papadopoulos**

*University of California, Berkeley, **University of California, Berkeley

ABSTRACT

Surface growth and resorption occur in a variety of engineering applications and natural phenomena including the accretion of layers in tree trunks and shells, polymerization of filaments aiding locomotion of cells, additive manufacturing, and metal solidification. The deposition of mass onto the surface of a physical body generates material points whose reference configurations depend on their time of deposition. Furthermore, the removal of mass through a given surface defines an ablated boundary along a formerly interior portion of the domain. Both addition and removal of mass characterize a rate-dependent process in which the spatial representation of a given subregion in a physical body relies on an evolving reference configuration [1]. In this work, a numerical framework is developed to capture the surface growth and resorption of a solid undergoing finite deformation using a methodology which extends the classical arbitrary Lagrangian-Eulerian (ALE) finite element method [2]. To this end, an intermediate configuration is defined which tracks the evolving reference state of the body based on the position of its surface and thus provides a means for enforcing balance laws at a given time. Examples illustrating the effects of surface growth and resorption on the spatial and temporal convergence of a two-dimensional body in plane strain are discussed. Moreover, specific algorithmic procedures of growth-induced multibody interaction are introduced within the context of cell motility. References [1] G. A. Ateshian, “On the theory of reactive mixtures for modeling biological growth,” Biomechanics and Modeling in Mechanobiology, vol. 6, pp. 423–445, Nov 2007. [2] N. Hodge and P. Papadopoulos, “A continuum theory of surface growth,” Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences, vol. 466, no. 2123, pp. 3135–3152, 2010.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

ONERA Composite Material Law for Crash Simulation

Julien Berthe*, Frédéric Laurin**, Antoine Hurmane***

*ONERA, **ONERA, ***ONERA

ABSTRACT

To reduce the environmental impact and the weight of the vehicles, the transportation industry is increasingly using organic matrix composite materials in structural parts. Such parts are submitted to various kinds of loading, mechanical as well as thermal, during the life cycle of an aircraft. Due to the cost of full-scale testing, advanced numerical method are more and more used to predict the response of a composite aircraft structure regarding crash loading. Various improvements of advanced simulations can be considered: material law, cohesive law, contacts modelling… In this work, an advanced material law is considered and improved in order to accurately describe the rate dependency of organic matrix composite materials. The ONERA progressive failure model which has been well ranked in the second world wild failure exercise has been considered as a starting point. Firstly, some simplifications have been done to take into account the specificities of crash simulations. Secondly, based on test results available at ONERA and/or tests available in the literature, the introduction of rate dependencies in the material law has been considered. In order to validate or justify some hypothesis, new experimental procedures have been developed or proposed. An overview of the recent experimental results and of the future experimental tests for the material law validation will also be presented in this paper.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Stabilizing DG Methods on Polygonal Meshes via Computable Dual Norms

Silvia Bertoluzza*, Ilaria Perugia**, Daniele Prada***

*Consiglio Nazionale delle Ricerche, **University of Vienna, ***Consiglio Nazionale delle Ricerche

ABSTRACT

The choice of the stabilization terms (or, equivalently, of the definition of the numerical fluxes and/or traces) is a key issue in the design of DG methods. Usually, some form of penalization is somehow added, where some residual term is measured in a mesh dependent norm, designed so that it somehow mimics the norm of the dual space where the residual naturally exists. The treatment, in the analysis, of such mesh dependent norms calls for the use of direct and inverse inequalities, which, in turn, depend on some “shape regularity” assumptions on the underlying tessellation, which are not always easily satisfied in the polygonal framework. With the final aim of relaxing such requirement, we will present, in this talk, a way to design “cheap” computable norms (and scalar products) for the dual spaces where the residuals live, and of using them in designing the stabilization term for a DG type method for the Poisson equation on a polygonal mesh, in which the unknown in the polygonal elements, the fluxes and the unknown on the edges, are all, independently, approximated by polynomials of degree k.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Scalability and Portability of Large Scale Turbulent Combustion Problems

Martin Berzins*

*SCI INSTITUTE, UNIVERSITY OF UTAH

ABSTRACT

When solving large scale turbulent combustion problems using adaptive techniques, the coming of exascale computer architectures such as Argonne National Laboratory 's A21 and the presence of very different pre-exascale machines such as the fastest present machine the Tianhu SunwayLight and the DOE Summit and Sierra raises the challenge of being able to port codes across very different computer architectures. While the use of approaches based upon Asynchronous Many Task (AMT) Runtime Systems such as the Uintah framework considered here makes porting easier, the central challenge of obtaining performance from the actual loops of the adaptive code remains. In order to explore this issue this talk will examine the performance of the adaptive mesh-based radiation solver using approaches such as the Kokkos portability library within an AMT code. A suvccessful attempt to port Uintah to the the Tianhu SunwayLight will be described as a demonstrator of the overall portability approach. This is joint work with Zhang Yand iapm Beijin and Alan Humphrey, John Holmen, Damodar Shahasbarude, Brad Peterson and John Schmidt at Utah.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Hydraulic Fracturing in Naturally Fractured Reservoir Simulation Using Finite Elements with Embedded Discontinuities

Leila Beserra*, Leonardo Guimarães**, Osvaldo Manzoli***

*Federal University of Pernambuco, **Federal University of Pernambuco, ***São Paulo State University

ABSTRACT

Hydraulic fractures usually propagate perpendicular to the direction of least principal stress, because this is the direction that defines the lowest work. However, modeling hydraulic fracturing in the presence of a natural fracture network is a challenging task, due to the strong coupling that exists between fluid flow and mechanical behavior, as well as the complex interactions between propagating fractures and existing natural interfaces. From the mathematical point of view it is a coupled hydro-mechanical problem, where equations for fluid flow through porous media and fractures (fluid mass balance) and medium deformation and fracture propagation (mechanical problem) have to be solved simultaneously considering the constitutive equations that describe the material behavior. When a fracture propagates through a continuous media, discontinuities in the displacement and fluid pressure fields are introduced. The selection of an appropriate fracture propagation model is a critical task in modeling of hydraulic fracturing. In this paper, a strong discontinuity approach, proposed by Manzoli and Shing (2006), to embed discontinuities into finite elements was implemented in a numerical code that performs numerical analysis of fluid flow in a deformable reservoir. The presence of natural fractures includes an additional difficulty for the modeling of hydraulic fracturing, since they may affect the fluid flow in the reservoir and the orientation of the induced fracture. In order to apply the formulation presented in this paper, the hydraulic fracturing problem in reservoirs with pre-existing fractures was simulated. A numerical tool was used to embed the natural fracture network into the finite element mesh, with respect to the geological mapping of these fractures. To model the mechanical behaviour of material, was adopted a tensile damage model proposed by Sánchez et al. (2014). The resulting numerical code was used to model hydraulic fracture propagation through naturally fractured reservoirs with relatively coarse meshes in a reasonable computational time. Furthermore, the results provided an important insight into the mechanisms that generate microseismicity that occurs during hydraulic fracture stimulation. The interpretation of microseismicity based on geomechanical analysis gives a more realistic estimation of the stimulated reservoir volume (SRV), otherwise SRV can be overestimated. REFERENCES Manzoli, O.L. and Shing, P.B. [2006] A general technique to embed non-uniform discontinuities into standard solid finite elements. Computers & Structures, 84, 742–757. Sánchez, M.; Manzoli, O. L.; Guimarães, L. J. N. [2014] Modeling 3-D desiccation soil crack networks using a mesh fragmentation technique. Computers and Geotechnics, 62, 27-39.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Data-driven Design of New Materials and Structures

Miguel Bessa*

*Delft University of Technology

ABSTRACT

A data-driven computational framework [1] combining Bayesian machine learning for imperfection sensitive quantities of interest, uncertainty quantification and multi-objective optimization is developed to analyze and design new materials and structures. This talk intends to demonstrate the generality of the proposed framework, highlighting key challenges and possible solutions illustrated by three different design problems: toughening composite materials by tuning the plastic behavior of the constituents, improving collapse behavior of ultra-thin satellite structures with uncertain ultimate buckling strength, and finding unprecedented properties by exploring a new material concept. [1] Bessa, M.A., Bostanabad, R., Liu, Z., Hu, A., Apley, D.W., Brinson, C., Chen, W., Liu, Wing Kam, “A framework for data-driven analysis of materials under uncertainty: Countering the curse of dimensionality,” Computer Methods in Applied Mechanics and Engineering, 320, 633–667 (2017).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

The GENERIC formalism for the thermodynamically consistent formulation and discretization of coupled thermomechanical solids

Peter Betsch*, Mark Schiebl**

*Institute of Mechanics, Karlsruhe Institute of Technology (KIT), Germany, **Institute of Mechanics, Karlsruhe Institute of Technology (KIT), Germany

ABSTRACT

GENERIC (General Equation for the Non-Equilibrium Reversible-Irreversible Coupling) is a double-generator formalism for the thermodynamically consistent formulation of problems from continuum mechanics. The GENERIC-based formulation relies on an additive decomposition of the evolution equations into a reversible part and a dissipative part. While the reversible part is generated by the total energy of the system, the irreversible part is generated by the total entropy. Originally, GENERIC has been developed in the context of complex fluids (H.C. Öttinger, Beyond Equilibrium Thermodynamics, Wiley, 2005). More recently, the GENERIC framework has been extended to solid mechanics. Romero (I. Romero, Thermodynamically consistent time-stepping algorithms for nonlinear thermomechanical systems, IJNME, 79(6): 706-732, 2009) realized soon the great potential of the GENERIC formalism for the design of structure-preserving numerical schemes and coined the notion of a thermodynamically consistent (TC) method. Alternatively, TC schemes may be termed Energy-Entropy-Momentum (EEM) schemes. These methods can be viewed as extension to dissipative systems of earlier developed Energy-Momentum (EM) schemes for conservative systems with symmetry such as large strain elastodynamics and flexible multibody dynamics (P. Betsch, editor, Structure-preserving Integrators in Nonlinear Structural Dynamics and Flexible Multibody Dynamics, Vol. 565 of CISM Courses and Lectures, Springer, 2016). Previously developed GENERIC-based TC methods for thermomechanically coupled solids are typically subject to serious limitations such as (i) the use of the entropy density as thermodynamical variable, and (ii) the restriction to isolated (or closed) systems in which the boundaries are neglected. In the present talk we propose a generalized GENERIC-based formulation that (i) allows for the free choice of the thermodynamical variable among either the temperature, internal energy density or entropy density, and (ii) takes into account the boundaries of the system. The new formulation lays the ground for the design of structure-preserving (e.g. TC) methods for the solution of initial boundary value problems for thermomechanically coupled solids. In the talk we focus on the dynamics of thermoelastic solids with heat conduction.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Closed-Form Solution and Comparison for the One-Dimensional Orthorhombic Quasicrystal and Crystal Plate

Arpit Bhardwaj*, Koushik Roy**

*Undergraduate Student, IIT BHU, **Assistant Professor, IIT Patna

ABSTRACT

Quasicrystals (QCs) are solids with a long-range quasi-periodic translational order, and a long-range orientational order was ?rst discovered around in 1984. The work includes derivation of the exact-closed form solution for simply supported quasicrystal and crystal plates by using propagator matrix method under surface loading, free vibration, and patch loading. As a numerical example a quasicrystal and a crystal plate are considered, and after investigation, the variation of displacement and stress ?elds along the thickness of these two plates are presented. Further, it includes analyzing the displacement and stress ?elds for two plates having two different stacking arrangement, i.e., QuasiCrystal/Crystal/QuasiCrystal and Crystal/QuasiCrystal/Crystal and comparing their results. This will not only tell us the change in the behavior of displacement and stress ?elds in two different materials but also how these get changed after trying their different combinations. For the free vibration case, Crystal and Quasicrystal plates along with their different stacking arrangements are considered, and displacements are plotted in all directions for different Mode Shapes. At last, effect of patch loading is considered as a result of dynamic loading on multi-layered 1D plate and numerous results were obtained such as, displacement and Stress fields for different area of patch along with different normalized frequencies, displacement and Stress fields for different ratios of Phason-Phonon Coupling constant & C66 along the thickness direction, displacement and Stress fields variation along one of the Length's direction. The numerical results can be further used as a benchmark for investigating various properties of quasicrystals which make them different from crystals. Using the results from the stacking arrangement QuasiCrystal/Crystal/QuasiCrystal, we can use properties of Quasicrystal such as less friction coef?cient and low conductivity which will lower the frictional losses in machines if we can use brittle Quasicrystal as a coating over a strong crystal axle. Keywords: Quasicrystals, Multilayered Plates, Surface Loading, Patch Loading, Free Vibration References: [1] L.-Z. Yang, Y. Gao, E. Pan, and N. Waksmanski, "An exact closed-form solution for a multilayered one-dimensional orthorhombic quasicrystal plate," Acta Mechanica, vol. 226, no. 11, pp. 3611–3621, 2015. [2] Waksmanski N, Pan E, Yang L, Gao Y. Free Vibration of a Multilayered One-Dimensional Quasi-Crystal Plate. ASME. J. Vib. Acoust. 2014;136(4):041019-041019-8. doi:10.1115/1.4027632. [3] T. Fan, The Mathematical Elasticity of Quasicrystals and its Applications. Springer, 2011.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Certified Model Order Reduction of an Elastic Body with Large Deformations

Ashish Bhatt*, Dennis Grunert**, Jörg Fehr***, Bernard Haasdonk****

*University of Stuttgart, **University of Stuttgart, ***University of Stuttgart, ****University of Stuttgart

ABSTRACT

Model order reduction (MOR) of nonlinear mechanical systems is a technique of reducing the computational complexity of the corresponding mathematical model by reducing associated degrees of freedom and thereby obtaining a model of reduced dimension. This reduced model can then be simulated efficiently in multi-query scenarios. The gain in simulation efficiency often comes at the cost of the low fidelity of the reduced model. Model verification or certification of the reduced method by estimating the error incurred is important to use the simulation for management decisions and engineering applications. We derive the equation of motion of an elastic body under large rigid motion in the absolute coordinate formulation (ACF) using principles of continuum mechanics. For this purpose, the motion of the elastic body is decomposed into a large rigid body displacement and a small elastic displacement with respect to some fixed inertial frame. The principle of virtual work is then used to derive a second order nonlinear differential equation, with a constant mass matrix, governing the motion of the body with respect to the inertial frame. Constraints to the elastic body are modeled with additional algebraic equations. The overall motion of the body is therefore governed by a nonlinear DAE. The parametrized equation obtained from the spatial discretization of the DAE is often very high dimensional and is therefore computationally prohibitive to solve especially in multi-query scenarios. One, therefore, needs a reduction strategy [1] to simulate the system dynamics efficiently. In the absence of rigid body motion, the resulting DAE is linear and we investigate the error incurred in such systems in [3]. We are interested in the reduction and estimation of the error incurred in the nonlinear DAE in [2]. References: [1] Benner, Peter, and Tatjana Stykel. "Model order reduction for differential-algebraic equations: a survey. " Surveys in Differential-Algebraic Equations IV. Springer International Publishing, 2017. 107-160. [2] Bhatt, Ashish, and Fehr, Jörg, and Bernard Hassdonk. "Error Estimation in Model Order Reduction of an Elastic Body under large rigid motions." In A.F. Radu (Ed.) European Conference on Numerical Mathematics and Advanced Applications, submitted, 2017. [3] Fehr, Joerg, and Grunert Dennis, and Bhatt, Ashish, and Bernard Haasdonk. "A Sensitivity Study of Error Estimation in Reduced Elastic Multibody Systems. " In 9th Vienna International Conference on Mathematical Modelling, submitted, 2018.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Design of Morphing Shape Memory Polymer Structures Via Topology Optimization

Anurag Bhattacharyya*, Kai A. James**

*University of Illinois at Urbana-Champaign, **University of Illinois at Urbana-Champaign

ABSTRACT

We present a novel approach to the design of morphing structures using topology optimization, while incorporating shape memory polymers (SMPs). The thermomechanical characteristics of SMPs can be exploited to actuate structural deflection to enable morphing toward a target shape. Structures displaying multiple target shapes can be designed by leveraging SMPs with specific deformation characteristics. In the current study, topology optimization is used to optimally distribute a combination of active (SMP) and passive material phases within the design domain. In this way, we are able to tailor the nonlinear response of the structure to achieve the desired morphology. The large-scale deformation undergone by the structure is modeled using a hybrid theory that combines deformable media with a hyperelastic material model. An isoparamteric finite element model is used for modeling the deformation characteristics of the structure, and the non-linear structural equilibrium equations are solved using a displacement-controlled Newton-Raphson procedure. The material distribution is parameterized using a modified multi-material SIMP formulation, and the resulting design optimization problem is solved using a gradient-based approach. The design sensitivities are derived and implemented using an adjoint sensitivity formulation. Optimization results will include two-dimensional planar structures capable of deforming into target configurations in response to controlled thermal loads.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Computational Model of Transcatheter Aortic Valve Replacement: a Patient-Specific Approach to Minimize Clinical Complications

Matteo Bianchi*, Gil Marom**, Ram Ghosh***, Giorgia Bosi****, Danny Bluestein*****

*Stony Brook University, **Tel Aviv University, ***Stony Brook University, ****University College London, *****Stony Brook University

ABSTRACT

Introduction Transcatheter aortic valve replacement (TAVR) is a minimally invasive procedure which often represents the only lifesaving solution for patients with severe calcific aortic valve (AV). Despite its promising outcomes, adverse events such prosthesis migration and peri-procedural complications such as paravalvular leakage (PVL) have been reported. New lower-profile stents have shown to exert higher mechanical compression on the conduction fibers, thus leading to cardiac conduction abnormalities (CCAs) as a result of suboptimal placement. This work focuses on a patient-specific approach to study the effect of heart beating and the correspondent risk of CCAs following TAVR. Secondly, the effect of valve positioning and balloon inflation on stent anchorage and degree of post-procedural PVL are investigated. Methods Refined patient-specific models were reconstructed from pre-TAVR CT scans of patients suffering from PVL and CCAs after TAVR. AV leaflets were modeled with variable thickness and calcifications were embedded in the aortic root [1]. The crimping, the catheterization process and the deployment of the stent was modeled in Abaqus Explicit. Stent anchorage was quantified in terms of contact area and pressure. Transient diastolic flow analyses were conducted in Ansys Fluent and the degree of PVL was quantified as total regurgitant flow rate during diastole. The effect of the heart beating on TAVR valve performance was studied using Simulia Living Heart Human Model (LHHM). The LHHM AV motion was applied to CCAs patient-specific models to assess the strain distribution in the region of the atrio-ventricular node. These results were compared to healthy subjects to determine a mechanical threshold predictive of CCAs. Results Three PVL and three CCAs cases have been reconstructed and analyzed with three positions (aortic, midway, ventricular) and two expansions (nominal and over-expansion). PVL quantities showed agreement with correspondent patients' echocardiographic data. A self-expandable Evolut R and a balloon-expandable SAPIEN stents were deployed in the heart beating for three successive cycles, with ventricular deployments and over-expansions leading to higher logarithmic strains in the region in proximity of the left bundle branch, suggesting an increased risk of CCAs. Discussion Our study offers a comprehensive methodology to evaluate TAVR valves' performance using patient-specific reconstructed geometries and incorporating novel aspects such as the effect of cardiac motion on the procedure outcome. This would ultimately offer the possibility to develop predictive models to reduce the impact of post-procedural complications. Acknowledgements: Funding ? NIH (1U01HL131052, DB). References [1] Bianchi, M, et al., Artif Organs, 40:E292-E304, 2016.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Synchrotron measurement and simulation of the heterogeneous internal strain state evolution during in-situ heating in commercial purity titanium with two different crystallographic textures

Thomas Bieler*, Philip Eisenlohr**, Darren Pagan***, Armand Beaudoin****, Fionn Dunne*****, Benjamin Britton******, Zebang Zheng*******

*Michigan State University, **Michigan State University, ***Cornell High Energy Synchrotron Source, ****Cornell High Energy Synchrotron Source, *****Imperial College, ******Imperial College, *******Imperial College

ABSTRACT

Computational modeling of anisotropic materials such as titanium is commonly done with a starting assumption of a zero-stress state. However, most non-cubic materials have anisotropic coefficients of thermal expansion. A consequence of this is that upon cooling from a heat treatment temperature, crystals shrink at different rates with decreasing temperature, leading to buildup of elastic strains. In materials with a high yield strength, this can lead to elastic strains that are a significant fraction of the yield stress. To assess this effect, two samples of commercial purity titanium, one with near-random texture, and the other with a strong texture with a preferred c-axis orientation with about 8 x random, were heated in-situ in the CHESS beamline F-2 while collecting diffraction patterns. From averages of the <a> and <c> dimensions as a function of temperature, the expansion coefficients for the two alloys showed a similar cross over where the c-axis expansion exceeded a-axis expansion between 700 and 800°C, but the slopes were slightly different. Analysis of internal strain data indicate that some grains have internal stresses as large as 150 MPa at room temperature. The neighborhood of near-zero stress grains was compared with highly stressed grains, revealing different relationships between averages of grain neighbor misorientation vs. distance from each grain in the near-random and textured samples. Anisotropic crystal elastic and plastic simulations of the experiments using the measured microstructures (grain morphology and crystallographic orientations) and thermal history, with the experimentally characterized initial stresses, anisotropic thermal expansion, and temperature dependent elastic moduli have been carried out to compare with measurements to assist interpretation of the experiment and to assess the credibility of the microstructural models.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

On the Form-Finding Problem of a New Class of Tensegrity Metamaterials

Zbigniew Bieniek*, Ida Mascolo**, Ada Amendola***, Gianmario Benzoni****, Fernando Fraternali*****, Mariella De Piano******, Francesco Fabbrocino*******

*Rzeszów University of Technology, Poland, **University of Salerno, Italy, ***University of Salerno, Italy, ****University of California, USA, *****University of Salerno, Italy, ******University of Salerno, Italy, *******Pegaso University, Italy

ABSTRACT

Keywords: Metamaterials, tensegrity, soft modes The category of “extremal materials” has been introduced to define materials that simultaneously show very soft and very stiff deformation modes [1], and are called unimode, bimode, trimode, quadramode and pentamode materials, depending on the number of soft modes. Extremal materials that are receiving increasing interest are the so-called pentamode lattices, which consist of diamond-like lattices featuring five soft modes of deformation. The unit cell forming the this lattice is made of four rods meeting at a point. Previous studies show that pentamode lattices confined between stiffening plates have the ability to carry unidirectional compressive loads with sufficiently high stiffness, while behaving very soft in shear [2]. Because of their unusual mechanical features, these structures have been proposed for transformation acoustics, elasto-mechanical cloak, and seismic isolation (refer, e.g., to [2]-[3] and the references therein). This study examines the mechanical behavior of a novel class of mechanical metamaterials alternating class ? tensegritry structures [4] and stiffening plates. Analytical formulae for the vertical and bending stiffness properties are developed, and the dependence of such quantities on the main design parameters, which include the lattice constant, the solid volume fraction, the cross-section area of the rods, and the layer thickness, is studied. The potential use of the analyzed metamaterials as novel seismic-isolation devices and impact-protection equipment is highlighted. References [1] Milton, G.W., Cherkaev, A.V., “Which elasticity tensors are realizable?”, Journal of Engineering Materials and Technology, 117(4), 483-493 (1995). [2] Fraternali, F., Amendola, A., “Mechanical modeling of innovative metamaterials alternating pentamode lattices and confinement plates”, Journal of the Mechanics and Physics of Solids, 99, 259-271 (2017). [3] Bückmann, T., Thiel, M., Kadic, M., Schittny, R., Wegener, M., “An elastomechanical unfeelability cloak made of pentamode metamaterials”. Nature Communications 5:4130 (2014). [4] Bieniek, Z.W., “The self-equilibrium configurations for the class ? triangular tensegrity prism”, Proc. XXIII Aimeta Congress, 1093-1097 (2017).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

High-dynamic Strengthening of Cementitious Materials: Structural Effect and Influence of Concrete Hardening

Eva Binder*, Yong Yuan**, Herbert Mang***, Bernhard Pichler****

*TU Wien - Vienna University of Technology; Tongji University, **Tongji University, ***TU Wien - Vienna University of Technology; Tongji University, ****TU Wien - Vienna University of Technology

ABSTRACT

During the service of infrastructural facilities, spanning typically over 100 years, exceptional load cases such as explosions and traffic accidents need to be considered. Both load cases result in high-dynamic loading of the structure, herein assumed to be made out of concrete. In this contribution the focus is split. In the first part, strengthening of cementitious materials under high-dynamic loading is quantified by means of the dynamic increase factor (DIF). In the second part, the influence of hardening of concrete on the dynamic strength and the DIF is investigated. The present contribution follows the approach of Fischer et al. [1], who developed a model for the dynamic increase factor, based on the loading rate, the quasi-static strength, the Young's modulus, the shear modulus, and the crack length, which is related to the specimen size. In the first part, the model predictions are compared with experiments by Zhang et al. [2] on mortar cylinders with two different heights. In the second part, the same model for the DIF is combined with a validated multiscale model for cementitious materials to determine the influence of the hardening process on the dynamic behavior. In this context, the concrete used for the immersed tunnel of the Hong Kong-Zhuhai-Macao-Bridge is analysed, and a high-dynamic compression test is simulated, see [3]. As regards the first part, it is concluded, that strengthening of cementitious materials includes a structural effect. Concerning the second part, the results imply, that the dynamic strength of concrete increases and that the DIF decreases with progressive hardening of concrete. Acknowledgment The authors are indebted to the Austrian Science Fund for their financial support in the frame- work of the FWF-project "Bridging the Gap by Means of Multiscale Structural Analyses" (project number: P 281 31-N32). References [1] I. Fischer, B. Pichler, E. Lach, C. Terner, E. Barraud and F. Britz, Compressive strength of cement paste as a function of loading rate: Experiments and engineering mechanics analysis, Cement and Concrete Research 58 (2014) 186-200. [2] M. Zhang, H. Wu, Q. Li and H. Huang, Further investigation on the dynamic compressive strength enhancement of concrete-like materials based on split Hopkinson pressure bar tests. Part I: Experiments, International Journal of Impact Engineering 36 (2009) 1327-1334. [3] H. Wang, E. Binder, H. Mang, Y. Yuan and B. Pichler Multiscale structural analysis inspired by exceptional load cases concerning the immersed tunnel of the Hong Kong-Zhuhai-Macao Bridge, submitted to Underground Space.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Mixed Discrete-Continuum Approach for Modelling the Fracture Behaviour of Soft Collagenous Tissues

Kevin Bircher*, Alexander Edmund Ehret**, Edoardo Mazza***

*Department of Mechanical and Process Engineering, ETH Zurich, Switzerland, **Department of Mechanical and Process Engineering, ETH Zurich, Switzerland; Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland, ***Department of Mechanical and Process Engineering, ETH Zurich, Switzerland; Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland

ABSTRACT

While the deformation behaviour of soft collagenous tissues, such as the fetal membranes (FM) and the liver capsule (LC), has been investigated intensively, the mechanisms underlying their fracture are still poorly understood, despite their importance for events of tissue failure and damage. In particular, investigations regarding the defect tolerance of fetal membranes would provide valuable input for therapies to prevent their premature rupture. Based on our characterization of the multiscale deformation behaviour of collagenous membranes, we introduced a numerical tool that is capable of efficiently performing fracture-related simulations by combining a discrete fiber network model in the near-field of a crack with a continuum representation of the far field. This tool was applied to investigate the crack propagation in soft collagenous tissues for strip biaxial fracture tests and compared to corresponding experiments of bovine LC, human FM and soft elastomers (PDMS). The near field of a defect in LC and FM was also visualized with a multiphoton microscope (MPM) in order to characterize the compaction behaviour and the reorientation of fibers. With the discrete fiber network model, a fibre-level failure criterion was implemented which dictates material failure. This allowed avoiding the stress singularity present in the crack near field of a continuum model. Systematic parameter variation indicated the influence of fiber deformation and failure behaviour on tissue rupture properties. Simulations and corresponding MPM observations showed that the crack near field size is in the sub-milimeter range and therefore much shorter than for elastomers such as PDMS. Interestingly, our simulations for soft collagenous tissues show that large sample-sizes are required for the determination of the tearing energy. Thus, conventional fracture mechanical approaches are not applicable for defects of few milimeters in the tissues as typically occurring in clinically and physiologically relevant cases.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Partitioned Adaptive Parallel Multirate Methods for Coupled Stiff Systems

Philipp Birken*, Peter Meisrimel**, Azahar Monge***

*Lund University, **Lund University, ***Lund University

ABSTRACT

The efficient numerical simulation of stiff multiphysics systems remains a core challenge in scientific computing. Examples are fluid structure interaction, earth system models or turbulent flames. We consider problems with the following characteristics: They are large scale, all components are stiff, possibly on different time scales and there are codes for the subproblems available. Thus, we want a partitioned numerical method, meaning that reuse of the existing codes is possible. Thereby, we assume that while we have access to the source codes, we want to edit that code as little as possible. In particular we assume that we can repeat a time step. We are then looking for numerical methods that are implicit and at least order two, time adaptive, allow the subsolvers to run in parallel and allow for different time steps in the different models. We are not aware of a method that fulfills all of these properties and suggest two methods of our own for the case of two systems being coupled. The core idea is the following: We have a time integration method of at least order two for each subproblem and assume that we can restart these with new initial data and that during time integration, information for the other solver at all times can be provided using interpolation. This continuous representation of the numerical solution is updated after each local time step. Then the solvers run in parallel over a macro time window and are free to choose their own timesteps in an adaptive way without outside interference. At the end of the macrostep, it is checked if the coupled system is fulfilled up to a tolerance, if not, the time window is repeated. Crucial questions are order of the time integration method and convergence of the time window iteration, also called waveform relaxation. This is shown numerically for representative test cases. For the specific case of two linear heat equations with different material properties coupled across an interface, we suggest to do the waveform relaxation in the form of a Neumann-Neumann coupling, known from domain decomposition. There, the choice of the relaxation parameter is crucial and previous analysis by Gander and Kwok for the semidiscrete case does not apply. We thus perform a fully discrete analysis for the case of fixed but different time steps for the subproblems. Numerical results show that this can be used for the time adaptive case as well.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

3D Mapping of the Osteocyte Lacunae Network with the Adaptive Bone (Re)modeling Dynamics

Annette Birkhold*, Pouyan Asgharzadeh**, Lydia Farack***, Sara Checa****, Oliver Röhrle*****, Paul Zaslansky******, Bettina Willie*******

*Charité - Universitätsmedizin Berlin, Germany; University of Stuttgart, Germany, **University of Stuttgart, Germany, ***Charité - Universitätsmedizin Berlin, Germany, ****Charité - Universitätsmedizin Berlin, Germany, *****University of Stuttgart, Germany, ******Charité - Universitätsmedizin Berlin, Germany, *******Charité - Universitätsmedizin Berlin, Germany; McGill University, Canada

ABSTRACT

Bone is a highly adaptive biomaterial that optimizes its microstructure depending on the mechanical loads placed on it. The exact mechanisms by which a network of interconnected mechanical strain-sensing cells, embedded in the bone matrix, termed osteocytes, orchestrate bone turnover and mineral homeostasis remains largely unknown. Here, we present a multimodal preclinical tomographic imaging approach to correlate the 3D osteocyte lacunar network with bone formation and resorption dynamics in a mouse tibia after in vivo mechanical loading. Using a mouse model we analyze bone (re)modeling occurring over a short period of time. Female C57Bl/6J mice were subjected to of in vivo cyclic compressive loading of the left tibia (2 weeks, approx. 5 min/day; F_max=11N; 1200 µ? at the medial surface of the tibia midshaft) with the right tibia as internal control (1). Dynamic in vivo µCT-based time-lapsed microcomputed tomography (day 0 – day 15; isotropic voxel size 10.5 µm) was used to monitor bone micro-architecture response to load. In vivo images were registered and segmented to extract formation patches and resorption cavity geometries (2). High-resolution 3D Synchrotron-µCT imaging was performed on the same bones (isotropic voxel size 876 nm). SR-µCT images were registered with in vivo images and locally segmented to extract osteocyte lacunae geometries. 3D individual osteocyte lacunar descriptors and and global osteocyte lacunar network descriptors were extracted. A correlation of the 3D osteocyte cellular level network topology with the dynamic bone surface (re)modeling processes at the tissue level was performed. Our data reveals that the 1) osteocyte lacunae network changes as the tissue ages (formation ? mineralization ? maturation) and during resorption. 2) The osteocyte lacunae network influences the probability of formation and resorption processes occurring. 3) Adaptive processes, such as an earlier alignment of new osteocyte lacunae in response to loading, were identified. Our 3D-correlation imaging approach will enhance our understanding of regulation of bone remodeling and homeostasis following physiological development, pathological conditions, or pharmaceutical intervention. 1. Willie et al. Diminished response to in vivo mechanical loading in trabecular and not cortical bone in adulthood of female C57Bl/6 mice coincides with a reduction in deformation to load. Bone 55, 335–346 (2013). 2. Birkhold et al. Mineralizing surface is the main target of mechanical stimulation independent of age: 3D dynamic in vivo morphometry. Bone 66, 15–25 (2014).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Direct Volumetric Manufacturing of Composites via Addressable Joule Heating

Andrew Birnbaum*, Athanasios Iliopoulos**, John Steuben***, John Michopoulos****

*US Naval Research Laboratory, **US Naval Research Laboratory, ***US Naval Research Laboratory, ****US Naval Research Laboratory

ABSTRACT

Despite increasing levels of acceptance in a number of niche areas, traditional additive manufacturing (AM) techniques continue to suffer from a number of fundamental drawbacks that act to limit their broad adoption. There exist a wide variety of AM methods and technologies that can be classified according to various criteria, including energy source type (e.g. laser beam, electron beam, UV lamp, etc.) power requirements and material systems. Each of these methods also tend to have added requirements such as inert atmospheres, high vacuum processing and powder handling, that represent a significant overhead and inhibit cost reduction. Furthermore, the vast majority of additive manufacturing methods rely on an ultra-serialized approach for building parts. Often described as "layer-by-layer," in reality, these are hierarchically serial, point-by-point, path-by-path and layer-by-layer approaches. The multi-scale stratification of mass and accompanying complex thermal histories introduced by such hierarchical processes give rise to a series of deleterious consequences in terms of scaling behavior/build times, structural anisotropy, microstructural defects, mesoscopic deficiencies and macroscopic geometric deviations. This work proposes a new methodology that addresses many of these drawbacks by implementing a truly volumetric approach to additive manufacturing. That is, instead of building parts a single point at a time in a hierarchical manner, by spatially controlling the energy distribution within a three-dimensional build domain, one can build composite parts from large constituent volumes, in parallel, by addressable, resistive heating. The presented work consists of a theoretical treatment of the underlying physics, a computational approach to discretization into geometrical sub-domains, process planning via the solution of an inverse problem for implementing the proper control, and, finally, the demonstration of a preliminary prototype along with our plans for the future.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Simplified Fatigue Procedure for Analyzing the Postbuckling Behavior of a Composite Single-Stringer Specimen

Chiara Bisagni*

*Delft University of Technology

ABSTRACT

Fatigue life of postbuckled composite stiffened panels is a complex issue which remains difficult to predict due to the interaction of several damage modes and geometric nonlinearities. Composite stiffened panels are particularly used in the aerospace industry, and are capable to sustain loads that far exceed their buckling load. The skin-stringer separation is one of the most common types of damage in composite stiffened structures, and can initiate and propagate under both static and fatigue loading. Therefore, the ability to assess the fatigue mechanisms is essential for the design of aerospace structures that satisfy damage tolerance and lifetime requirements. A composite single-stringer specimen is here analyzed, as it exhibits most of the challenges that characterize the analysis of a multi-stringer panel and at the same time reduce the computational effort. The fatigue capabilities of the new Abaqus procedures are investigated to predict the life and collapse of the composite single-stringer specimen in the postbuckling field, that is highly dependent on the nonlinear mode of deformation. In particular, a simplified fatigue procedure is used [1]. It solves linear elastic fatigue crack growth problems considering a load or displacement envelope strategy instead of a cycle-by-cycle based approach. It means that the applied numerical load remains constant at the maximum value of the cyclic load and interface elements are degraded based on a discrete number of elapsed cycles after each time increment. Avoiding the need to explicitly model each individual fatigue cycle provides greater computational efficiency. The simplified fatigue procedure demonstrated to account for geometric nonlinearities and for stiffness change after buckling, and to capture the separation onset and some stages of the propagation. The numerical results are compared with test data obtained by the author in previous experimental campaigns [2-3]. Future investigation of the fatigue algorithm will consider stress ratio effects, and various mixed-mode fatigue delamination growth laws so to be able to consider changes in mixed-mode ratio during the analysis. 1. Di Memmo I. and Bisagni C., “Fatigue Simulation for Damage Propagation in Composite Structures”, Proceedings American Society of Composites Conference, pages 1009-1019, 2017. 2. Dávila C.G. and Bisagni C., “Fatigue Life and Damage Tolerance of Postbuckled Composite Stiffened Structures with Initial Delamination”, Composite Structures, 161:73-84, 2017. 3. Dávila C.G. and Bisagni C., “Fatigue Life and Damage Tolerance of Postbuckled Composite Stiffened Structures with Indentation Damage”, Journal of Composite Materials, https://doi.org/10.1177/0021998317715785, 2017.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Brainware for Sciences – A Distributed HPC Competence Centre to Link Experts, Users and Computing Centres

Christian Bischof*, Dörte Carla Sternel**

*TU Darmstadt, **TU Darmstadt

ABSTRACT

The efficient use of HPC systems requires users in most instances scientist to be aware of both architecture, underlying system software and operating procedures such as scheduling. While this complexity can be masked in certain cases for well-established workflows around well-maintained community software, a university setting with its variety of application scenarios for the most part falls outside of this carefree domain. Instead, in order to make good use of expensive HPC resources, scientists using HPC resources need to be made aware of issues such as efficient programming or scheduling, and be cogniscent of the strength and weaknesses of certain computing architectures. Most scientists, however, are mainly interested (and trained) in getting their science done, and not so much in the more computer sciency issues mentioned before. To close this gap, the term brainware was coined to denote HPC experts that can fill this gap, and support users with their scientific codes, both hands-on and by educating them. In the German state of Hesse, such a brainware center was established with funding from the Hessian State Ministry of Higher Education, Research and the Arts. Altogether, seven scientists are funded at the five universities in Darmstadt, Frankfurt, Gießen, Kassel, and Marburg, as well as a managing director. Together, these "brainware" people are a place that every scientist with questions pertaining to the HPC systems at those sites can turn to. They are catalysts for a focussed collaboration of application scientists, computer scientists and computing centres towards an efficient use of the Hessian HPC landscape and, ultimately, for accelerating the scientific outcomes depending on simulation. The Hessian Competence Center for High Performance Computing has been in operation since 2013, and is now in its second round of funding. On the basis of this experience, we will report on the activities of the centre, the feedback we obtained from users on the topics of interest, and the social engineering challenges faced in such a distributed competence network. The results underscore the pivotal role that good software engineering practices play in HPC software stewardship, i.e. the "taking care" of program over time.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Influence of the Microstructure on the Deformation Behaviour of cp-titanium with Large Grains

Robert Bischof*, Luisa Böhme**, Charlotte Kuhn***, Ralf Müller****, Eberhard Kerscher*****

*Institute of Applied Mechanics, University of Kaiserslautern, **Materials Testing, University of Kaiserslautern, ***Institute of Applied Mechanics, University of Kaiserslautern, ****Institute of Applied Mechanics, University of Kaiserslautern, *****Materials Testing, University of Kaiserslautern

ABSTRACT

Manufacturing processes on small scales are of high importance. Simulation techniques, such as the Finite-Element-Method (FEM), are important tools to predict the workpiece behaviour in manufacturing processes. In mirco-cutting the machining tool is about the same scale as the grains of the crystalline workpiece. Thus the crystal structure has to be considered in the FEM material model. The material to be examined is commercially pure (cp-) titanium with a hexagonal-closed-packed (hcp) crystal structure. The influence of the crystalline material is modeled by a crystal plastic material model. It considers the reversible elastic behaviour through a compressible Neo-Hookean material law. The anisotropic plastic deformation is considered by specifiying the slip planes and slip direction of the hcp crystal structure. One problem of elasto-plastic material models with several slip systems is the possible non-uniqueness of the set of active slip systems. To avoid this problem, a viscoplastic material formulation is used. The viscoplastic parameters are chosen such that the viscoplastic material behaviour approximates the elasto-plastic limit. Locking effects, which arise due to the volume preserving plastic deformations, are alleviated by a modified F-bar deformation gradient [1]. The results of the FEM simulations are compared with experimental data for further development and validation of the material model. Small scale tensile tests of cp-titanium are performed to investigate the material behaviour. The dimension of the specimen are small enough that the crystal structure has an influence on the material behaviour, but large enough that the material can be considered as polycrystal. The grain orientation of the specific sample is provided by electron backscatter diffraction (EBSD) investigations. The influence of the grain orientation on the micro-cutting process is shown. [1] de Souza Neto, E. A.; Peric, D.; Owen, D. R. J.: Computational Methods for Plasticity: Theory and Applications. New York: John Wiley & Sons, 2011.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Variational Method to Avoid Locking – Independent of the Discretization Scheme

Manfred Bischoff*, Simon Bieber**, Bastian Oesterle***, Ekkehard Ramm****

*University of Stuttgart, **University of Stuttgart, ***University of Stuttgart, ****University of Stuttgart

ABSTRACT

We present a variational method for problems in solid and structural mechanics that is designed to be intrinsically free from locking when using equal order interpolation for all involved fields [1]. The method is inspired by the DSG (Discrete Strain Gap) method [2] and can be interpreted as its variational counterpart. As it involves displacement degrees of freedom as well as additional degrees of freedom obtained from integrated strains, which mostly have the physical units of displacements as well, it is denoted as Mixed Displacement (MD) method. The specific feature of the formulation is that it avoids all geometrical locking effects (i.e. locking effects related to geometric parameters, like the slenderness, as opposed to material locking effects, e.g. Poisson locking) for any type of structural or solid model, independent of the underlying discretization scheme. In the context of thin-walled structures, the most important geometric locking phenomena are transverse shear locking and membrane locking. While the former can elegantly be circumvented via hierarchic shell models [3], a similar approach to remove membrane locking has not yet been found. The possibility to employ equal order interpolation for all involved fields circumvents the task of finding particular function spaces to remove locking and avoid artificial stress oscillations. This is particularly attractive for instance for isogeometric analysis using unstructured meshes or T-splines. Comprehensive numerical tests underline the promising behavior of the proposed method for geometrically linear and non-linear problems in terms of displacements and stress resultants using standard finite elements, isogeometric finite elements and a meshless method. The method can also be applied in the context of collocation.
[1] S. Bieber, B. Oesterle, E. Ramm, M. Bischoff. A variational method to avoid locking – independent of the discretization scheme, International Journal for Numerical Methods in Engineering, accepted for publication. [2] K.-U. Bletzinger, M. Bischoff, E. Ramm, A unified approach for shear-locking-free triangular and rectangular shell finite elements, Computers and Structures, 2000; 75(3); 321-334. [3] B. Oesterle, Ramm E. and Bischoff M., A shear deformable, rotation-free isogeometric shell formulation, Computer Methods in Applied Mechanics and Engineering, 2016; 307; 235-255.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Modeling Electroactive Polymers and Electromechanical Instability

Dana Bishara*, Mahmood Jabareen**

*Technion – Israel Institute of Technology, **Technion – Israel Institute of Technology

ABSTRACT

Electroactive polymers (EAPs) are an emerging class of smart materials, which has gained a wide popularity among researchers in the last two decades. EAPs are considered promising materials due to their ability to undergo large deformations when they are subjected to external electric stimuli. Therefore, various applications have been proposed in the literature including artificial muscles, medical devices and soft robotic applications. A typical EAP based actuator consists of a thin film of dielectric elastomer, which on its major surfaces, two flexible electrodes are smeared, and an electric potential difference between the electrodes is applied. The mode of action is principally based on Coulomb forces generated by the electric field, which causes the polymer membrane to exhibit geometrical changes, i.e., contraction in the thickness direction and expansion of the surfaces. Despite the high-level of actuation performances enabled by EAPs, their extensive use is conditioned by the requirement of high driving electric fields. As a result, the applied electric field may cause an electromechanical instability or electric breakdown. Unlike gases or liquids, as the electric breakdown in solid dielectrics takes place, tubular conductive channels evolve, and they do not recover when the voltage is discharged. In this work, a computational model including the electromechanical coupling and the large deformation combined with time dependent behavior of EAPs is developed. This model has been calibrated to provide a quantitative tool for predicting the realistic behavior of the widely used dielectric elastomer VHB. Moreover, the electromechanical instability has been studied within the proposed model using a general convexity condition, from which the Hessian matrix must be positive definite at the equilibrium state.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Review of Boundary and Interface Representations in Meshfree Solid Mechanics for Extreme-deformation Applications

Joseph Bishop*, Mike Tupek**

*Sandia National Laboratories, **Sandia National Laboratories

ABSTRACT

Meshfree methods for solid mechanics have been in development for over 25 years. Initial motivations included alleviation of the burden of mesh creation and the desire to overcome the limitations of traditional mesh-based discretizations in extreme deformation applications. One challenge for meshfree methods is maintaining an accurate representation of the domain boundary and internal interfaces during extreme deformation. Without an accurate boundary representation, it becomes difficult to implement a self-contact algorithm that avoids pathological material welding. Furthermore, it becomes challenging to update the connectivity of the meshfree discretization (semi-Lagrangian) in highly non-convex domains. Here, a review of boundary and interface representations in meshfree methods is presented. The various techniques are critically compared for several applications in extreme mechanics.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Non-Isothermal Thermodynamically Consistent Phase Field Framework for Structural Damage and Fatigue in Plasticity

Marco Bittencourt*, Geovane Haveroth**, José Boldrini***

*University of Campinas, **University of Campinas, ***University of Campinas

ABSTRACT

We present a general thermodynamically consistent non-isothermal non-local phase field framework for the evolution of damage, fatigue and fracture in plasticity under the hypothesis of small deformation. The damage phase field is considered a continuous dynamical variable whose evolution equation is obtained by the Principle of Virtual Power. The fatigue phase field is a continuous internal variable whose evolution equation is considered as a constitutive relation to be determined in a thermodynamically consistent way. In this work, we use high order finite elements for approximation and a semi-implicit scheme to perform the time integration of the equations, which allows us to decouple the variables and use larger time steps. We compare different degradation functions for the damage variable.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Influence of Deformation Induced Topological Anisotropy on Mechanical Properties of Silica Glass: An Atomistic Study

Erik Bitzek*, Sudheer Ganisetti**

*FAU Erlangen-Nürnberg, **FAU Erlangen-Nürnberg

ABSTRACT

Glasses are generally believed to be isotropic materials. However, it is well known that anisotropy can be introduced in silica glass, e.g., by wire drawing, and that the mechanical properties are subsequently anisotropic. Since topology plays an important role for the mechanical properties, it is necessary to understand the physics behind the development of topological anisotropy on the atomic scale. Here we present the results of atomistic simulations using an ab-initio based polarisable force field. Isotropic silica glass was prepared by the melt quenching method. Anisotropy was introduced at different temperatures by either elongating, compressing or shearing the glass at different rates. During load, transient anisotropy is observed, as characterized by the anisotropy factor. Significant persistent anisotropy, which remains after load removal, could only be introduced by compression and shear. The conditions favourable to the formation of persistent anisotropy, the underlying mechanisms and the relationship between transient and persistent anisotropy are analysed in detail. Samples with persistent topological anisotropy also show a pronounced anisotropy in the mechanical properties, in particular on the elastic constants and fracture strain. The results are compared to simulations on bulk metallic glasses and discussed in the framework of mesoscale and continuum models for the deformation of amorphous materials.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Homogenisation-based Modelling of Skeletal Muscle Tissue across the Scales

Christian Bleiler*, Pedro Ponte Castañeda**, Oliver Röhrle***

*University of Stuttgart, **University of Pennsylvania, ***University of Stuttgart

ABSTRACT

Like for many biological materials, the elastic properties of skeletal muscle tissue can vary quite significantly between different persons or between different muscle types of one single person. It is well known that these distinct mechanical properties are due to variations in the microstructure of the material. For skeletal muscles, especially the arrangement and the stiffness of collagen fibres in the connective tissue define the macroscopic passive stiffness, while the sarcomeres (contractile units) enable an active contractility of the muscles. Moreover, the microstructural arrangement not only influences the stiffness, but also the anisotropy of the material at the macroscale. Continuum-mechanical muscle models based on phenomenological approaches are easy to implement, but lack the ability to take microstructural properties into account in a natural way. Hence, experimental data for every desired muscle type to be modeled is required, but usually not available. To overcome this issue, we propose a novel, homogenisation-based material model, which predicts the mechanical behaviour of muscle tissue by incorporating the decisive parts of the underlying microstructure, here, (i) the connective tissue and (ii) the muscle fibres. Furthermore, instead of computationally expensive numerical homogenisation methods, like FE2, we proceed from well-founded analytical methods [1] in order to get the effective material response on the macroscale. The description of the collagenoeus tissue is based on angular integration models [3]. Therefore, the direction-dependent properties of the macroscopic tissue are direct consequences of the arrangement and the mechanical properties of the micro-constituents, especially of the collagen fibres. The present model is able to predict the specific anisotropy (transverse isotropy) of muscle tissue as observed in experiments [2] simply by including the arrangement of the microstrcture without the need of further constitutive assumptions as it would be the case for standard phenomenological models. Concluding, this study presents a novel, hyperelastic muscle model, which includes microstructural data in order to obtain the effective response of the overall muscle tissue by using analytical homogenisation methods. [1] Avazmohammadi R., Ponte Castañeda P.: Tangent Second-Order Estimates for the Large-Strain, Macroscopic Response of Particle-Reinforced Elastomers. J Elasticity 112:139-183, 2013. [2] Böl M., Ehret A. E., Leichsenring K., Weichert C., Kruse R.: On the anisotropy of skeletal muscle tissue under compression. Acta Biomater 10:3225-3234, 2014. [3] Lanir Y.: Constitutive equations for fibrous connective tissues. J Biomech 16:1-12, 1983.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Phase-field Modeling of Anisotropic Brittle Fracture in Fiber-reinforced Composites

Jeremy Bleyer*, Roberto Alessi**

*Ecole des Ponts ParisTech, Laboratoire Navier, Université Paris-Est, **SAPIENZA, University of Rome

ABSTRACT

The phase-field approach to fracture is an effective method to describe and simulate complex fracture phenomena and is therefore gaining increasing attention by the computational mechanics community. Many extensions have already been considered ranging from dynamic aspects, plasticity, fluid transport in porous media, finite deformation, etc. However, few works have dealt with anisotropic effects. In particular, these works have considered only an anisotropic fracture energy with an underlying isotropic elastic material. As a result, no work has extended yet the phase-field approach to consider fracture in anisotropic media, in particular fiber-reinforced composites. The present contribution aims at closing this gap by proposing a phase-field approach for brittle fracture in an anisotropic material. In particular, it is shown that standard models including one phase-field variable and possibly an anisotropic fracture energy are not well suited to describe complex crack paths in such materials. Instead, we propose to endow the phase-field energy functional with multiple damage mechanisms, e.g. longitudinal fiber cracking and transverse matrix cracking in the case of fiber-reinforced composites. Although, numerical examples focus on this situation, the proposed framework is sufficiently general to be also applied to all situations where different fracture mechanisms are involved within the same material such as different failure mechanism in tension and compression, fracture anisotropy depending on mode mixity, cracking of composite laminates, etc. Illustrative applications demonstrate that the proposed model is able to capture well known features of crack propagation in fiber-reinforced media such as propagation in the fiber preferential direction, straight propagation under mode II loading but also non trivial behaviors such as crack kinking, whereas a standard phase-field model, even if equipped with an anisotropic fracture energy, is not. Although our work does not focus on an exhaustive description of the complex constitutive behavior of fiber-reinforced composites, we hope that it will contribute to a decisive advance in the development of the phase-field approach for this extremely important class of materials.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Peridynamic Modeling of Corrosion Damage and Fracture

Florin Bobaru*, Siavash Jafarzadeh**, Jiangming Zhao***

*University of Nebraska-Lincoln, **University of Nebraska-Lincoln, ***University of Nebraska-Lincoln

ABSTRACT

We present a peridynamic model for corrosion damage and stress-dependent fracture. We find that corrosion changes the material properties in a layer near the corrosion front [3]. The peridynamic model introduced here [1] captures the growth of corrosion pits [2] and verifies the measured properties of the embrittled layer. The corrosion process is autonomous in a peridynamic model, freeing the model from geometrical restrictions that would otherwise be present. Examples will also be shown from numerical tests spanning intergranular corrosion to uniform corrosion. The numerical examples are compared with experimental results and we observe a good match between the two. We also discuss future steps to be taken in peridynamic modeling of corrosion processes. References [1] S. Li, Z. Chen, L. Tan, F. Bobaru, “Corrosion-induced embrittlement in ZK60A Mg alloy”, Materials Science & Engineering A, 713: 7-17 (2018) https://doi.org/10.1016/j.msea.2017.12.053 [2] S. Jafarzadeh, Z. Chen, F. Bobaru, “Peridynamic modeling of repassivation in pitting corrosion of stainless steel”, Corrosion (2017). https://doi.org/10.5006/2615 [3] Shumin Li, Ziguang Chen, Fei Wang, Bai Cui, Li Tan, and F. Bobaru, “Analysis of Corrosion-Induced Diffusion Layer in ZK60A Magnesium Alloy”, Journal of The Electrochemical Society, 163(13): C784-C790 (2016). doi: 10.1016/j.cma.2016.08.012

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Optimization-based, Property Preserving Finite Element Methods

Pavel Bochev*, Marta D'Elia**, Denis Ridzal***, Mauro Perego****

*Sandia National Laboratories, **Sandia National Laboratories, ***Sandia National Laboratories, ****Sandia National Laboratories

ABSTRACT

We present an optimization-based approach for the accurate, property preserving finite element solution of Partial Differential Equations (PDEs) in which the solution is obtained by solving a suitably defined constrained optimization problem. The objective is to minimize the distance to a given finite element target, computed by a formally accurate but not necessarily property preserving scheme, while physical properties such as maximum principle and/or preservation of local solution bounds define the constraints. This divide-and-conquer strategy separates solution accuracy from the preservation of the relevant physical properties and always finds a globally optimal, with respect to the given target, solution that also satisfies these properties. To illustrate the approach we consider the finite element solution of a model scalar advection-diffusion equation and present some preliminary numerical studies. The talk will also examine connections between the optimization-based property preserving solution of PDEs and algebraic flux correction techniques for the preservation of local solution bounds. This material is based upon work supported by the U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research. D. Ridzal also acknowledges funding by the Advanced Simulation & Computing (ASC) Program.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Optimal Design of Bio-inspired Multi-material Soft Robots

Narasimha Boddeti*, Oliver Weeger**, Pablo Valdivia y Alvarado***, Martin Dunn****

*Singapore University of Technology and Design, **Singapore University of Technology and Design, ***Singapore University of Technology and Design, ****Singapore University of Technology and Design

ABSTRACT

Animals make use of biological structures with tailored distribution of materials with different properties to achieve a variety of desired functions such as fins for swimming and wings for flying. Recent advances in robotics have recognized this and moved towards realizing designs for robots with soft materials that mimic biology to achieve improved performance and versatile functionality under disparate operating conditions. Advances in additive manufacturing technologies have also aided in this by allowing arbitrary yet precise placement of desired materials in a component. Even as bio-inspired designs offer considerable performance gains over traditional robots, they are not necessarily the most optimal designs for engineering applications as biological designs are a result of evolutionary pressures and constraints while engineering applications are devoid of such constraints. With that in mind, our goal here is to develop a topology optimization based framework for design of bio-inspired structures with optimal distribution of materials (either isotropic or anisotropic) to realize desired performance criterion such as target deformation, minimum compliance and optimal power consumption while accounting for constraints imposed by the fabrication approach. We will exercise the abilities of our framework in the context of design and fabrication of an under-actuated batoid-like soft robot fabricated via multi-material 3D printing. Batoids (e.g. stingrays, manta rays) are a group of fish species that are flat bodied with enlarged pectoral fins. They make an ideal basis for autonomous underwater robotics due to their simple body kinematics with excellent maneuverability and efficient operation. We will seek optimal batoid-like designs tailored for different 3D printing techniques (viz. voxel based material jetting and embedded 3D printing) with single or multiple objectives including target dynamic deformation behavior and placement of the actuator.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Modeling Coulomb Interactions in Ionic Solids for Atomistic-to-Continuum Methods

Vishal Boddu*, Denis Davydov**, Bernhard Eidel***, Paul Steinmann****

*University of Erlangen-Nuremberg, **University of Erlangen-Nuremberg, ***University of Siegen, ****University of Erlangen-Nuremberg

ABSTRACT

Existing atomistic-to-continuum multiscale methods, such as the quasicontinuum method, are applicable exclusively in cases where the atomic interactions are short-ranged. This restriction on the nature of atomic-level interactions for the multiscale methods exclude an extremely large class of materials, essentially--all dielectrics, polarizable solids and ionic solids, that are central to numerous scientifi c and industrial applications. So far there has been only one approach, to the best of our knowledge, that enables the applicability of atomistic-to-continuum methods for ionic crystals. The method involves coarse-graining of the long-range Coulomb interactions in ionic crystals [1]. In doing so, the ionic charges are expressed in terms of a charge density fi eld defi ned on two different length scales, namely the length scale of atomic unit cell and the characteristic continuum length scale. However, this approach assumes complete separation of scales and for a fi nite atomistic system this is naturally not true. Furthermore, realizing adaptive refi nement and seamless coarse-graining using this approach is not trivial. Unphysical artifacts of the direct cutoff based truncated sum to evaluate Coulomb interactions in ionic solids have been pointed out in a number of studies. However, recently it is understood that the artifacts of the direct cutoff based truncated sum can be signifi cantly minimized if a suitable correction term is added [2]. In this work we examine whether or not such cutoff-based methods are suitable to carry out the accumulation of the Coulomb interactions within the context of atomistic-to-continuum multiscale methods. In this regard, we choose the quasicontinuum method from the existing collection of the multiscale methods for demonstration. References: [1] Marshall, J. and Dayal, K., 2014. Journal of the Mechanics and Physics of Solids 62, 137-162. [2] Fukuda, I. and Nakamura, H., 2012. Biophysical reviews, 4.3, 161-170.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Modeling Transient Aircraft Engine Operation

Christoph Bode*, Jens Friedrichs**, Andreas Kellersmann***, Florian Herbst****, Joerg Seume*****

*Institute of Jet Propulsion and Turbomachinery TU Braunschweig, **Institute of Jet Propulsion and Turbomachinery TU Braunschweig, ***Institute of Jet Propulsion and Turbomachinery TU Braunschweig, ****Institute of Turbomachinery and Fluid Dynamics Leibniz University Hannover, *****Institute of Turbomachinery and Fluid Dynamics Leibniz University Hannover

ABSTRACT

Due to the multidisciplinary design approach of large-scale and high complex capital goods there exist several different forms of operational behavior and deterioational effects depended to the typical case of application. In case of a jet engine these effects are most often unknown or at least not accurately considered because of the large product cycles which are linked to the high costs of these goods. This means that for a jet engine a detailed understanding of the above mentioned effects for single components and for the overall system for stationary and transient operational behavior is necessary. This is even more pronounced when it comes to the interaction (amplification or reduction) of multiple components under the influence of wear as well as repair and overhaul in sense of parameters like performance as well as reliability and safety of the overall system. The Collaborative Research Center ´871 “Regeneration of complex capital goods” is investigating these issues. To investigate the transient engine performance effects, the Institute of Jet Propulsion and Turbomachinery (IFAS) of Technische Universität Braunschweig is developing the simulation tool ASTOR (Aircraft Engine Simulation for Transient Operation Research) within the research center. The objective is to create an analytical simulation environment for gas turbine processes where the operational behavior of an existing gas turbine could be modeled accurately. This basic model is to be retained while arbitrary modifications to the engine are examined. These modifications could include additional bleed systems, power off take or the deterioration of engine components. Since the basic engine model is retained, this model would also be accurate in predicting the operational performance of the engine if the same modifications are applied in an experiment. The general application of the gas path analysis is difficult since every additional parameter which has to be calculated requires additional boundary conditions which affect the entire engine model. To avoid this, a system theory approach is used to establish a model which could be used similar to the model of an electric or hydraulic circuit. Circuit models consist of interconnected building blocks where each block models the behavior of an individual component. With this method it is possible to describe even the most complex circuits with sufficient accuracy and the basic circuit model could be retained and validated while additional components are added or single components modified. Thus the dedicated effects of the modification could be observed in the model.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Model Order Reduction for Additive Manufacturing Process

Brice Bognet*, Olivier Desmaison**, Francisco Chinesta***

*GeM, Ecole Centrale Nantes, **ESI Group, France, ***Arts et Métiers ParisTech

ABSTRACT

Key Words: Model Reduction, Powder Bed Fusion, Separated representation Additive manufacturing (AM) processes are of increasing interest in today 's industrial context. Several different technologies are getting mature, allowing the production of complex quality parts, however the simulation associated to such processes is still a challenge for the scientific community. In the present work, we focus on the simulation of residual stresses and distortion of parts produced by Powder Bed Fusion (PBF) technologies. The inherent complexity of the process, including many possible process parameters and various possible tool path, lead to a necessity of running simulations prior to the manufacturing in order to determine optimal parameters, correct for eventual process induced distortions and check the actual printability of a design. Simulation of such processes implies various difficulties, including: - multi-scale process (powder scale, heat source scale, part scale, tool-path length) - multi-physics with non-linearity (phase change, plasticity, large displacement) - geometric complexity, including supporting structures being optimized for heat dissipation and/or distortion reduction - layers thickness(issue for standard discretization techniques) All those difficulties combined together lead to failure of standard discretization based numerical strategies. In order to overcome some of those difficulties, the physics is first simplified: we consider the activation of full layers at the time in the simulation (eventually lumping several of them), ignoring the actual tool-path and filling strategy. Moreover, and equivalent shrinkage is applied directly in a mechanical simulation, ignoring the actual heat transfer problem and phase changes. Secondly, we use a specially developed model reduction approach to keep down the number of degrees of freedom. Our approach is based on the so-called Proper Generalized Decomposition, where quantities of the model are described using a separation of variables approach. When solving the elasto-plastic problems, a space variables separation is used, such that all quantities of the model are expressed as sums of products of the in-plane coordinates {x,y} (coordinates on the bed surface), the out-of-plane coordinate {z} (stacking direction) and the number of the domain {n}. The last discrete coordinate n being associated to a domain decomposition strategy, and representing the domain number associated to one or a group of layers depending on the layers lumping strategy. Thanks to the use of such separated representation, the 3D problem to be solved is reduced to a set of 2D and 1D sub-problems, reducing drastically the number of degrees of freedom, and therefor reducing the simulation time.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Loosely Coupled Scheme for Fictitious Domain Approximations of Fluid-Structure Interaction Problems with Immersed Thin-Walled Structures

Ludovic Boilevin-Kayl*, Miguel Ángel Fernández**, Jean-Frédéric Gerbeau***

*a) Inria Paris, 75012 Paris, France and b) Sorbonne Universités, UPMC Université Paris 6, UMR 7598 LJLL, 75005 Paris, France, **a) Inria Paris, 75012 Paris, France and b) Sorbonne Universités, UPMC Université Paris 6, UMR 7598 LJLL, 75005 Paris, France, ***a) Inria Paris, 75012 Paris, France and b) Sorbonne Universités, UPMC Université Paris 6, UMR 7598 LJLL, 75005 Paris, France

ABSTRACT

We are interested in the simulation of elastic thin-walled bodies immersed in an incompressible viscous fluid. Cardiac valves are the main motivation of the present study. To our knowledge, the coupling schemes used in this context are usually implicit or semi-implicit. This yields unconditional stability but at the price of solving a computationally demanding coupled system at every time step. The design of explicit coupling schemes – i.e. schemes that call the two solvers only once per time-step – is of major interest, especially for three-dimensional simulations. However, the major drawback of the existing approaches (e.g., [1]) is that either stability or accuracy demands severe time-step restrictions (e.g., parabolic CFL) or correction iterations. We propose a new solution that overcomes these difficulties. The fluid is modelled with the Navier–Stokes equations, in a Eulerian setting, and the valves are described by a Reissner-Mindlin shell type model in Lagrangian formulation. The interface coupling is enforced through Lagrange multipliers approximated with Dirac masses (e.g., [2]). The proposed coupling scheme is an extension of the Robin-Neumann splitting proposed in [3] to the present unfitted mesh framework. It treats implicitly the coupling of the fluid with the solid inertia and explicitly the coupling with the solid elastic effects. In addition, the choice of Dirac masses for the Lagrange multipliers, combined with a consistent lumped-mass approximation in the solid, yields a very efficient implementation in the fluid solver which makes the coupling scheme explicit. The resulting numerical method is provably stable in the energy norm. Numerical examples, including cardiac valves, will be presented. Comparisons in terms of accuracy and computational efficiency with respect to the implicit scheme will be discussed and will illustrate the benefits of the explicit scheme. This new method is very promising and outperforms the coupling schemes we are aware of. This work has been supported by the project MIVANA and the companies Kephalios and Epygon. References: [1] D. Boffi, N. Cavallini and L. Gastaldi. Finite element approach to immersed boundary method with different fluid and solid densities. Math. Models Methods Appl. Sci., 21, (2011), 2523–2550. [2] N. Diniz dos Santos, J.-F. Gerbeau and J.-F. Bourgat, A partitioned fluid–structure algorithm for elastic thin valves with contact, Comput. Methods Appl. Mech. Engrg., 197, (2008), 1750–1761. [3] M.A. Fernández, J. Mullaert and M. Vidrascu, Explicit Robin-Neumann schemes for the coupling of incompressible fluids with thin-walled structures, Comput. Methods Appl. Mech. Engrg., 267, (2013), 566–593.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Shear Transformation Activation and Distribution in the Deformation of Amorphous Materials

Francesca Boioli*, Tristan Albaret**, Anne Tanguy***, David Rodney****

*LEM UMR-104, CNRS-ONERA, Chatillion, **ILM, University of Lyon 1, ***LaMCoS, INSA Lyon, ****ILM, University of Lyon 1

ABSTRACT

Amorphous solids are characterized by high strength and low ductility. The latter property is a consequence of the localization of the plastic deformation in shear bands, which leads to catastrophic failure. As a consequence, understanding the localization of plastic deformation and the formation of shear bands is of utmost importance. Generally, it has been accepted that local irreversible rearrangements of small clusters of atoms, Shear Transformations (STs), are the elementary processes involved in the deformation of amorphous systems and several mesoscale models based on STs have been proposed. Still the fundamental mechanisms underlying ST occurrence and shear bands formation are not yet clear. In this context, atomistic simulations can provide significant details that would otherwise be unavailable. In this work we investigate amorphous silicon by performing quasi-static and molecular dynamics shear simulations with Stillinger-Weber type potentials. First, the analysis of the shear simulations allow to identify local plastic rearrangements. By fitting their displacement field on collections of Eshelby spherical inclusions, we characterize their size and plastic strain. This result provides atomic-scale parameters to characterize the local shear rearrangements needed to build mesoscale simulations. Second, using the Nudged Elastic Band method, we calculate the energy barriers and the activation volumes involved in the plastic rearrangements caused either by isolated STs or by cascades of interacting STs accessing the strain-rate sensitivity of glass plasticity, another important parameter for mesoscale models. Finally, we investigate the dynamic process of ST formation, determining the characteristic time involved in the development of STs and the influence of the strain rate on the STs distribution and organization.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Thermodynamically Consistent Model for Shape-Memory Ionic Polymers

Alain Boldini*, Abdolhamid Akbarzadeh Shafaroudi**, Stefano Mariani***

*Politecnico di Milano, **McGill University, ***Politecnico di Milano

ABSTRACT

Smart materials have recently attracted the attention of many researchers due to their unique multifunctional properties; however, their practical applications are still somehow limited due to the lack of constitutive models capable of accurate description of their multiphysics behavior. Dealing with ionic polymers with shape memory effects, e.g. the commercially available Nafion™, we propose a thermodynamically consistent model for the fully coupled chemo-electro-thermo-mechanical response to external stimuli. Moving from continuum thermodynamics, the relevant conservation laws are discussed. The constitutive equations are then obtained via an appropriate choice of the Helmholtz free-energy function, through the standard Coleman-Noll procedure. The free-energy function is set by properly linking recognized models for the description of electro-mechanical effects in ionic polymers on one side, and of shape memory effects in polymers on the other side. The instantaneous (elastic) and time-delayed (viscous) response of the polymer in a finite strain setting and the fixation of alternate shape configurations through a thermo-mechanical training are discussed. The obtained model is then implemented in the commercial finite element software Abaqus™ through a UEL (user element) interface. The model and its implementation are validated by comparing calculated numerical results with data obtained from tests conducted in an ad-hoc designed experimental campaign. Results are finally reported on the use of these shape-memory polymers as triggering mechanisms of folding/unfolding of an origami-inspired deployable structure.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Adaptive Discontinuous Galerkin Schemes for Unsteady Under-resolved Problems

Thomas Bolemann*, Gregor Gassner**

*University of Cologne, University of Stuttgart, **University of Cologne

ABSTRACT

Unsteady multi-scale problems pose high requirements on the resolution, both in space and time, for appropriately covering the relevant physical phenomena. In recent years high-order methods in general and discontinuous Galerkin methods in particular have made substantial progress. Investigations have shown that these methods have highly favorable properties for multi-scale problems, such as LES in the field of fluid dynamics, due to their superior scale-resolving capabilities. It is valid to assume that practically all simulations for these problems are under-resolved due to the high resolution requirements, thus making efficient schemes a key requirement. In this work we use the discontinuous Galerkin Spectral Element Method (DGSEM), which is among the most efficient high-order schemes, due to consequent use of tensor-product operators, with split-form fluxes ensuring the stability of the scheme. Since unsteady phenomena lead to strongly varying resolution requirements, the basic scheme is combined with an octree-based adaptive mesh refinement. To avoid the global impact of small time-steps in refined areas, we utilize a local-time stepping approach based on a space-time formulation, where the time steps are linked to groups of octants. Most numerical frameworks of this complexity are implemented using statically typed low-level programming languages such as C/C++ or Fortran, mainly for performance reasons. We take another approach, using Julia a modern high-level, dynamic language. Focused on numerical computing, it provides performance on par with low-level languages. By this choice we can keep the numerical framework as compact and user-friendly as possible and retain the feasibility for rapid-prototyping complex algorithms. In the talk we will present the novel Julia-based DGSEM framework and outline the basics of the numerical method and provide details on the parallel implementation of the octree-based AMR and LTS algorithm. We will furthermore compare it to the established open-source solver Flexi (https://www.flexi-project.org/), a Fortran-based DGSEM framework already operating at Petascale level, developed by the same authors. We will detail on implementation differences and present benchmarks for selected model problems with a focus on fluid dynamics.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Discrete Element Modeling of Powder Spreading for Metal Additive Manufacturing

Dan Bolintineanu*, Jeremy Lechman**

*Sandia National Laboratories, **Sandia National Laboratories

ABSTRACT

Metal additive manufacturing technologies such as selective laser melting rely on layer-by-layer deposition of powder. Spreading of the powder in layers of controlled thickness forms the basis for subsequent selective laser melting or sintering. It is therefore essential to quantify and understand the relationships between powder properties, powder processing parameters and powder bed structure. We present discrete element method (DEM) simulations pertaining to the processing of metal AM powders in the context of additive manufacturing. DEM simulations can account for arbitrary variations in particle-scale properties such as size and shape distribution, as well as various aspects of interparticle contact mechanics, such as variations in friction (e.g. due to particle surface roughness) or variations in interparticle cohesion (e.g. due to chemical composition and particle surface morphology variability). We present a detailed sensitivity study relating the detailed structure of the powder bed to variations in these powder properties as well as powder processing parameters (e.g. layer thickness, spreader blade geometry and speed). In characterizing the powder bed, we examine a variety of spatial statistics, including descriptors of the powder bed surface and the spatial distribution of porosity within the bulk of the powder bed. We note significant variability on length scales relevant to the AM process (e.g. typical laser spot size and powder layer thickness). While such metrics are challenging to determine experimentally, they provide important information for uncertainty quantification efforts in the context of full AM process modeling. Both interparticle friction and cohesion are shown to have notable effects on powder bed structure. As these properties are difficult to measure experimentally, we also discuss preliminary efforts to incorporate powder rheology measurements as both input and validation for our models. Due to the particle-level detail in these simulations, we are able to explore a wide range of particle properties, and therefore provide quantitative insight into powder selection and handling decisions for additive manufacturing. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Shape Identification and Optimization in Elastoplastic Boundary Value Problems Using Parametric Integral Equation System (PIES) and Particle Swarm Optimization (PSO)

Agnieszka Boltuc*

*University of Bialystok

ABSTRACT

Shape optimization (identification) is one of the stages of the design of mechanical structures. The solution of these problems is usually achieved by minimization of the objective function describing the optimization criterion. In practice, it leads to multiple solving of a direct problem with the modified geometry. Therefore, it is extremely important, especially in the case of complex elastoplastic problems, to choose the appropriate method for solving direct problems. It can be carried out using FEM or BEM, however both have a serious disadvantage – they require discretization of the boundary and the domain (at least the plastic zone). In the literature are attempts to modelling the optimized boundary by curves. It significantly reduces the number of design variables, but the numerical solution of the direct problem still requires division into elements. Considering the above, the PIES method [1] is proposed for solving direct elastoplastic problems. It is characterized by the separation of shape approximation from solutions approximation and allows for elementless modeling of the boundary (by curves) and the domain (by surface patches). Its effectiveness stems from a reduced number of design variables (only control points of curves), the lack of discretization and automatic adaptation of its mathematical formalism to the changing shape. The latter results from PIES's main feature - the shape is analytically integrated into its mathematical formula. Additionally, the area of the plastic zone is not discretized repeatedly, but is defined once by a single surface, whose shape, if coincident with the shape of the boundary, automatically adjusts to the changes. For optimization purposes the particle swarm optimization method is applied. As indicated in recent publications it is more effective than classical evolutionary algorithms, because allows for greater diversity and exploration over a single population with lower computational costs. This is especially important in elastoplastic problems solved by incremental–iterative scheme, because in inverse problems we have to deal with nested iterative processes, which significantly increases the computational effort. The proposed strategy was tested on several examples. Shape identification was performed basing on values from selected measurement points on the boundary, while shape optimization consisted in minimizing plastic deformation areas. Obtained results confirm the efficiency of the method. References: [1] A.Boltuc, Parametric integral equation system (PIES) for 2D elastoplastic analysis, Engineering Analysis with Boundary Elements, 69, 21-31, 2016. Acknowledgements: These investigations were supported by the National Science Centre, Poland (Project NCN MINIATURA no.2017/01/X/ST8/00534).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Formulation of Plasticity Models through Symbolic Regression

Geoffrey Bomarito*, Kathryn Esham**, Saikumar Yeratapally***, Jacob Hochhalter****

*National Aeronautics and Space Administration, Langley Research Center, Hampton, VA, **The Ohio State University, Columbus, OH, ***National Institute of Aerospace, Hampton, VA, ****National Aeronautics and Space Administration, Langley Research Center, Hampton, VA

ABSTRACT

Material plasticity models typically consist of an assumed functional form and fitting parameters. The functional form is often derived from a simplified analytical model. The fitting parameters exist in order to give flexibility to the model to fit many materials. In most cases, the real material deviates from the idealized analytical model and the functional form of the plasticity model is not completely accurate. Traditionally, the revision and iteration on the analytical model and functional form relies on human intuition and interaction. Production of accurate models in this way can take decades. In this work, an alternate approach is taken whereby a plasticity model is formulated based on a representative volume element (RVE) simulated with the finite element method. The approach can be seen as a method of computational homogenization. Rather than relying on an assumed functional form and tuning the parameters to match the homogenized response of the RVE, the response is used directly as an input to a symbolic regression routine. Symbolic regression is a machine learning method that fits data with an equation of arbitrary functional form. The result is a plasticity model that fits the response of the RVE, without assumption of its functional form. A verification of the method is performed showing that the Von Mises plasticity model can indeed be derived from symbolic regression of simulated response data.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

LES-type Models for the Simulation of Flows Past Hydraulic Structures

Fabian Bombardelli*, Juan Pablo Toro**, Joongcheol Paik***

*Univ. of California, Davis, **Andres Bello University, Chile, ***Gangneung-Wonju National University, South Korea

ABSTRACT

Several works have been presented in recent years regarding the use of LES-type models to simulate the flow past hydraulic structures. These models serve the purpose of providing evidence on the turbulence coherent structures at a much smaller computational cost and larger Reynolds numbers than LES or DNS. These simulations have a tremendous promise in giving notable insight into the flow mechanisms. Here, we first discuss the development of a detached eddy simulation (DES) for the flow past stepped spillways, and we compare the results to those of standard Reynolds-Averaged Navier-Stokes (RANS) simulations. Comparisons not only highlight the power of the DES in terms of its prediction, but they also underscore the good agreement with data. Further, we show that the entrainment of air seems to be the consequence of well-organized thin tubes which interact with the free surface. Then, we present simulations of the flow past a gate, developed with a modified Scale-Adaptive Simulation (SAS) model and results of a simulation of flow past a bridge pier. We address the ratio between the eddy viscosity to the fluid kinematic viscosity and its impact on the first type of flow. We corroborate that the SAS has a nice property of a weak dependence on the mesh size close to the wall (obviously in relative terms), and assess its computational cost. We further obtain the coherent structures associated with both flows explaining some of the interesting features of the flow.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Automatic Quadrilateral and Hexahedral Mesh Generation via Integer-Grid Maps

David Bommes*

*RWTH Aachen University

ABSTRACT

Automatically generating quadrilateral and hexahedral meshes that smoothly align to freeform surfaces and offer a high amount of regularity and low distorted elements is a notoriously challenging task. Novel algorithms based on global optimization rely on the construction of integer-grid maps, which pull back a Cartesian grid of integer isolines from a 2D or 3D domain onto a structure aligned quadrilateral or hexahedral mesh. Such global optimization algorithms do not suffer from limitations known from local advancing front methods, as for instance a high rate of irregularity, and enable meshes comparable to manually designed ones by finding a good compromise between regularity and element distortion. In my talk, I will give an overview of the state of the art and discuss the strengths and weaknesses of available algorithms, including open challenges for hexahedral meshing. Through rapid progress in the last years, nowadays for quadrilateral meshing a high level of robustness, performance and quality is available. It is expected that such algorithms will soon conquer commercial applications and strongly relieve users from the time-consuming task of manually generating quadrilateral meshes.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Two-Level Nested Model Reduction Framework for a Class of Optimization Problems Characterized by a High-Dimensional Parameter Space

Gabriele Boncoraglio*, Spenser Anderson**, Charbel Farhat***

*Stanford University, **Stanford University, ***Stanford University

ABSTRACT

Optimization problems in computational mechanics typically involve the solution of a combination of linear and nonlinear PDEs to evaluate the objective function, and/or enforce complex constraints. Most often, they involve a large number of optimization parameters. They are usually solved using a Nested Analysis and Design approach, and therefore incurs the repeated solutions of the aforementioned PDEs at different parameter points. The computational expense of these solutions is often reduced by replacing the underlying High-Dimensional Models (HDMs) by less computationally intensive surrogate models such as a, for example, Projection-based Reduced-Order Models (PROMs). This defines the context of this talk which will describe a novel computational framework for solving PDE-constrained optimization problems using PROMs. Specifically, the focus will be set on those problems characterized by a high-dimensional design space and at least one linear and steady PDE. The framework is based on the concept of a database of local PROMs and the associated concept of interpolation on matrix manifolds [1]. To address the challenges raised by high-dimensional parameter spaces, adaptive least-squares radial basis functions [2] are first introduced to facilitate interpolation in tangent spaces to matrix manifolds. Then, the dimensionality of the parameter space itself is reduced by representing its elements using low-dimensional affine subspace approximations. This results in a two-level nested model reduction framework where first, the parameter space is restricted to a low-dimensional subspace to yield an optimization problem with fewer variables, then a constructed or interpolated PROM is used to reduce the dimensionality of the linear PDE. This framework will be illustrated with the solution of several realistic constrained optimization problems in aeronautics, including design optimization problems under flutter constraints. Its online speed, flexibility, and its enabling of multi-start approaches to global optimization will also be demonstrated. 1. D. Amsallem and C. Farhat, An Online Method for Interpolating Linear Parametric Reduced Order Models, SIAM Journal for Scientific Computing, Vol. 33, pp. 2169–2198 (2011) 2. G.E. Fasshauer, Adaptive Least squares Fitting with Radial Basis Functions on the Sphere, Mathematical Methods for Curves and Surfaces, Vanderbilt University Press, Nashville, pp. 141-150 (1995)

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Flow and Mechanics in Fractured Media as Mixed-Dimensional PDEs

Wietse Boon*, Jan Nordbotten**

*University of Bergen, **University of Bergen

ABSTRACT

In the mixed-dimensional representation of fractured media, the fractures are considered as lower-dimensional manifolds. This concept is successively applied to the lines and points at the intersections between fractures leading to a hierarchical geometry of manifolds of codimension one. By imposing these modelling assumptions a priori in the continuous setting, the basis is formed for the introduction of coupled PDEs on the mixed-dimensional geometry, which we refer to as mixed-dimensional PDEs. In this work, we consider Darcy flow combined with linear elasticity on mixed-dimensional representations of fracture networks. Since the associated, governing equations are fully coupled, the systems of equations are presented using mixed-dimensional differential operators which map between the different dimensions. In turn, the resulting system of equations is considered as mixed-dimensional and is analysed as such, before the introduction of the discretization scheme. We present theoretical results related to the structure of mixed-dimensional elliptic partial differential equations from which multiple conforming discretization schemes arise using dimensionally hierarchical finite elements. Keeping later purposes such as transport problems and fracture propagation in mind, our main interest lies in obtaining accurate flux fields and stress states which respect physical conservation laws. Therefore, we employ mixed finite elements which allow for a local preservation of such laws. The symmetry of the stress tensor is imposed in a weak sense, thus leading to the use of familiar, conforming, finite elements with relatively few degrees of freedom. Results concerning convergence and stability of the mixed finite element schemes are shown. These are supported by numerical examples in two- and three-dimensional domains in which the lower-dimensional inclusions, intersection lines, and points have significantly different material properties compared to the surroundings.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

An Adaptive Multi-Model Approach to Simulate the Damage of Composite Panels with Initial Defect under Compressive Loading

Eva Borakiewicz*, Vincent Chiaruttini**, Antoine Hurmane***, Frédéric Laurin****

*Airbus Operations, Université Paris Saclay, Onera - The French Aerospace Lab, **Onera - The French Aerospace Lab, ***Onera - The French Aerospace Lab, ****Onera - The French Aerospace Lab

ABSTRACT

The growing industrial interest for predictive virtual testing makes the development of advanced numerical tools essential to achieve confident and realistic complex numerical simulations. For instance, one may wonder to what extent an initial defect affects the global behavior of a slender composite structure under compressive loading. The resolution of this problem necessitates expertises in both numerical approaches and material constitutive behaviors while several non-linearities sources are arised such as large deformation and material on-going degradation. Responding to those problematics, this work presents an adaptive multi-model method to predict the residual strength of a structure with an initial defect. Like other multiscale approaches [1], our technique attempts to put in each location of the structure just the right amount of complexity in terms of meshing and material behavior. In this respect, the structure is divided in two parts separated by a boundary that is allowed to evolve during the simulation in order to gain in overall computation time. The first part concentrates non-linearities using a complex non-linear damage constitutive law and a multi-layered mesh. An advanced mesoscale model [2] is chosen in order to take into account several material non-linearities and to correctly predict a laminate 's degradation processes. The second part, which is complementary to the first one, has a simpler elastic behavior. The local area, which is at first concentrated around the defective zone, evolves according to the progression of damage during the simulation process. Such an approach induces dealing with remeshing, field transfer and coupling between models aspects which will be detailed related to our implementation within a commercial finite element solver. Various numerical assessments (from both academic and industrial applications of the aeronautical domain) will be presented in the context of composite structures to demonstrate the efficiency of this strategy. [1] Multiscale strategy for solving industrial problems, O. Allix, Computational Mechanics, pp 107-126, 2006 [2] A multiscale progressive failure approach for composite laminates based on thermodynamical viscoelastic and damage models, F. Laurin, N. Carrère, J.-F. Maire, Composites: Part A, 38, pp 198-209, 2007

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Predicting Failure in High-Strength Steels Using Phase-Field Methods

Michael Borden*, Pulama Bhattacharya**, Michael Scott***

*Brigham Young University, **Brigham Young University, ***Brigham Young University

ABSTRACT

In this presentation, we will describe our recent efforts to enhance phase-field methods to accurately predict failure in high-strength steels. This work will extend recent advances in phase-field models for fracture in ductile materials to include additional failure criteria, such as the Cockroft-Latham fracture criteria. We will also describe our efforts to develop a methodology to determine the various parameters required by the models. A number of numerical results that demonstrate the performance of the models with respect to benchmark experimental results will be shown.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Weakly Intrusive Level-Set Topology Optimization for Multiphysics Problems

Felipe Bordeu*, Julien Cortial**

*Safran SA, **Safran SA

ABSTRACT

The majority of commercial topology optimization software available on the market relies on a tightly coupled simulation package to compute the state of the system and the sensitivities at every iteration of the optimization. In general these solvers are dedicated to only one (or at best two) type(s) of physics (solid, thermal, fluid…) making the topology optimization of inherently multiphysics problems difficult, if not impossible. Also, the virtually universal use of variable density (or SIMP) methods complicates the modeling of interface phenomena and further increases the level of intrusiveness. In this work we propose a new architecture to construct topology optimization software. The approach is based on two key ideas. The first ingredient is the use of the level-set method [1] to track the optimization interface combined with a remeshing strategy [2] to maintain a body-fitted physical discretization. The use of conformal meshes enables to model the physics on the interface (i.e. interface thermal behavior, boundary layer behavior…) more accurately. Also in the case of weakly coupled problem the different physics can be solved by dedicated, highly performant solvers. The second ingredient is the separation of the equations of the optimization problem into two sets, one related to the physical problems and the other to the computation of the gradient and the shape evolution mechanism. The first set of equations can be solved by any (commercial/parallel) simulation software, ideally one that is already available and in routine use. The second set of equations, including the calculation of the next candidate (new iterate), calculation of the gradient and the manipulation of the level-set, are delegated to an independent, Python-based library. We call this approach "weakly intrusive" because even if we use a commercial code to compute the physical solution in a "black box" fashion, we still need to solve auxiliary (adjoint) problems to generate the next candidate. These auxiliary problems can be solved by the same commercial software (if supported) or by an independent finite element solver. Examples of topology optimization for parts with realistic, industrial geometries will illustrate the proposed methodology and software architecture. [1] Allaire G., Jouve F., Toader A-M, "A level-set method for shape optimization", CR Acad. Sci. Paris, Serie I, 334, 1125-1130, 2002. [2] C. Dapogny, C. Dobrzynski and P. Frey, "Three-dimensional adaptive domain remeshing, implicit domain meshing, and applications to free and moving boundary problems", J. Comput. Phys., 262, 358-378, 2014.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

An Adaptive Mesh Refinement Approach for Eulerian Turbulent Fluid-Structure Interaction Computations

Raunak Borker*, Sebastian Grimberg**, Phil Avery***, Charbel Farhat****

*Stanford University, **Stanford University, ***Stanford University, US Army Research Laboratory, ****Stanford University

ABSTRACT

Embedded Boundary Methods (EBMs) [1] for the solution of Fluid-Structure Interaction (FSI) problems are typically formulated in the Eulerian setting. This makes them more attractive than alternative computational frameworks for FSI problems where the structure undergoes large structural motions and/or deformations, or topological changes. For viscous problems however, EBMs suffer from a major drawback in that they do not track the boundary layers [2]. In principle, this disadvantage can be overcome using Adaptive Mesh Refinement (AMR). However, this approach raises several issues ranging from interpreting the concepts of anisotropy and aspect ratio in this setting, to achieving computational efficiency for a given Reynolds number. To this end, this talk presents an approach for performing AMR in Eulerian turbulent FSI computations that is based on the distance to the nearest wall boundary, which typically evolves and deform in time. It efficiently tracks every embedded discrete surface using a fast predictor-corrector estimation algorithm and adapts the embedding mesh so that all boundary layers stay resolved at all times. It is also equipped with a Hessian-based mesh adaptation criterion for capturing solution features. In general, AMR gives rise to non-conforming mesh configurations that can complicate the semi-discretization process. The proposed AMR approach addresses this issue by explicitly enforcing mesh conformity during the mesh adaptation process, via an appropriately designed scheme for adding and deleting edges and elements. It is implemented, together with a dynamic mesh repartitioning strategy for load balancing, in the massively parallel AERO Suite for highly nonlinear FSI problems, which features the FIVER (Finite Volume method with Exact two-material Riemann solvers) [3] EBM for CFD and FSI. Its potential for enabling the efficient solution of highly nonlinear, turbulent FSI problems is demonstrated with numerous examples associated with the simulation of supersonic parachute inflation dynamic problems. 1. R. Mittal and G. Iaccarino, Immersed Boundary Methods, Annual Review of Fluid Mechanics, Vol. 37, pp. 239-261 (2005) 2. C. Farhat and V. Lakshminarayan, An ALE Formulation of Embedded Boundary Methods for Tracking Boundary Layers in Turbulent Fluid-Structure Interaction Problems, Journal of Computational Physics, Vol. 263, pp. 53-70 (2014) 3. C. Farhat, J.-F. Gerbeau and A. Rallu, FIVER: A Finite Volume Method Based on Exact Two-Phase Riemann Problems and Sparse Grids for Multi-Material Flows with Large Density Jumps, Journal of Computational Physics, Vol. 231, pp. 6360-6379 (2012)

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Dislocation-Phase Boundary Interaction – a Peierls-Nabarro Finite Element Approach

Franz Bormann*, Ron Peerlings**, Marc Geers***

*Eindhoven University of Technology, **Eindhoven University of Technology, ***Eindhoven University of Technology

ABSTRACT

ABSTRACT To get a better insight into the interaction of edge dislocation pile-ups with a phase boundary we perform a numerical study of a simplified two-phase continuum microstructure. The model comprises a soft Phase A that is flanked by a harder Phase B. Embedded in both phases lies a single glide plane, perpendicular to and continuous across the phase boundary. Centred within Phase A lies a dislocation source that emits dislocation dipoles under sufficiently high shear stress. On the remote boundary, a shear stress is applied that triggers dislocation nucleation and drives the dislocations towards the phase boundary. Due to the phase contrast between both phases, a natural source of dislocation obstruction is present. This leads to the formation of dislocation pile-ups. Eventually, the driving forces on the dislocations exceed a critical threshold such that i) the leading dislocation of the pile-up is transmitted into Phase B or ii) the leading dislocation is absorbed into the phase boundary inducing local decohesion. Other scenarios such as dislocation reflection or dislocation nucleation at the phase boundary are not considered. For this study we adopt the Peierls-Nabarro model [1] in a 2D plane strain finite element framework. Both phases are split into two linear elastic media that are connected by the glide plane. Along the glide plane a relative tangential displacement, or disregistry, is allowed for that is mapped to the intrinsic misfit energy. The employed potential is periodic, and thus nonconvex, to capture the effect of lattice periodicity. Along the phase boundary an exponential cohesive zone law is introduced to include decohesion. The model is discretised by finite elements and solved with the Truncated Newton method, along the lines proposed by Nash [2]. The modelling thus obtained provides a natural interplay between dislocations, external boundary conditions and the phase boundary, including the possibility of decohesion. No additional criteria for the dislocations' interaction with the phase boundary is required. The numerical solutions obtained allow us to study the interplay between dislocations and interface decohesion as a function of material properties of the two phases and the phase boundary, as well as the current internal dislocation configuration. REFERENCES [1] J.P. Hirth, J. Lothe, Theory of dislocations, Wiley, New York, Vol. II., 1982. [2] S.G. Nash, "A survey of truncated-Newton methods", J. Comput. Appl. Math., 124, 45-59, 2000.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Bayesian Calibration of Expensive Computer Models

Ramin Bostanabad*, Weizhao Zhang**, Jian Cao***, Wei Chen****

*Northwestern University, **Northwestern University, ***Northwestern University, ****Northwestern University

ABSTRACT

As the role of computer models in investigating physical phenomena increases, more efficient and rigorous uncertainty quantification and propagation methods are pursued in various fields of science and engineering. This is because, regardless of the scale and purpose of the physical process under study, computer models are not perfect and differ from the reality for a variety of reasons including our lack of knowledge which result in discrepancies between the model predictions and the observed values. Additionally, computer models are often developed to be applicable to a wide range of applications. However, to use a model for prediction in a specific context, one may have to adjust some of its inputs by calibrating them against some experimental data. Lack of data is another prevalent source of uncertainty in mechanics since most computer simulations and experimental data are rather costly and time-consuming to gather. The goal of this work is to employ a modular Bayesian approach [1-3] to calibrate a high-dimensional phenomenological material law developed for modeling fiber composites in finite element simulations. Following the seminal work of Kennedy and O'Hagan [1], our goal is to (i) model the (potential) bias of the computer model by placing a Gaussian process prior on it and finding its posterior distribution, and (ii) estimate the calibration parameters. However, special care is exercised to address the identifiability issues (between the posterior of the calibration parameters and the posterior of the bias function) commonly faced in Bayesian calibration since (i) the calibration parameters of our model have distinct physical meaning, and (ii) there are certain physical constraints that the posterior of the computer model has to satisfy,. Additionally, artificial simulations are added to the training dataset to enforce the physical constraints and partially address the lack of data due to considerable costs in running the computer model. 1. Kennedy, M.C. and A. O 'Hagan, Bayesian calibration of computer models. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 2001. 63(3): p. 425-464. 2. Bayarri, M., et al., Computer model validation with functional output. The Annals of Statistics, 2007: p. 1874-1906. 3. Arendt, P.D., et al., Improving identifiability in model calibration using multiple responses. Journal of Mechanical Design, 2012. 134(10): p. 100909.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Application of a Multi-Scale Hysteresis Model to Dynamic Seal Friction

Johan Steffen Bothe*, Matthias Wangenheim**

*Leibniz Universitaet Hannover, Institut fuer Dynamik und Schwingungen, **Leibniz Universitaet Hannover, Institut fuer Dynamik und Schwingungen

ABSTRACT

Dynamic seals prevent mass transfer across system boundaries while allowing relative motion of the corresponding sealing surfaces with minimum friction loss. For this presentation, a multi-scale analysis originally created for the simulation of hysteresis friction in tire-road contact is adapted and applied to dynamic seal friction. Adhesive, viscous and cohesive friction mechanisms are ignored. The multi-scale analysis uses viscoelastic material data in the form of prony parameters including temperature dependence. The countersurface is approximated by a set of sine waves, which have the same height-difference correlation as the original countersurface when superposed. The effect of lubrication on hysteresis friction is implemented by surface data modification. Simulation results are validated against experimental data.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Hybrid High-Order Method for Nonlinear Elasticity on General Polyhedral Meshes

Michele Botti*, Pierre Sochala**, Daniele A. Di Pietro***

*Université de Montpellier, **Bureau de Recherches Géologique et Minières, ***Université de Montpellier

ABSTRACT

We formulate and analyze a novel Hybrid High-Order discretization of a class of (linear and) nonlinear elasticity models in the small deformation regime which are of common use in solid mechanics. The proposed HHO discretization is inspired by the recent works on linear elasticity [2] and Leray--Lions operators [1]. It hinges on degrees of freedom that are discontinuous polynomials on the mesh and on the mesh skeleton. Based on these degrees of freedom, we reconstruct discrete counterparts of the strain and of the displacement by solving local linear problems inside each mesh element. These reconstruction operators are used to formulate a local contribution composed of two terms: a consistency term inspired by the weak formulation of problem and a stabilization term penalizing cleverly designed face-based residuals. The resulting method is valid in two and three space dimensions, it supports general meshes including polyhedral elements and nonmatching interfaces, enables arbitrary approximation order, and can be efficiently implemented thanks to the possibility of statically condensing a large subset of the unknowns for linearized versions of the problem. Additionally, the method satisfies a local principle of virtual work on each mesh element, with interface tractions that obey the law of action and reaction. For monotone stress-strain relations, convergence to minimal regularity solutions is proved following the ideas of [3]. Moreover, optimal error estimates hold under the additional conditions of Lipschitz continuity and strong monotonicity on the stress-strain law. The performance of the method is investigated on a extensive panel of model problems using two types of nonlinear stress-strain laws. [1] D. A. Di Pietro and J. Droniou, A Hybrid High-Order method for Leray--Lions elliptic equations on general meshes. Math. Comp., 2017. [2] D. A. Di Pietro and A. Ern, A hybrid high-order locking-free method for linear elasticity on general meshes. Comput. Meth. Appl. Mech. Engrg. 283, pp 1--21, 2015. [3] J. Droniou and B. P. Lamichhane, Gradient Schemes for Linear and Non-linear Elasticity Equations. Numer. Math. 129 (2), pp 251--277, 2015.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Analysis of Local Strain in Nodular Graphite Cast Iron at the Onset of Coalescence by Means of 3D Numerical Modeling Combined with X-Ray Laminography and Digital Volume Correlation

Pierre-Olivier Bouchard*, Victor Trejo-Navas**

*Mines ParisTech, PSL-Research University, CEMEF - Centre de mise en forme des matériaux, CNRS UMR 7635, CS10207 rue Claude Daunesse 06904 Sophia Antipolis Cedex, France., **Mines ParisTech, PSL-Research University, CEMEF - Centre de mise en forme des matériaux, CNRS UMR 7635, CS10207 rue Claude Daunesse 06904 Sophia Antipolis Cedex, France.

ABSTRACT

Ductile fracture for metallic materials is generally resulting from void nucleation, growth and coalescence mechanisms. Thanks to advanced in situ Synchrotron Radiation Computed Laminography techniques [1], it is now possible to observe these mechanisms during mechanical tests with different stress states. However, in order to understand and model such mechanisms, it is necessary to assess local mechanical fields within the microstructure all along the tests. This can now be achieved thanks to Digital Volume Correlation (DVC) for displacement measurements and strain calculations in the bulk of the microstructure [2]. The work presented herein uses both techniques and describes a finite element (FE) framework in which 3D heterogeneous microstructures are meshed and studied for large plastic strains [3]. Thanks to this framework, immersed microstructures and DVC boundary conditions are considered for more realistic numerical simulations at the microscale of nodular graphite cast iron submitted to tensile loading with various stress states [4]. Equivalent strain values prior to coalescence in the intervoid ligament resulting from DVC and FE simulations are compared for different pairs of coalescing voids with either internal necking or void-sheet coalescence mechanisms. The numerical study is generalized to a bigger group of void pairs in the cast iron microstructure in order to get more representative data and to discuss the possibility of validating a strain-based coalescence criterion while taking into account the occurrence of the two aforementioned coalescence mechanisms. This work was performed within the COMINSIDE project funded by the French Agence Nationale de la Recherche (ANR-14-CE07-0034-02 grant). 1. A. Buljac, T. Taillandier-Thomas, T. F. Morgeneyer, L. Helfen, S. Roux and F. Hild. Early strain localization during flat to slant crack transition in AA 2198 T8 sheet: In situ 3D measurements. International Journal of Fracture, 200(1):49-62, 2015 2. T. F. Morgeneyer, T. Taillandier-Thomas, L. Helfen and F. Hild. On strain and damage interactions during tearing: 3D in situ measurements and simulations for a ductile alloy (AA2139-T3). Journal of the Mechanics and Physics of Solids, 96:550-571, 2016 3. A. Buljac, M. Shakoor, J. Neggers, M. Bernacki, P.-O. Bouchard, L. Helfen, T. F. Morgeneyer and F. Hild, Numerical Validation Framework for Micromechanical Simulations based on Synchrotron 3D Imaging, Computational Mechanics, 59(3): 419–441, 2017

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Frequency Response of Assembled Structures with Identified Multi-interface Proportional Damping

Noureddine Bouhaddi*, Mohamed Krifa**, Scott Cogan***, Najib Kacem****

*Univ. Bourgogne Franche-Comté, FEMTO-ST Institute, CNRS/UFC/ENSMM/UTBM, Department of Applied Mechanics, **Univ. Bourgogne Franche-Comté, FEMTO-ST Institute, CNRS/UFC/ENSMM/UTBM, Department of Applied Mechanics, ***Univ. Bourgogne Franche-Comté, FEMTO-ST Institute, CNRS/UFC/ENSMM/UTBM, Department of Applied Mechanics, ****Univ. Bourgogne Franche-Comté, FEMTO-ST Institute, CNRS/UFC/ENSMM/UTBM, Department of Applied Mechanics

ABSTRACT

The severe dynamic environment of take-off and flight of launchers presents risks of damage and life cycle limitation of the payload. To improve the dynamic comfort of the payload, damping treatments are employed at the final stage of the launcher assemble. One well-known solution is the limitation of the vibration amplitudes by dissipating the energy at the bolted joints between the stages. To our knowledge, there is not a simple and effective method that allows an accurate damping prediction at the full structure level from the knowledge of localized dissipation between the components. Indeed, to model the damping of an assembled structure made up of several components, one carries out a 3D modeling of the interfaces [1] to have a good representation of the dissipation. The result is a damping model identified by interface, which is difficult to exploit in the prediction of the dynamic behavior of the full model. Moreover, for uniformly distributed dissipation, it is common to use the Rayleigh damping assumption to represent the damping matrix in the equivalent viscous model. In general, common methods [2] identify this matrix at a single interface. In this work, we propose a method of modeling the multi-interface Rayleigh damping which consists of the following steps: (i) calculation of the modal damping of each interface taken separately by using the modal effort method [3] or the modal displacement method developed in PERMAS finite element software; (ii) identification of the proportional damping matrix of each interface (proportionality coefficients of stiffness and mass matrices); (iii) assembly of the identified damping matrices; (iv) prediction of the dynamic response of the complete structure from the global model. The proposed method was validated on a reduced model of the ARIANE 5 launcher to calculate the dynamic responses taking into account the different types of dissipation in the interfaces for the asymmetric load case and successfully compared to the reference results. The main advantages of the proposed method are the simplicity of the numerical implementation, the reduction of the CPU, the quality of prediction and the perspective of integration in an optimization procedure of interfaces design with high damping performances. References [1] S. Bograd, P. Reuss, A. Schmidt, L. Gaul and M. Mayer, Mechanical Systems and Signal Processing, 25(8), 2801–2826, 2011. [2] S. Adhikari, 293(1), 156–170, 2006. [3] A. Caignot, P. Ladevèze, D. Néron and J. F. Durand, Engineering Computations, 27(5), 621-644, 2010.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Model for Cellular Mechanotransduction and Contractility at Finite Strain

Nikolaos Bouklas*, Selman Sakar**, William Curtin***

*Cornell University, **EPFL, ***EPFL

ABSTRACT

In this work we introduce a theoretical and computational modeling framework for the contractile response of single cells triggered by external mechanical stimuli. The structural response due to the formation and dissociation of stress fibers is modeled following isotropic anisotropic contractile phases with an orientation that evolves with time and strain. The passive and active structural components are postulated to act in parallel, and the re-orientation process drives the anisotropic phase of stress fiber orientation to align with the direction of the maximum principal stretch. A reduced form of the Hai-Murphy model is used to follow kinetics of myosin states considering the combined effect of "latch"- and "cross"-bridge states. The introduction of distinct isotropic and anisotropic activation allows modeling of the contractile intensity of each phase. Tractions on the cell surface initiate bio-chemical signaling through the RhoA pathway, which in turn controls both myosin contraction and F-actin polymerization. A signaling model is introduced to effectively connect intracellular events with the tractions on the cell surface. The overall model is defined by a free energy density function that couples the deformation and the activation, and associated equilibrium and kinetic models for evolution. Features of the model are highlighted via implementation in a finite element model and application to benchmark problems. The model captures the dynamic contractile responses of cells and stress fiber re-alignment under complex load histories. For example, physiologically relevant scenario such as relaxation of cells to their initial state upon removal of applied loads can be simulated.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Haemodynamic Analysis in Arterial Models in Relation to Pulmonary Valve Treatment in Adults with Congenital Heart Disease

Maria Boumpouli*, Mark Danton**, Terence Gourlay***, Asimina Kazakidi****

*University of Strathclyde, **Golden Jubilee National Hospital, ***University of Strathclyde, ****University of Strathclyde

ABSTRACT

Introduction Pulmonary artery stenting and valve replacement (PVR) are common interventions in an increasing population of adult patients with previously repaired congenital heart disease [1]. Indications for intervention include assessing regional haemodynamics and effects on right ventricular volume and function [2]. The criterion for intervention remains largely empirical and the optimal timing remains unknown. This work aims to investigate the altered haemodynamic environment of adults with congenital heart disease, pre- and post- operative PVR to establish a computational fluid dynamic (CFD) derived metric for determining the optimal requirement for PVR and stenting. In this initial work, we present CFD results in simplified geometries representing the proximal pulmonary artery and bifurcation. Methods Blood flow simulations were performed using an implementation of the finite volume method. The flow was assumed to be incompressible and governed by the Newtonian Navier-Stokes equations. Physiological vessel dimensions and boundary conditions were used in the models. Local velocities and wall shear stress values were evaluated numerically. Results and Discussion Blood flow in the pulmonary bifurcation is strongly dependent on the local geometrical characteristics and haemodynamic conditions. An increase in the flow separation is observed when the angle of the bifurcation increases. In addition, the geometry has a significant effect on the velocities and shear stresses developed on the vessel wall. Future work will involve anatomically-correct reconstructions from CT and MRI image data of adult congenital heart patients that have or are about to undergo pulmonary valve replacement. Numerical studies of these models will provide an insight into the underlying flow mechanisms of more complex 3D patient-specific geometries. Acknowledgements This work is funded by the University of Strathclyde Research Studentship Scheme (SRSS) Research Excellence Awards (REA), Project No 1208. References [1] Kogon B.E., et al (2015) Seminars in Thoracic and Cardiovascular Surgery. 27 p57 [2] Buechel, E.R.V., et al. (2005). European Heart Journal. 26 p2721

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Crack Nucleation in Variational Phase Field Models of Fracture

Blaise Bourdin*, Jean-Jacques Marigo**, Corrado Maurini***, Erwan Tanné****

*Department of Mathematics and Center for Computation & Technology, Louisiana State University, Baton Rouge, LA 70803, USA, **Laboratoire de Mécanique des solides, École Polytechnique, Route de Saclay, Palaiseau 91120, France, ***Sorbonne Universités, UPMC Univ Paris 06, CNRS, UMR 7190, Institut Jean Le Rond d'Alembert, Paris F-75005, France, ****Department of Mathematics, University of British Columbia, Vancouver, Canada

ABSTRACT

Since their inception in the mid-90's, variational phase-field models of fracture have steadily gained popularity. Part of this success is undoubtedly due to their ability to capture complex fracture behavior, including nucleation and propagation along complex unknown path in 2 and 3 dimensions without the need for ad-hoc criteria and geometric restrictions on crack path. In this talk, I will focus on crack nucleation. I will show that carefully constructed variational phase-field models can account for crack nucleation in the strength and toughness regimes, and for scale effects. I will give arguments in favor of identifying the model regularization parameter and the classical concept of a cohesive length. I will illustrate my claims with validation and verification experiments in a broad range of brittle materials and geometries.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Isogeometric Hierarchical Model Reduction for Parameter-Dependent Problems

Yves Antonio Brandes Costa Barbosa*, Simona Perotto**, Alessandro Veneziani***

*Politecnico di Milano, **Politecnico di Milano, ***Emory University / IUSS Pavia

ABSTRACT

In engineering applications, numerical models have evolved to account for the demands in speed and accuracy. In particular, different model reduction techniques have been properly incorporated to compute, with a reasonable level of precision, the solution of partial differential equations in a constrained time and with a contained computational burden. In particular, our interest is for Hierarchical Model (HiMod) Reduction techniques [1], suitably combined with Isogeometric Analysis (HigaMod), according to the setting proposed in [2] and successively applied in a data assimilation context [3]. HigaMod is a reduction procedure suited to downscale models when the phenomenon at hand presents a preferential direction of flow, e.g., when modelling the blood flow in arteries or the water flow in a channel network. The method showed a significant improvement in reducing the computational power and simulation time, while giving enough information to analyze the problem at hand. In this communication, we generalize HigaMod approach to a parameter-dependent framework, setting the so-called HigaPOD formulation, which merges the computational benefits of HigaMod with the ones characterizing a Proper Orthogonal Decomposition (POD). In particular, we will refer either to linear and nonlinear problems by setting ad-hoc procedures for both the cases. The results so far obtained, although preliminary, are very promising. Thus, after introducing the basic HigaMod framework, we will focus on the HigaPOD approach by verifying the corresponding performances on some benchmark configurations. [1] S. Perotto. A survey of hierarchical model (Hi-Mod) reduction methods for elliptic problems. In Numerical Simulations of Coupled Problems in Engineering. Series: Computational Methods in Applied Sciences, Vol. 33, Springer, S.R. Idelsohn Ed. (2014), 217-241. [2] S. Perotto, A. Reali, P. Rusconi and A. Veneziani. HIGAMod: a Hierarchical IsoGeometric Approach for MODel reduction in curved pipes. Comput. & Fluids, 142 (2017), 21-29. [3] Y. A. Brandes C. Barbosa, S. Perotto, A. Veneziani. A Kalman filtering data assimilation procedure based on Hierarchical Isogeometric Model reduction. In preparation.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Multiscale Design of Nonlinear Composites Using an Interface-Enriched Generalized FEM

David Brandyberry*, Philippe Geubelle**

*University of Illinois at Urbana-Champaign, **University of Illinois at Urbana-Champaign

ABSTRACT

Advances in manufacturing technology such as additive manufacturing are enabling the creation of new composite materials with microstructures of increasing complexity. These material microstructures can be designed to fit desired macroscopic responses by changing the geometry and constituent properties. The shape and layout of inclusions, and the properties of their interfaces can greatly affect the constitutive and failure behavior of the composite. These two microstructural parameters, i.e., the shape and properties of the inclusion/matrix interfaces, constitute the design parameters of this study. In this work, a multiscale, parallel Interface-Enriched Generalized FEM (IGFEM) solver is developed to efficiently solve large 3D structural problems involving complex internal microstructures, extract the homogenized macroscopic material properties, and compute the analytic design sensitivities to drive a gradient-based design optimization algorithm. In this study, material interfaces are represented on the highest level by simple geometric shapes which can be described by functions such as spheres and ellipsoids. Standard finite element methods are capable of modeling the constitutive response of complex microstructures. However, generalized finite element methods such as IGFEM have much greater flexibility in representing the discretized geometry without the complex and costly meshing process. Because IGFEM uses a fixed non-conforming mesh, it offers major advantages in shape optimization studies over regular FEM since large shape changes do not cause mesh distortion or require remeshing. To capture the nonlinear behavior of material interfaces, a cohesive law is introduced to govern their traction-separation behavior. A smoothed trapezoidal model provided by (Scheider & Brocks, 2003) is chosen here for its flexibility, allowing us to capture high initial stiffness of the ‘intact interface’ while controlling the progressive failure of the inclusion/matrix interface. Gradient-based design optimization presents a very efficient method for determining optimal microstructure shape and constituents. The optimal set of shape and cohesive interface parameters are found to match the homogenized response to a given desired macroscopic nonlinear constitutive behavior. An analytic shape and material sensitivity is derived to capture the gradients of the described nonlinear problem with respect to our design variables extremely efficiently. Scheider, I., and Brocks, W. (2003). Simulation of cup–cone fracture using the cohesive model. Engineering Fracture Mechanics, 70:14, 1943–1961.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Novel Approaches towards the Efficient Simulation of Falling Nano-Ribbons

Michael Braun*, Raúl Radovitzky**

*Massachusetts Institute of Technology, **Massachusetts Institute of Technology

ABSTRACT

Nano-ribbons are flexible structures whose length is much larger than their width which in turn is much larger than their thickness. These different length scales equip nano-ribbons with some remarkable motion and deformation characteristics when being immersed in certain fluid flows. In this talk, we present our ongoing work towards an efficient simulation tool suitable for exploring these characteristics: We utilize our finite element code SumMIT to simulate the falling behavior of elastic nano-ribbons in an ambient viscous fluid. On the one hand, this task requires the solution of a structural dynamics problem that involves large deformations and different length scales; on the other hand, it also requires an efficient computation of the deformation-dependent viscous forces exerted by the fluid on the nano-ribbons. As for the structural part of our approach to this fluid-structure interaction problem, we model the nano-ribbons using discontinuous Galerkin shell finite elements [1] which have been shown to be effective in the thin shell limit. Regarding the fluid part, we are not aimed at discretizing the fluid domain and solving the full Navier-Stokes equations since we are primarily interested in the motion and deformation of the nano-ribbons under low Reynolds number conditions. Instead, the resulting viscous forces acting onto the nano-ribbons are computed using different fluid models that are based on the assumption of Stokes flow. They comprise a boundary element method for open surfaces [2] and the recently published slender-ribbon theory [3]. In our talk, we elaborate on the coupling of these fluid models to the structural problem, discuss their verification, and present our findings on the falling behavior of elastic nano-ribbons in air. References [1] B. Talamini and R. Radovitzky. A discontinuous Galerkin method for nonlinear shear-flexible shells. Computer Methods in Applied Mechanics and Engineering, 303:128–162, 2016. [2] L. Heltai, J. Kiendl, A. DeSimone, and A. Reali. A natural framework for isogeometric fluid-structure interaction based on BEM-shell coupling. Computer Methods in Applied Mechanics and Engineering, 316:522–546, 2017. [3] L. Koens and E. Lauga. Slender-ribbon theory. Physics of Fluids, 28(1):013101, 2016.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Sediment Transport over Evolutionary Bedforms by the Particle Finite Element Method

Rafael Bravo*, Pablo Becker**, Pablo Ortiz***, Sergio Idelsohn****

*University of Granada, **International Center for Numerical Methods in Engineering, ***University of Granada, ****International Center for Numerical Methods in Engineering

ABSTRACT

The numerical simulation of sediment transport coupled with evolutionary erodible bedforms is essential for the analysis of the morphodynamics of sediment structures. The erosion and evolution of a bedform is a dynamical coupled problem that must be studied with methods able to simulate the interface between the sediment flow and erodible bed. The Particle Finite Element Method (PFEM) with movable mesh was successfully applied in the past to model free surface flows problems such as the interaction of flows with boundaries, or the strong erosion of beds subjected to high velocity flows [1]. A numerical strategy based on the new version of the Particle Finite Element Method with fixed mesh (PFEM-2) is presented for the simulation of sediment flows coupled with evolu-tionary erodible boundaries. The present approach models in a Lagrangian frame with fixed mesh the evolution of a bed-form using an advection–diffusion equation and is solved with the explicit time integration method PFEM-2 from [2], which permits to employ intermediate-large time steps and takes advantage of its easy computer parallelization. This approach overcomes the restrictions of previous PFEM developments applied to model the erosion, see [1], that was simulated by the conversion of soil to fluid elements leading to sudden changes in the geometry. In this work flow and bedform are coupled in a staggered way. Flow is solved using an stand-ard Finite Element fluid solver compatible with Arbitrary Lagrangian–Eulerian (ALE) tech-niques, which allows the deformation of the mesh at every time step. The evolution of bedform and flow is linked by the empirical sediment flux relation of Meyer-Peter-Müller. The model is able to reproduce with good agreement the lab experiments of the evolution of subaqueous small dunes under different flow conditions from [3]. This research is supported by MICIIN Grant #BIA-2015-64994-P (MINECO/FEDER) REFERENCES [1] Oñate E, Celigueta MA, Idelsohn SR (2006) Modeling bed erosion in free surface flows by the particle finite element method. Acta Geotechnica 1(4):237–252. [2] Bravo, R Becker P, Ortiz P (2017) Numerical simulation of evolutionary erodible bedforms using the particle finite element method. Computational Particle Mechanics 4(3):297–305. [3] Leclair S (2002) Preservation of cross-strata due to the migration of subaqueous dunes: an experi-mental investigation. Sedimentology 49(6):1157–1180.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Modeling of Actual-Size Organic Electronic Devices from Efficient Molecular-Scale Simulations

Jean-Luc Bredas*, Haoyuan Li**

*Georgia Institute of Technology, **Georgia Institute of Technology

ABSTRACT

The rational development of organic electronic devices requires to gain a molecular insight into the structure-performance relationships for the organic semiconductor active layers. To this end, molecular-scale simulation techniques, such as the kinetic Monte Carlo (KMC) method, have been exploited in the modeling of organic electronic devices.[1-2] However, such simulations are computationally expensive and, as a result, limited to nanometer-size systems; this is well below the micrometer-size systems that would be needed in order to consider actual-scale morphologies and to reliably model low dopant concentrations and trap densities. An alternate molecular-scale simulation technique, the master equation (ME) approach, is in principle less computationally demanding. However, up to now, ME methodologies have been scarcely applied to device modeling because of their lesser accuracy, which mainly originates in their inability to (fully) account for the electrostatic interactions among charge carriers.[3] Here, we overcome this limitation and show that both short-range and long-range electrostatic interactions can be properly included in ME simulations. The important result is that efficient, reliable molecular-scale simulations can now be applied to systems 100 times the size of those previously accessible. In addition, by exploiting GPU acceleration, we demonstrate that ME simulations of micrometer-sized systems can be completed in a matter of hours on a desktop computer, while the estimated computational cost for an equivalent KMC simulation reaches 300 years. This quantum leap in the modeling capability has allowed us to investigate a micrometer-size diode device and to uncover, in the case of a single-component active layer, that there exist large inhomogeneities in the charge carrier distributions. In the case of a blend morphology, the charge transport in an actual-scale device is found to evolve differently as a function of applied voltage, in comparison to the case of a uniform, single-component film. By now offering the possibility of incorporating such features in the description of realistic-scale systems, our methodology represents a major step into a deeper understanding of the operation of organic electronic devices. References: [1] P. K. Watkins; A. B. Walker and G. L. B. Verschoor, Nano Lett., 2005, 5, 1814. [2] M. Mesta; M. Carvelli; R. J. de Vries; et al., Nat. Mater., 2013, 12, 652. [3] J. J. M. van der Holst; F. W. A. van Oost; R. Coehoorn and P. A. Bobbert, Phys. Rev. B, 2011, 83, 085206.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Task-based Parallelism for Finite-Element Models of Shallow Water Flows

Max Bremer*, Kazbek Kazhyken**, Hartmut Kaiser***, Craig Michoski****, Clint Dawson*****

*The University of Texas at Austin, **The University of Texas at Austin, ***Louisiana State University, ****The University of Texas at Austin, *****The University of Texas at Austin

ABSTRACT

The advent of exascale computing has introduced a massive increase in the amount of concurrency within modern supercomputers. The efficient utilization of these new architectures necessitates a change in programming models. In this talk, we present a task-based implementation of a discontinuous Galerkin finite element method for the shallow water equations. The results have been implemented within a new C++ open-source project, called dgswem-v2, which is a discontinuous Galerkin fork of ADCIRC and parallelized using High Performance ParallelX (HPX). HPX is a novel task-based C++ runtime designed to execute lightweight threads while avoiding costly synchronizations. Scaling results will be presented on the latest architectures including Intel 's Knights Landing as well as Skylake chips. Particular emphasis will be placed on contrasting HPX's performance with a traditional MPI parallelization in order to provide practical insights.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Dynamics of Human Thoracic Aorta under Pulsatile Blood Pressure

Ivan Breslavsky*, Marco Amabili**

*McGill University, **McGill University

ABSTRACT

Introduction and Methods Deformations of a thoracic segment of the human descending aorta under static and dynamic pressure is studied. The aortic segment is modeled as a circular cylindrical shell with three layers (intima, media, and adventitia). The material of each layer is considered to be viscoelastic, hyperlelastic and reinforced by two families of collagen fibers. The anisotropic hyperelastic law used in this study is the Holzapfel-Gasser-Ogden model [1]. As is well known, aortas in vivo are not stress-free even without the blood pressure load. We account for two types of residual stresses – circumferential and axial ones. The shell has spring boundary conditions that simulate the connection with the remaining parts of the aorta and it is filled with pressurized blood, simulated by potential flow theory. The material parameters are taken from the literature [2]. We compare two sets of material parameters, corresponding to middle-aged and old man. Results and Discussion Initially we applied static pressure to obtain the configuration corresponding to the average contribution of the dynamical blood pressure. Subsequently, nonlinear dynamics under physiological pulsatile pressure was analyzed with the local models method [3]. The contribution off the added masses of blood into the inertia has been taken into account, as well as the dynamic stiffening effect. It was found that for the both middle-aged and old patients the amplitude of the dynamical response increases with the heart beating rate in the physiological range. At heart beating rates higher than 100 beats per minute, the dependence of the amplitudes of the aorta response on the frequency of the pulsatile pressure is very significant. This is a strong evidence that nonlinear dynamics is important in evaluating the aorta deformations. References [1] Holzapfel, G.A., Gasser, T.C., and Ogden, R.W., “A New Constitutive Framework for Arterial Wall Mechanics and a Comparative Study of Material Models”, J. Elasticity, 61, pp. 1-48 (2000). [2] Weisbecker, H., Pierce, D.M., Regitnig, P., and Holzapfel, G.A., “Layer-specific damage experiments and modeling of human thoracic and abdominal aortas with non-atherosclerotic intimal thickening”, J. Mech. Behav. Biomedical Mater., 12, pp. 93-106 (2012). [3] Breslavsky, I.D., Amabili, M., and Legrand, M., “Physically and Geometrically Non-Linear Vibrations of Thin Rectangular Plates”, Int. J. Non-Linear Mech., 58, pp. 30-40 (2014).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Successes and Challenges from the Performance Optimisation and Productivity Centre of Excellence

Sally Bridgwater*, Nick Dingle**, Jonathan Boyle***, Jon Gibson****, Wadud Miah*****

*Numerical Algorithms Group Ltd, **Numerical Algorithms Group Ltd, ***Numerical Algorithms Group Ltd, ****Numerical Algorithms Group Ltd, *****Numerical Algorithms Group Ltd

ABSTRACT

The Performance Optimisation and Productivity (POP) Centre of Excellence in Computing Applications was funded by the European Union 's Horizon 2020 programme to help people in the EU write more efficient parallel code and thus boost their productivity. In two and a half years of operation POP has completed approximately 150 investigations of codes drawn from a wide range of scientific domains of which around one third were computational mechanics or fluid dynamics codes. This talk will look at the types of improvements that POP's users have been able to achieve because of engaging with the project. POP's success stories include a CFD code, for which the user reported a 3x performance improvement, an OpenFOAM solver which achieved a 25% performance improvement along with other computational mechanics and CFD examples. We will also draw out some common performance issues identified by the analyses relevant to computational mechanics and fluid dynamics codes as well as highlighting some of the technical and orgnaisational challenges we have had to overcome. The methodology used within the project for analysis of parallel codes, provides a quantitative way of measuring the relative impact of the different factors inherent in parallelisation. A feature of the methodology is that it uses a hierarchy of metrics, each metric reflecting a common cause of inefficiency in parallel programs. These metrics then allow comparison of parallel performance (e.g. over a range of thread/process counts, across different machines, or at different stages of optimisation and tuning) to identify which characteristics of the code contribute to inefficiency. This provides the knowledge necessary to decide the best course of action to get performance, and determine how much effort is needed with a clear view of the potential reward via reproducible and comparable measurements of the performance. POP is a collaboration between Barcelona Supercomputer Center, High Performance Computing Center Stuttgart, Juelich Supercomputing Centre, Numerical Algorithms Group Ltd, RWTH Aachen, and TERATEC.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Semi-automatic Method to Characterize the Mechanical Properties of Specific Patient: Application on Pelvic System

Mathias Brieu*, Guillaume Dufaye**, Olivier Mayeur***, Jean-françois WITZ****, Pauline Lecomte-Grosbras*****, Laurent Patrouix******

*LAMcube, Centrale Lille, France., **Satt nord, LAMcube, France., ***LAMcube, Centrale Lille, France., ****LAMcube, Centrale Lille, France., *****LAMcube, Centrale Lille, France., ******LAMcube, Centrale Lille, France.

ABSTRACT

Female genital prolapse represents a major problem with 60% of women over 60 years old being concerned [1]. To prevent from such problem, numerical simulation of the pelvic mobility aims to evaluate pelvic floor disorder in order to further help for pelvic floor surgery planning [2]. Such application of numerical simulation for surgical evaluation and planning will only be possible if patient-specific anatomy and mechanical properties are known [3]. The aim of the study is to introduce a semi-automatic reconstruction of the pelvic system and the characterization of the mechanical properties of a specific patient. This approach will be validated according to a physical model, based on a representative pelvic system. The Patient-Specific geometric model is obtained from images analysis on MRI allowing to generate a pelvic cavity FE model [3]. Since the principal difficulty is to estimate the intra-abdominal pressure, medical device has been developed to measure the intravaginal pressure during coughing. This probe is compatible with MRI examination to synchronise the pressure and dynamic MRI and motion tracking algorithm. The proposed inverse method is based on the minimization of the gap between Finite Element (FE) analysis and dynamic MRI observation, to finally identify the patient-specific tissue's mechanical properties of anatomical structures. To evaluate this numerical approach, we manufactured a physical model of the pelvic system, compatible with MRI techniques, where every input parameters are totally controlled (imposed pressure, material properties and geometry), in order to mimic the geometry, behaviour, pressure level and compare results. The application to the physical model allows us to quantify uncertainties of the proposed method based on MRI data treatment. The comparison between the imposed pressure and the intravaginal sensor are same with constant gap, which validate the sensor application. Results on the physical model are in range of the experimental data bank of the constitutive material (silicone rubber). This non-destructive identification approach is also validated on patient-specific geometry and works are in progress to apply this method in clinical case, with patient-specific pressure measured with our probe imposed on our FE model. [1] Samuelsson et al. American Journal of Obstetrics and Gynecology, 1999, 180 : 299-305 [2] Chen et al. Journal of Biomechanics, 2015, 48 : 238–245. [3] Mayeur et al. Annals of Biomedical Engineering, 2016, 44(1) : 202-212.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Nanomine – Polymer Nanocomposite Data Resource to Design Next Generation Materials

L. Cate Brinson*, Claire Lin**, Bingyin Hu***, Wei Chen****, Yixing Wang*****, Linda Schadler******, Deborah McGuinniss*******, Jim McCusker********, Rui Yan*********

*Duke University, **Duke University, ***Duke University, ****Northwestern University, *****Northwestern University, ******RPI, *******RPI, ********RPI, *********RPI

ABSTRACT

Nanocomposites can exhibit significant physical property changes with very small loadings of nanofiller. However, the properties of nanocomposites can be influenced by many factors, including chemical synthesis details where small changes in the composition of the constituents can lead to unexpected large changes in resultant properties. Consequently trial-and-error iterative experiments have mainly been used to develop and study these materials. Although systematic approaches and databases have been developed in some areas for metallic alloy systems on top of the processing-structure-property (p-s-p) paradigm, the field of polymers and their composites have largely been lacking. The materials genome concept however offers compelling advantages to enhance our understanding of and design of polymer nanocomposites. In this presentation, we present the Nanomine data resource, the schema and ontology supporting the database, as well as the application of this data resource and case studies. Nanomine is a data-driven web-based infrastructure combining a database, data search and visualization tools, data-driven material analysis tools and physics-based modeling for polymer nanocomposites. Our infrastructure is developed based on the NIST Materials Data Curation System (MDCS). MDCS is inherently a No-SQL based database system and organizes the data using a user-defined XML schema. To appropriately capture the full features of possible data for nanocomposite, we designed the basic structure of the NanoMine schema and continue expanding to incorporate more features during our development. We also developed a robust ontology for polymer nanocomposites based on our XML schema that was used to support organization, search and visualization services of the material data. This ontology also formalizes relationships inherent in our XML schema and can act as a translator to accept multiple XML formats, enhancing ability to share across different data resources. Using the XML schema and the ontology, we have developed a prototype web-based system for polymer nanocomposite material data archiving, data exploration and visualization, characterization and analysis, as well as simulation and design. Current database contained over 1500 samples manually collected from over 150 papers and is continuously expanding. Nanomine aims to capture the physical properties, processing conditions and microstructure information reported in literature or individual research labs using standardized format and terminology. With sufficient data in each p-s-p domain, we are creating case studies to link processing conditions with the quantified microstructure information, interphase properties and bulk composite response by building statistical correlations coupled by image analysis and physics-based simulation tools.

AN ERROR INDICATOR BASED ON A WAVE DISPERSION ANALYSIS FOR THE VIBRATION EIGENMODES OF ANISOTROPIC ELASTIC SOLIDS DISCRETIZED BY THE ENERGY-ORTHOGONAL TWENTY-NODE HEXAHEDRAL FINITE ELEMENT

Francisco J. Brito

Departamento de Ingeniería Industrial, Universidad de La Laguna
Calle Méndez Núñez 67-2C
Santa Cruz de Tenerife 38001, Spain
E-mail address; fjbrito@ull.es

Key words: energy-orthogonal stiffness, numerical dispersion, vibration eigenmodes.

Summary. *This contribution studies the dispersion of the bulk elastic waves in homogeneous and anisotropic elastic media discretized by the twenty-node hexahedral finite element. The element stiffness matrix is split into basic and higher order components which are respectively related to the mean and deviatoric components of the strain field. This decomposition is applied to the elastic energy of the finite element assemblage. By a dispersion analysis the higher order energy is related to the energy error for the propagating waves. An averaged correlation is proposed to apply the higher order energy as an error indicator for vibration eigenmodes*.

1 INTRODUCTION

It is well known that the wave scattering at boundaries creates an interference field that, if composed solely of waves of frequency equal to a natural frequency of the solid, takes the form of a standing-wave field which is an eigenmode of the continuum [1]. For a homogeneous, anisotropic and linearly elastic solid this standing-wave field could be considered essentially composed of bulk quasi-longitudinal and quasi-shear waves. In this case the goal of determining the finite element mesh required to accurately represent a given number of eigenmodes could be approached by analysing the effect of the spatial discretization over the propagation of such bulk waves in unbounded media. This effect becomes apparent by observing the dispersive behavior of the waves, a phenomenon that is not present in the physical system, the analysis of which will be approached in this contribution. A recent sample of the extensive research about the subject of the wave propagation in discretized solid media can be found in reference [2].

The anisotropic elastic media considered in this research cover laminated composites with periodic layering. The oriented plies can be reduced to a unit cell geometry with repeats throughout the laminate. The unit cell is generally composed of alternating uniaxial layers in two or more directions and can also include isotropic layers [3, 4], Fig. 1.

It is supposed that the wavelength of the elastic waves is much larger than the thickness of the unit cell. In this case the laminated composite could be replaced by an effective homogeneous medium with elastic properties computed by the Backus' procedure [5]. Specifically, the laminated composites considered in this research are made combining epoxy, aluminum and diverse fibers. In Table 1, the density ρ and the non-null components of the

elasticity matrix $\mathbf{C}^c$, relating the stresses and engineering strains components, in the material coordinate system, Fig. 1, are shown for the uniaxial basic materials [6, 7, 8, 9].

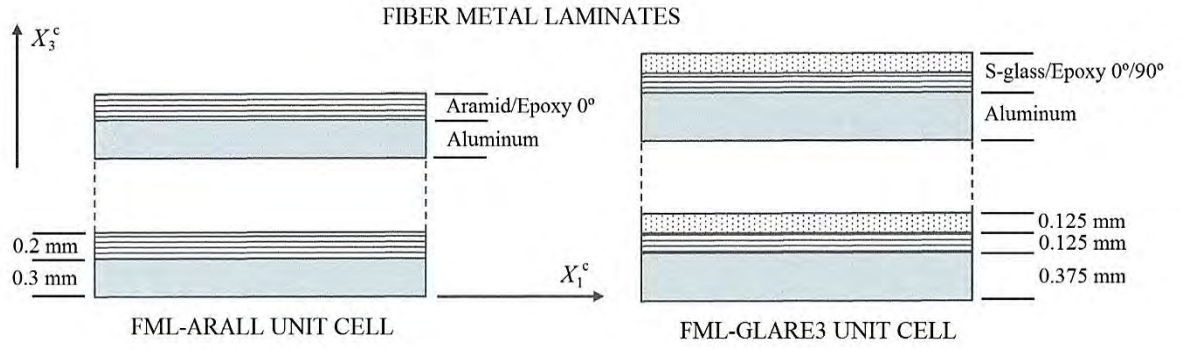


Figure 1. Laminated composites with periodic layering.

C_{IJ}^c	Uniaxial Carbon/Epoxy [6]	Uniaxial Aramid/Epoxy [6]	Uniaxial S-glass/Epoxy [8, 9]	Uniaxial Bo-Al [7]	Isotropic Aluminum [6]
11	162.00	60.00	59.52	269.07	110.00
12	11.80	1.70	8.08	58.50	56.00
13	11.80	5.00	8.08	58.50	56.00
22	17.00	5.80	20.14	188.60	110.00
23	8.20	5.00	8.72	76.34	56.00
33	17.00	8.50	20.14	188.60	110.00
44	4.40	1.80	5.71	56.13	27.00
55	8.00	2.30	7.60	60.19	27.00
66	8.00	2.10	7.60	60.19	27.00
ρ	1610.00	1600.00	2000.00	2520.00	2700.00

Table 1. Elastic properties (GPa) and density (kg/m^3) of the uniaxial basic materials.

1.1 Finite element formulation

In a solid medium discretized by the finite element method the equations of equilibrium governing its linear dynamic response for time-harmonic waves with damping neglected may be cast in matrix form [10],

$$(\mathbf{K} - \omega^2\mathbf{M})\mathbf{x} = \mathbf{F}; \quad \mathbf{x} = \tilde{\mathbf{x}}\exp(-i\omega t), \quad \mathbf{F} = \tilde{\mathbf{F}}\exp(-i\omega t) \tag{1}$$

where: **K** (**M**), stiffness (mass) matrix of the finite element assemblage; $\tilde{\mathbf{x}}$ ($\tilde{\mathbf{F}}$), column matrix containing the complex amplitude of the nodal displacements (nodal external loads); $\omega = 2\pi/T$, circular frequency; T, period of wave; t, time. The elastic energy of the finite element assemblage will be

$$E = \tfrac{1}{2}\,\mathrm{Re}[\mathbf{x}^t]\mathbf{K}\,\mathrm{Re}[\mathbf{x}] \tag{2}$$

Considering the matrix $\mathbf{B}^e$ at element level, relating the engineering strain components to the nodal values of displacement, and the elasticity matrix **C**, the element stiffness matrix will be

$$\mathbf{K}^e = \int_{\Omega e} (\mathbf{B}^e)^t \mathbf{C} \mathbf{B}^e dV \tag{3}$$

If the matrix $\mathbf{B}^e$ is partitioned into mean and deviatoric components,

$$\mathbf{B}^e = \bar{\mathbf{B}}^e + \mathbf{B}_d^e; \quad \bar{\mathbf{B}}^e V^e = \int_{\Omega e} \mathbf{B}^e dV, \quad \mathbf{B}_d^e = \mathbf{B}^e - \bar{\mathbf{B}}^e \tag{4}$$

the matrix Eq. (3) would be decomposed as addition of basic and higher order components,

$$\mathbf{K}^e = \mathbf{K}_b^e + \mathbf{K}_h^e; \quad \mathbf{K}_b^e = (\bar{\mathbf{B}}^e)^t \mathbf{C} \bar{\mathbf{B}}^e V^e, \quad \mathbf{K}_h^e = \int_{\Omega e} (\mathbf{B}_d^e)^t \mathbf{C} \mathbf{B}_d^e dV \tag{5}$$

In this case it is said that the element stiffness matrix is formulated in energy-orthogonal form [11]. The decomposition in Eq. (5) holds for the complete model,

$$\mathbf{K} = \mathbf{K}_b + \mathbf{K}_h \tag{6}$$

For a stationary wave, the amplitude of nodal displacements $\tilde{\mathbf{x}}$ is a real-valued vector. Then, from Eq. (2), the period-averaged elastic energy for the discretized domain will be

$$\bar{E} = \tfrac{1}{2} \tilde{\mathbf{x}}^t \mathbf{K} \tilde{\mathbf{x}} \int_0^1 \cos^2(2\pi\tau) d\tau = \tfrac{1}{4} \tilde{\mathbf{x}}^t \mathbf{K} \tilde{\mathbf{x}} \tag{7}$$

where: $\tau = t/T$, $0 \le \tau \le 1$, dimensionless time. By introducing Eq. (6) into Eq. (7), the basic and higher order period-averaged elastic energies will be obtained. The latter component will be

$$\bar{E}_h = \tfrac{1}{4} \tilde{\mathbf{x}}^t \mathbf{K}_h \tilde{\mathbf{x}} \tag{8}$$

2 DISPERSION ANALYSIS

The unbounded elastic domain is discretized by a regular mesh of standard twenty-node hexahedral finite elements HE20 [10], Fig. 2. The nodal lattice formed by the finite element assemblage has four nodes per unit cell. Different meshes with the same element volume can be obtained by selecting the aspect ratio parameter, $0 < \gamma \le 1$; and the skew angle, $0 \le \beta < 90º$. The angle of rotation α between the finite element mesh coordinate system and the material coordinate system can also be selected, Fig. 2.

For uniform plane harmonic waves, the displacement vector field will be

$$\mathbf{u} = \tilde{\mathbf{u}}(\mathbf{r}) \exp(-i\omega t), \quad \tilde{\mathbf{u}}(\mathbf{r}) = A \hat{\mathbf{a}} \exp(i\kappa \mathbf{n} \cdot \mathbf{r}) \tag{9}$$

where: A, amplitude of the wave; $\hat{\mathbf{a}}$, polarization vector, unit vector indicating the direction of the particle displacement; $\mathbf{n}$, wave normal, unit vector indicating the direction of the wave propagation; $\kappa = 2\pi/\lambda = \omega/c$, wave number; λ, wavelength; c, phase velocity of the continuum.

The wave normal has the components $n_1 = \cos\phi\sin\theta$, $n_2 = \sin\phi\sin\theta$ and $n_3 = \cos\theta$, where: ϕ, azimuthal angle, $0 \le \phi \le 360º$; θ, polar angle, $0 \le \theta \le 180º$, Fig. 2.

The polarization vectors and phase velocities are solution of the Christoffel Equation [12],

$$(l_{iK} C_{KL} l_{Lj}) \hat{a}_j = \rho c^2 \hat{a}_i, \quad i, j = 1, \ldots, 3; \quad K, L = 1, \ldots, 6 \tag{10}$$

where the non-null values of l_{iK} are: $l_{11} = n_1$, $l_{15} = n_3$, $l_{16} = n_2$, $l_{22} = n_2$, $l_{24} = n_3$, $l_{26} = n_1$, $l_{33} = n_3$, $l_{34} = n_2$, and $l_{35} = n_1$.

The elasticity matrix in the finite element mesh coordinate system and the one in the material coordinate system are related by the equation $C_{KL} = M^B_{KI} C^c_{IJ} M^B_{LJ}$, where $\mathbf{M}^B$ is the Bond matrix.

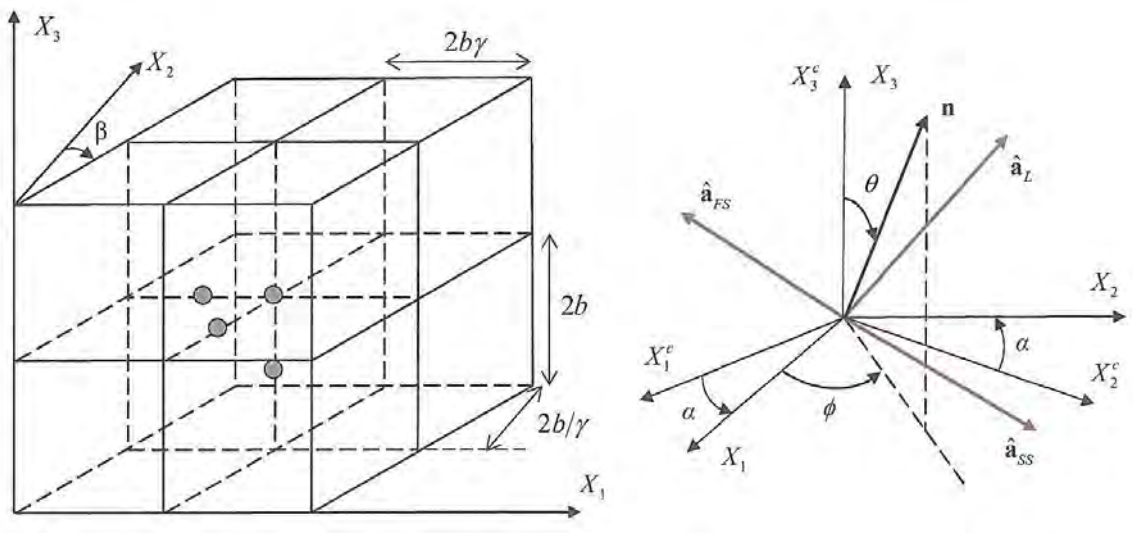


Figure 2. Elastic domain discretized by a regular mesh of HE20 elements and polarization vectors.

The three mutually orthogonal waves computed by solving the eigenproblem Eq. (10) are, Fig. 2: ($\hat{\mathbf{a}}_{SS}$, c_{SS}), slow quasi-shear wave, SS; ($\hat{\mathbf{a}}_{FS}$, c_{FS}), fast quasi-shear wave, FS; and ($\hat{\mathbf{a}}_L$, c_L), quasi-longitudinal wave, L.

For a plane elastic wave Eq. (9) the density of period-averaged elastic energy can be computed by the equation [6],

$$\overline{E}_0 = \tfrac{1}{4}\rho\omega^2 A^2 \tag{11}$$

2.1 Characteristic equations

The characteristic equations can be found assuming harmonic waves Eq. (9) with different amplitudes in each node of the unit cell,

$$\tilde{\mathbf{u}} = A_j \hat{\mathbf{a}} \exp(i\kappa \mathbf{n}\cdot\mathbf{r}), \quad j = 1,\ldots,4 \tag{12}$$

Inserting the solutions Eq. (12) into the homogeneous part of Eq. (1), the characteristic equation for each node of the unit cell is yielded by equilibrium of nodal forces into the direction of the particle displacement [13],

$$\mathbf{F}_K \cdot \hat{\mathbf{a}} - \omega^2 \mathbf{F}_M \cdot \hat{\mathbf{a}} = 0 \tag{13}$$

where: $\mathbf{F}_K$, nodal force associate to the global stiffness matrix; $\mathbf{F}_M$, nodal force associate to the global mass matrix.

By considering Eq. (13) for each node of the unit cell, a homogeneous system of four algebraic equations is formed,

$$\mathbf{ZA} = \mathbf{0}$$
$$\left[a_{ij}(m,\phi,\theta,\alpha,\beta,\gamma) + \varpi^2 b_{ij}(m,\phi,\theta,\alpha,\beta,\gamma) \right] A_j = 0, \quad i,j = 1,\ldots,4 \tag{14}$$

$$m = b\kappa/\pi = 2b/\lambda, \quad \varpi = (2b/c)\,\omega \tag{15}$$

where: m, dimensionless wave number, $0 < m < 1$; b, half of the element size; ϖ, dimensionless frequency of the discretized elastic domain.

In this procedure the global stiffness matrix has been expressed in a suitable form,

$$\mathbf{K} = \rho c^2 (2b)\mathbf{K}^0 \tag{16}$$

Similarly, the global mass matrix has been expressed as $\mathbf{M} = \rho(2b)^3 \mathbf{M}^0$.

2.2 Dispersion equations

The system of homogeneous algebraic equations given in Eq. (14) has a non-trivial solution only if the matrix **Z** is singular; that is, det [**Z**] = 0. Then it is yielded the following polynomial equation which is called the characteristic frequency equation for the plane wave propagation,

$$\sum_{r=0}^{4} c_r(m,\phi,\theta,\alpha,\beta,\gamma)\varpi^{2r} = 0, \quad c_4 = 1 \tag{17}$$

By computing the zeros of Eq. (17), the four dispersion equations are then yielded,

$$\varpi_k = \varpi_k(m,\phi,\theta,\alpha,\beta,\gamma), \quad k = 1,\ldots,4 \tag{18}$$

Substituting Eq. (18) into Eq. (14), the wave amplitudes corresponding to the nodes of the unit cell are yielded for each dispersion equation. The range of dimensionless wave number values where each dispersion equation represents the propagation of elastic waves in the discretized medium will be called the acoustical branch of the dispersion equation. In order to determine the acoustical branches the following constraint conditions are imposed,

$$A_1 = 1; \quad A_j(m,\phi,\theta,\alpha,\beta,\gamma) > 0, \quad j = 2,3,4 \tag{19}$$

$$(\partial\varpi/\partial m)_{\phi,\theta,\alpha,\beta,\gamma} > 0 \tag{20}$$

In molecular physics, condition Eq. (19) is called the restriction of the lattice spectrum to the acoustical branch [14]. The constraint condition Eq. (20) imposes that the normal component of the energy transport velocity must have the wave direction [6]. The preliminary constraint condition dim [**N**(**Z**)] = 1 over the dimension of the null space of matrix **Z** must be imposed in order to Eq. (19) would be a meaningful constraint condition. From this point, for each dispersion equation only the acoustical branch will be considered.

From Eq. (15) the indicators of numerical dispersion for the phase velocity and the normal component of the group velocity can be expressed as

$$e_p = c_p / c = (2\pi)^{-1} \varpi / m, \quad e_{gn} = c_{gn} / c = (2\pi)^{-1} \partial \varpi / \partial m \tag{21}$$

2.3 Elastic energy at the unit cell

From Eq. (2), (15) and (16) the density of period-averaged elastic energy is computed,

$$\bar{E} = \tfrac{1}{2} \rho (\omega / \varpi)^2 \int_0^1 \mathrm{Re}[\tilde{\mathbf{x}}^t \exp(-i2\pi\tau)] \, \mathrm{Re}[\tilde{\mathbf{F}}^0 \exp(-i2\pi\tau)] d\tau \tag{22}$$

where: $\mathbf{F}^0 = \tilde{\mathbf{F}}^0 \exp(-i2\pi\tau)$, column matrix of forces at the nodes of the unit cell.

From the decomposition in Eq. (6), the above computed density of period-averaged elastic energy Eq. (22) can be partitioned as addition of basic and higher order components. Then, the percentage of period-averaged higher order elastic energy can be defined as

$$e_h = \bar{E}_h / \bar{E}, \quad e_h = e_h(m, \phi, \theta, \alpha, \beta, \gamma) \tag{23}$$

From Eq. (22) and (11), the percentage indicator of elastic energy error associated with the spatial discretization that is introduced by the finite element model is defined as

$$\varepsilon = (\bar{E} / \bar{E}_0) - 1, \quad \varepsilon = \varepsilon(m, \phi, \theta, \alpha, \beta, \gamma) \tag{24}$$

From Eq. (23) and (24), a mapping between the elastic energy error and the percentage of higher order elastic energy can be also computed,

$$\varepsilon = \varepsilon(e_h, \phi, \theta, \alpha, \beta, \gamma) \tag{25}$$

2.4 Numerical research

For the SS, FS and L waves, the indicators Eq. (21), (23) and (24) are computed versus dimensionless wave number for different meshes, directions of wave propagation and media. An example of the indicators Eq. (23) and (25) is shown in Fig. 3. It is observed that Eq. (23) and it is deduced that Eq. (24) both vanish as dimensionless wave number goes to zero; that is, as the mesh is refined and in the limit of long waves. It must be remarked that the behavior of the higher order elastic energy as dimensionless wave number goes to zero is a consequence that the strain field inside each element becomes uniform. That is, given the mesh, in the limit of long waves, the density of elastic energy approaches to zero more slowly than its higher order component; and, given the wavelength, as the solution converges on account of mesh refinement, the density of elastic energy is increasingly dominated by its basic component.

Investigating the relationship between the elastic energy error and the percentage of higher order elastic energy Eq. (25), it can be observed from Fig. 3 that both variables could be related by a cubic function for moderate values of the higher order elastic energy,

$$\varepsilon = (A(\phi, \theta, \alpha, \beta, \gamma) * e_h + B(\phi, \theta, \alpha, \beta, \gamma)) * e_h^2 \tag{26}$$

For each of the waves (SS, FS, and L) and media considered in this research, an averaged correlation between the elastic energy error and the percentage of higher order elastic energy is sought by computing averaged values for the coefficients *A* and *B*.

First, two reference values of the percentage of higher order elastic energy are selected. Then, by Eq. (23) and Eq. (25), the related reference values of dimensionless wave number and percentage of elastic energy error are respectively computed,

$$e_{h1} = 0.10 \quad e_{h2} = 0.20 \quad \rightarrow \quad m_{1,2} = f_{m1,2}(\phi, \theta, \alpha, \beta, \gamma), \quad \varepsilon_{1,2} = f_{\varepsilon 1,2}(\phi, \theta, \alpha, \beta, \gamma) \tag{27}$$

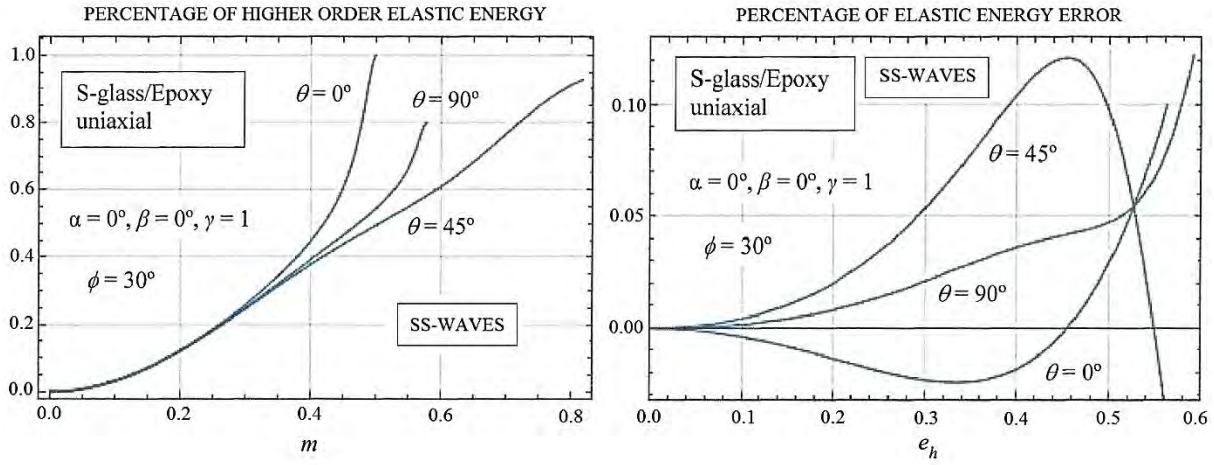


Figure 3. Higher order elastic energy versus dimensionless wave number and versus elastic energy error.

Next, the mean value of each reference dimensionless wave number and the root mean square value of each reference energy error are computed on the range of propagation angle,

$$m_{1,2}^{M}(\alpha, \beta, \gamma) = \tfrac{1}{\pi^2} \int_0^{\pi} \int_0^{\pi} m_{1,2} d\phi d\theta, \quad \varepsilon_{1,2}^{RMS}(\alpha, \beta, \gamma) = \sqrt{\tfrac{1}{\pi^2} \int_0^{\pi} \int_0^{\pi} \varepsilon_{1,2}^{2} d\phi d\theta} \tag{28}$$

The integrals in Eq. (28) are computed by a step of $\pi/36$ for the azimuthal and polar angles. For media with cross-ply fibers, the finite element mesh coordinate system and the material one are coincident ($\alpha = 0^{\circ}$); however, for media with uniaxial fibers, the finite element mesh coordinate system is oriented both in the direction of the fibers ($\alpha = 0^{\circ}$) and perpendicular to them ($\alpha = 90^{\circ}$), being averaged the values of the integrals computed in each case.

Then, the mean reference values above computed are averaged by selecting three different meshes having the same element volume, Fig. 2: Q_1, square section: $\beta = 0^{\circ}$, $\gamma = 1$; Q_2, rectangular section with aspect ratio (1:2): $\beta = 0^{\circ}$, $\gamma = 1/\sqrt{2}$; Q_3, skewed section: $\beta = 45^{\circ}$, $\gamma = 1$. That is,

$$\overline{m_{1,2}^{M}} = \tfrac{1}{3}\left[m_{1,2}^{M}(Q_1) + m_{1,2}^{M}(Q_2) + m_{1,2}^{M}(Q_3) \right], \quad \overline{\varepsilon_{1,2}^{RMS}} = \tfrac{1}{3}\left[\varepsilon_{1,2}^{RMS}(Q_1) + \varepsilon_{1,2}^{RMS}(Q_2) + \varepsilon_{1,2}^{RMS}(Q_3) \right] \tag{29}$$

The above computed mesh-averaged reference values Eq. (29) are shown in Tables 2 and 3 for each of the media and waves investigated. For details of ARALL and GLARE3 see Fig. 1.

Finally, by the mesh-averaged reference values of elastic energy error, the averaged values of the coefficients A and B for the cubic correlation Eq. (26) are then computed,

$$\overline{\varepsilon_{1,2}^{RMS}} = [\overline{A} * e_{h1,2} + \overline{B}] * e_{h1,2}^{2} \quad \rightarrow \quad \varepsilon = (\overline{A} * e_h + \overline{B}) * e_h^{2} \tag{30}$$

By similar procedure, the mesh-averaged reference values of the indicators of numerical dispersion for the phase velocity and the normal component of the group velocity Eq. (21) are also computed. The second mesh-averaged reference values are shown in Table 4.

		Carbon/Epoxy uniaxial	Aramid/Epoxy uniaxial	S-glass/Epoxy uniaxial	Bo-Al uniaxial	Aluminum
$\overline{m_1^M}$	SS	0.1755	0.1755	0.1755	0.1755	0.1755
	FS	0.1754	0.1754	0.1756	0.1755	0.1755
	L	0.1752	0.1751	0.1749	0.1749	0.1747
$\overline{m_2^M}$	SS	0.2570	0.2567	0.2569	0.2569	0.2569
	FS	0.2568	0.2566	0.2570	0.2570	0.2568
	L	0.2557	0.2555	0.2551	0.2548	0.2544
		HOMOGENIZED				
		Carbon/Epoxy Cross-ply	Aramid/Epoxy Cross-ply	S-glass/Epoxy Cross-ply	ARALL	GLARE3
$\overline{m_1^M}$	SS	0.1755	0.1755	0.1755	0.1755	0.1755
	FS	0.1756	0.1757	0.1757	0.1756	0.1757
	L	0.1751	0.1751	0.1750	0.1750	0.1749
$\overline{m_2^M}$	SS	0.2570	0.2568	0.2568	0.2568	0.2568
	FS	0.2573	0.2576	0.2574	0.2573	0.2574
	L	0.2557	0.2554	0.2551	0.2554	0.2548

Table 2. Mesh-average of the mean values of the first and second reference dimensionless wave number.

		Carbon/Epoxy uniaxial	Aramid/Epoxy uniaxial	S-glass/Epoxy uniaxial	Bo-Al uniaxial	Aluminum
$\overline{\varepsilon_1^{RMS}}$	SS	0.002755	0.002735	0.002756	0.002757	0.002781
	FS	0.003224	0.003424	0.002944	0.002831	0.002781
	L	0.003676	0.003843	0.004249	0.004426	0.004928
$\overline{\varepsilon_2^{RMS}}$	SS	0.011963	0.011687	0.011995	0.011988	0.011963
	FS	0.014300	0.015536	0.012862	0.012312	0.011963
	L	0.016685	0.018174	0.020068	0.021241	0.024421
		HOMOGENIZED				
		Carbon/Epoxy Cross-ply	Aramid/Epoxy Cross-ply	S-glass/Epoxy Cross-ply	ARALL	GLARE3
$\overline{\varepsilon_1^{RMS}}$	SS	0.002831	0.002756	0.002797	0.002801	0.002784
	FS	0.003025	0.003046	0.002828	0.002910	0.002831
	L	0.003800	0.003906	0.004256	0.004227	0.004540
$\overline{\varepsilon_2^{RMS}}$	SS	0.012340	0.011892	0.012252	0.012133	0.012201
	FS	0.012893	0.013034	0.012220	0.011945	0.012031
	L	0.016635	0.017561	0.020050	0.019338	0.021910

Table 3. Mesh-average of the rms values of the first and second reference percentage of elastic energy error.

From Table 2 it is deduced that the first and second mesh-averaged reference values of elastic energy error roughly correspond, in an averaged sense, to six and four elements per wavelength, respectively. The same conclusion can be applied to the mesh-averaged reference values of the indicators of numerical dispersion. In such averaged sense, the elastic energy error of the quasi-longitudinal waves is greater than the one of the quasi-shear waves, Table 3. The elastic energy error of the slow quasi-shear waves is weakly dependent on the elastic properties and its second

mesh-averaged reference value is slightly greater than one per cent. An opposite behavior is shown by the indicators of numerical dispersion, Table 4. In this case, the numerical dispersion of the quasi-shear waves is greater than the one of the quasi-longitudinal waves, and the indicator of numerical dispersion of the quasi-longitudinal waves is the variable weakly dependent on the elastic properties.

		Carbon/Epoxy uniaxial	Aramid/Epoxy uniaxial	S-glass/Epoxy uniaxial	Bo-Al uniaxial	Aluminum
$\overline{e_{p2}^{M}}$	SS	1.00320	1.00393	1.00317	1.00316	1.00348
	FS	1.00304	1.00275	1.00305	1.00312	1.00348
	L	1.00221	1.00225	1.00221	1.00219	1.00207
$\overline{e_{gn2}^{M}}$	SS	1.01584	1.01937	1.01570	1.01564	1.01723
	FS	1.01502	1.01366	1.01511	1.01545	1.01723
	L	1.01084	1.01104	1.01078	1.01065	1.01005
		HOMOGENIZED				
		Carbon/Epoxy Cross-ply	Aramid/Epoxy Cross-ply	S-glass/Epoxy Cross-ply	ARALL	GLARE3
$\overline{e_{p2}^{M}}$	SS	1.00286	1.00309	1.00290	1.00251	1.00275
	FS	1.00303	1.00282	1.00317	1.00333	1.00357
	L	1.00219	1.00227	1.00222	1.00217	1.00215
$\overline{e_{gn2}^{M}}$	SS	1.01419	1.01539	1.01435	1.01252	1.01366
	FS	1.01502	1.01404	1.01574	1.01649	1.01768
	L	1.01075	1.01112	1.01085	1.01061	1.01046

Table 4. Second mesh-averaged reference values of the indicators of numerical dispersion.

3 MODAL ANALYSIS

As application it is explored the use of the averaged correlation Eq. (30) as a reference to apply the higher order elastic energy as an error indicator for the finite element vibration eigenmodes. These ones are the solution of the eigenproblem [10],

$$(\mathbf{K} - \omega_j^2 \mathbf{M})\tilde{\boldsymbol{\psi}}_j = \mathbf{0}, \quad j = 1, \ldots, n \tag{31}$$

where ω_j and $\tilde{\boldsymbol{\psi}}_j$ are the finite element natural frequencies and eigenvectors, respectively.

By introducing the relation of **K**-orthogonality $\tilde{\boldsymbol{\psi}}_i^T \mathbf{K} \tilde{\boldsymbol{\psi}}_j = \delta_{ij} \omega_j^2$ into Eq. (7), the following expression for the modal elastic energy is yielded,

$$\overline{E}_j = \tfrac{1}{4} \omega_j^2, \quad j = 1, \ldots, n \tag{32}$$

The error for the modal elastic energy computed with the discretized elastic domain is estimated by a reference model that will be obtained by dividing each element of the actual mesh into eight elements. The modal elastic energies computed with the actual model and the ones computed with the reference model will be compared by the modal elastic energy error,

$$EEE = (\overline{E} / \overline{E}^{REF}) - 1, \quad EEE = (\omega / \omega^{REF})^2 - 1 \tag{33}$$

where $\overline{E}$ and $\overline{E}^{REF}$ are defined by Eq. (7), and Eq. (32) has been taking into account.

The modal elastic energy error computed by mesh halving Eq. (33) will be compared with the so-defined as standard modal elastic energy error which is computed by averaging the correlation Eq. (30) for the slow and fast quasi-shear waves, and by using the higher order elastic energy computed with the actual model,

$$SEEEs(PHE) = \tfrac{1}{2}(\varepsilon_{SS} + \varepsilon_{FS}) \tag{34}$$

where the percentage of higher order elastic energy computed with the actual model PHE will be evaluated by Eq. (7) and (8).

In order to select the standard modal elastic energy error Eq. (34), it has been taking into account the heuristic that given the frequency both the percentage of higher order elastic energy and the spatial discretization error should be mainly influenced by the slowest waves which have the shortest wavelengths.

Two test problems have been analyzed, Fig. 4: a tapered block fixed at its base and made of cross-ply carbon/epoxy homogenized, and a cantilever thick plate made of nine unit cells of FML-GLARE3 homogenized.

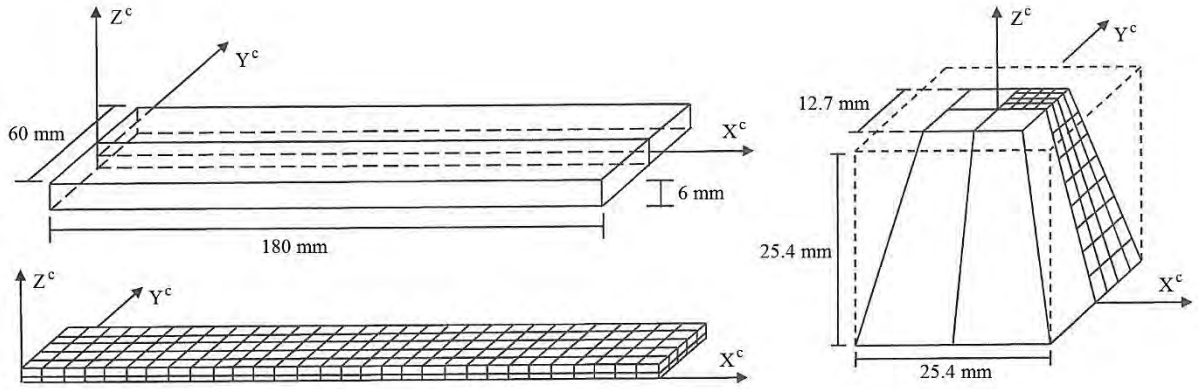


Figure 4. Tapered block fixed at its base and cantilever thick plate.

From Table 5 it is observed that the percentage of higher order energy PHE decreases as the mesh is refined for each of the eigenmodes computed. Then, this energy component behaves as a modal error indicator, which is in accordance with the numerical dispersion analysis.

From Fig. 5 it is observed that the standard modal energy error SEEEs Eq. (34) generally overestimates the modal energy error computed by mesh halving EEE Eq. (33). For the tapered block, which is a bulk solid, both indicators generally exhibit similar evolution shapes as the modal order increases. Clearly, by the standard modal energy error SEEEs the accuracy of the finite element eigenmodes could be confidently verified in order to select a cutoff modal order for values of energy error up to a neighbourhood of one per cent, an optimum upper bound to properly capture the eigenmodes from the engineering point of view.

4 CONCLUSIONS

The noteworthy conclusions of this contribution are:

#MODE	TYPE	PHE	PHE REF	#MODE	TYPE	PHE	PHE REF
1	AS	0.066156	0.017351	9	AS	0.083576	0.022333
2	AA	0.090874	0.026115	10	AS	0.076795	0.019839
3	AS	0.068166	0.017944	11	AS	0.086763	0.023320
4	AS	0.072159	0.019119	12	AA	0.103444	0.029204
5	AA	0.092516	0.026555	13	AS	0.099536	0.027649
6	AA	0.095225	0.027235	14	AS	0.094541	0.025594
7	AS	0.077795	0.020745	15	AA	0.109833	0.030844
8	AA	0.098722	0.028061	16	AS	0.112904	0.032069

Table 5. Cantilever thick plate. Percentage of higher order elastic energy computed with the actual model PHE versus the one computed by the reference model PHE REF.

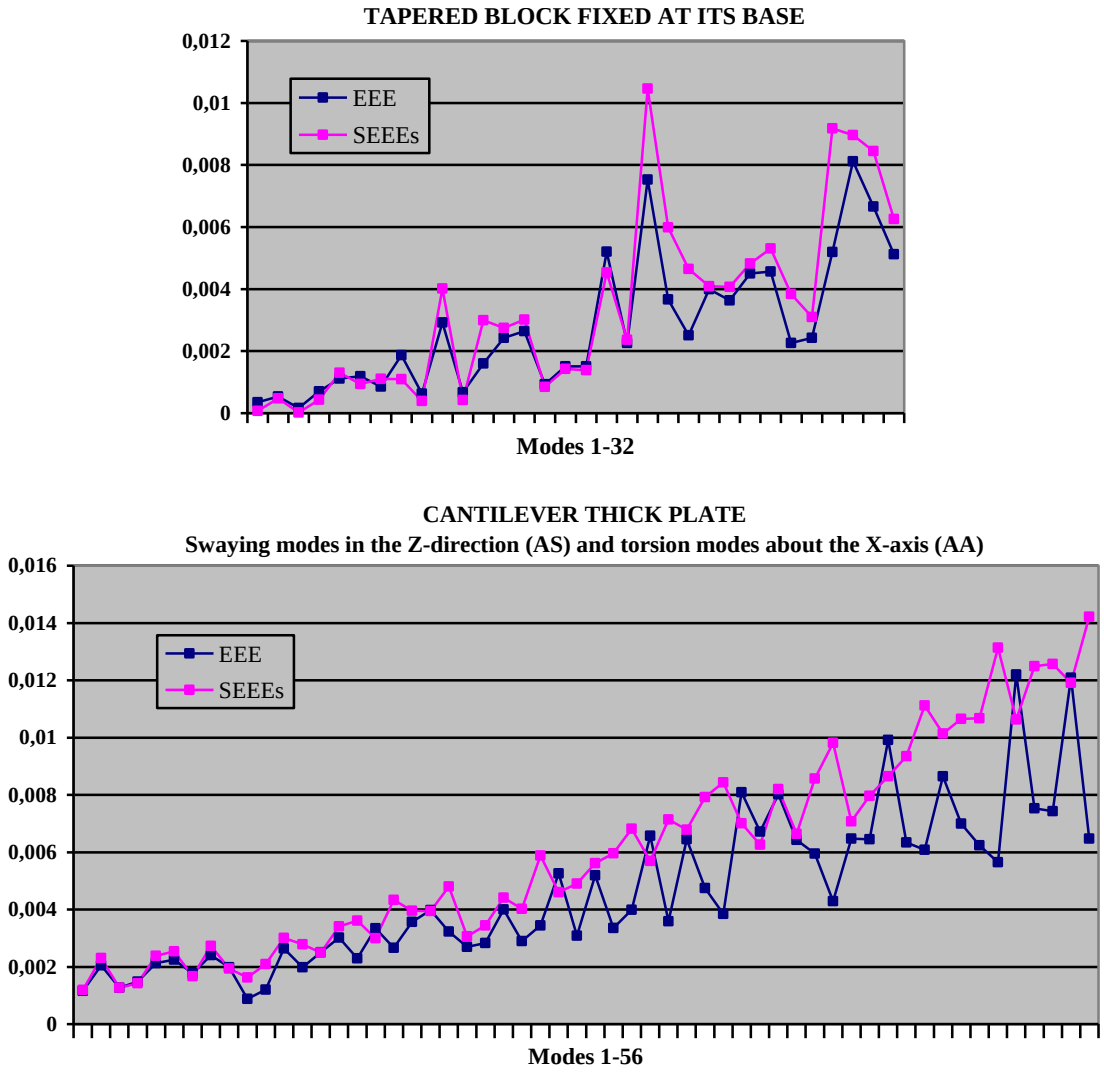


Figure 5. Standard modal elastic energy error SEEEs versus modal elastic energy error computed by mesh halving EEE for two test problems.

- - For homogeneous and anisotropic elastic media discretized by the energy-orthogonal twenty-node hexahedral finite element, by a dispersion analysis of plane harmonic waves an averaged correlation between the percentage of higher order elastic energy and the elastic energy error is yielded both for the quasi-longitudinal waves and the quasi-shear waves.
- - The use of the slow quasi-shear wave correlation and the fast quasi-shear wave correlation as reference to apply the higher order elastic energy as an error indicator for the finite element vibration eigenmodes is successfully tested.

REFERENCES

[1] Fahy, F. Sound and structural vibration. Academic Press, (1985).

[2] Kolman, R., Cho, S.S., Park, K.C. and Gonzalez, J.G. An explicit time scheme with local time stepping for one-dimensional wave and impact problems in layered and functionally graded materials. Proceedings COMPDYN 2017. Rhodes Island, Greece.

[3] Vlot, A. and Gunnink, J.W. Fibre metal laminates an introduction. Kluwer Academic Publishers, (2001).

[4] Alderliesten, R. Fatigue and fracture of fibre metal laminates. Springer, (2017).

[5] Milton, G.W. The theory of composites. Cambridge University Press, (2002).

[6] Rokhlin, S.I., Chimenti, D.E. and Nagy, P.B. Physical ultrasonics of composites. Oxford University Press, (2011).

[7] Datta, S.K. and Shah, A.H. Elastic waves in composite media and structures. CRC Press, (2009).

[8] Baker, A.A. and Scott, M.L. Composite materials for aircraft structures. American Institute of Aeronautics and Astronautics AIAA, (2016).

[9] Kollár, L.P. and Springer, G.S. Mechanics of composite structures. Cambridge University Press, (2003).

[10] Bathe, K.J. Finite Element Procedures. Prentice Hall, (1996).

[11] Felippa, C.A., Haugen, B. and Militello, C. From the individual element test to finite element templates: evolution of the patch test. Int. J. Meth. Eng. (1995) 38:199-229.

[12] Auld, B.A. Acoustic fields and waves in solids. Volume I. Krieger Publishing Company, (1990).

[13] Okrouhlík, M. and Höschl, C. A contribution to the study of dispersive properties of one-dimensional lagrangian and hermitian elements. Computers and Structures (1993) 49:779-795.

[14] Brillouin, L. Wave propagation in periodic structures. Dover Publications, (2003).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Virtualisation of Realistic Microstructures for 3D Crystal Plasticity Using Limited Information

Ben Britton*, Simon Wyatt**, Yi Cui***

*Imperial College London, **Imperial College London, ***Imperial College London/Brunel

ABSTRACT

As material scientists and engineers, we have developed the ability to extract data-rich information that describe the evolving deformation state from the surface of 3D materials, using techniques such as high angular resolution electron backscatter diffraction (EBSD) and high spatial resolution digital image correlation (DIC). This information can be used to understand the evolution of the deformation state of the material on the surface, and this data is now coupled with physically based simulations to explore the validity, and utility, of crystal plasticity models [1]. However, we know that the 3D state of the material can be important but that it can be expensive to access with high fidelity (e.g. using destructive sectioning methods or difficult to access X-ray synchrotron experiments) and for routine samples. In this talk, we will present a new framework to utilise a combined 2D morphology, stereology derived morphology information and crystallographic texture to create representative, and useful, microstructures for input into a 3D FFT based crystal plasticity simulation (using DAMASK [2]). In this talk, we will outline the methodology and discuss how it can be used to understand the efficacy of crystal plasticity models in predicting deformation. [1] Jiang, J., Dunne, F.P.E., and Britton, T.B. "Towards predictive understanding of fatigue crack nucleation in Ni-based superalloys " JOM (2017) http://dx.doi.org/10.1007/s11837-017-2307-9 [2] https://damask.mpie.de

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Nonlinear System Stochastic Response Determination Under Non-white and Non-Gaussian Excitation via the Wiener Path Integral Technique

Olga Brudastova*, Ioannis Kougioumtzoglou**, Apostolos Psaros***, Aaron Appelle****, Giovanni Malara*****

*Columbia University, **Columbia University, ***Columbia University, ****Columbia University, *****University of Reggio Calabria

ABSTRACT

Uncertainty propagation in engineering mechanics and dynamics is a highly challenging problem that requires development of analytical/numerical techniques for determining the stochastic response of complex engineering systems. In this regard, although Monte Carlo simulation (MCS) has been the most versatile technique for addressing the above problem, it can become computationally daunting when faced with high-dimensional systems or with computing very low probability events. Thus, there is a demand for pursuing more computationally efficient methodologies, such as the recently developed Wiener Path Integral (WPI) technique [1-3]. In this paper, the WPI technique for determining the joint response probability density function (PDF) of nonlinear systems subject to Gaussian white noise excitation is generalized to account for non-white, non-Gaussian, and non-stationary excitation processes. Specifically, modeling the excitation process as the output of a filter equation with Gaussian white noise as its input, it is possible to define an augmented response vector process to be considered in the WPI solution technique. A significant advantage relates to the fact that the technique is still applicable even for arbitrary excitation power spectrum forms. In such cases, it is shown that the use of a filter approximation facilitates the implementation of the WPI technique in a straightforward manner, without compromising its accuracy necessarily. Several numerical examples pertaining to both single- and multi-degree-of-freedom systems are considered, while comparisons with Monte Carlo simulation (MCS) data demonstrate the accuracy of the technique. [1] H. S. Wio, Path integrals for stochastic processes: An introduction. World Scientific, 2013. [2] I. A. Kougioumtzoglou, P. D. Spanos, An analytical Wiener Path Integral technique for non-stationary response determination of nonlinear oscillators, Probabilistic Engineering Mechanics 28 (2012) 125-131. [3] I. A. Kougioumtzoglou, P. D. Spanos, Nonstationary stochastic response determination of nonlinear systems: A Wiener Path Integral formalism, Journal of Engineering Mechanics 140 (9) (2014) 04014064.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Model Reduction and A Posteriori Error Estimation in the Context of Stable Variational Formulations of Parametrized Transport Equations

Julia Brunken*, Mario Ohlberger**, Kathrin Smetana***, Karsten Urban****

*University of Münster, **University of Münster, ***University of Twente, ****University of Ulm

ABSTRACT

Motivated by high-dimensional kinetic transport equations we consider in this talk stable variational formulations and model reduction techniques for possibly time-dependent transport equations. Kinetic equations describe densities in phase space consisting of independent space, time, and velocity variables. To tackle the high-dimensionality we employ the Reduced Basis-Hierarchical Model Reduction approach where we use a problem-adapted basis in the velocity variable to arrive at a hyperbolic system in the space-time domain [1]. In this context, stable discretizations and efficient error estimators are desirable both for the construction of the reduced basis and the validation of reduced solutions. To derive such stable variational formulations for general transport equations we use, similar to [2], an ultraweak approach to find an L^2 approximation of the solution. We introduce new pairs of optimally stable trial and test spaces: By first choosing a suitable test space and then defining the trial space by the application of the adjoint operator, we obtain optimally stable spaces with an inf-sup constant of one in the continuous as well as in the discrete case. The setting allows for an easy implementation of the solution procedure and is especially beneficial in the context of model reduction for parametrized transport equations: We apply the Reduced Basis method to parametrized equations within this framework and investigate possible a posteriori error estimators used in the construction of the reduced model. Due to the optimally inf-sup-stable setting, residual-based error estimators benefit from perfect constants, and, in contrast to previous works, no further stabilization is needed for the reduced spaces. Hence, also the reduced models can be constructed easily and efficiently. We exemplify the approach by presenting numerical results for full order and reduced order models for kinetic transport equations and compare our new framework to existing works [2, 3]. References: [1] J. Brunken, T. Leibner, M. Ohlberger, and K. Smetana. Problem adapted hierarchical model reduction for the Fokker-Planck equation. Proceedings of the Conference Algoritmy, pages 13–22, 2016. [2] W. Dahmen, C. Huang, C. Schwab, and G. Welper. Adaptive Petrov-Galerkin methods for first order transport equations. SIAM J. Numer. Anal., 50(5):2420–2445, 2012. [3] W. Dahmen, C. Plesken, and G. Welper. Double greedy algorithms: reduced basis methods for transport dominated problems. ESAIM Math. Model. Numer. Anal., 48(3):623–663, 2014.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Machine Learning and Sparse Optimization to Characterize and Control Fluids

Steven Brunton*

*University of Washintgon

ABSTRACT

The discovery of physical laws and governing equations from data is currently undergoing a revolution, driven by the rise of big data, algorithmic advances, and increasing computational power. In complex, multi-scale systems, physical laws often remain elusive, although data are abundant. This presentation will discuss recent approaches to leverage machine learning and sparse optimization to characterize and control multi-scale systems using the following generalized pipeline: 1) identify low-dimensional patterns in high dimensional data, 2) discover dynamical systems governing the evolution of these patterns, 3) compute embeddings defined by intrinsic coordinates in which the nonlinear dynamics appear linear, 4) identify optimized sensor locations to maximally inform real-time dynamics, and 5) design controllers to manipulate system behavior. The overarching perspective taken in this work is that of parsimony and interpretability, preferring simple, compact, and efficient model representations. First, we will describe the sparse identification of nonlinear dynamics (SINDy) framework to discover the governing equations underlying a dynamical system simply from data measurements, leveraging advances in sparsity-promoting techniques and machine learning. The resulting models are parsimonious, balancing model complexity with descriptive ability while avoiding overfitting. The only assumption about the structure of the model is that there are only a few important terms that govern the dynamics, so that the equations are sparse in the space of possible functions. This perspective, combining dynamical systems with machine learning and sparse sensing, is explored with the overarching goal of real-time closed-loop feedback control of complex systems. Next, connections to the Koopman operator will be discussed. Koopman operator theory has emerged as a dominant method to represent nonlinear dynamics in terms of an infinite-dimensional linear operator. A linear representation of nonlinear dynamics has tremendous potential to enable the prediction, estimation, and control of nonlinear systems with standard textbook methods developed for linear systems. Particular emphasis will be placed on the use of data-driven Koopman theory to characterize and control high-dimensional fluid dynamic systems. This presentation will focus primarily on applications in fluid dynamics, although many pressing applications stand to benefit from these methods, such as understanding cognition from neural recordings, inferring patterns in climate, determining stability of financial markets, predicting and suppressing the spread of disease, and controlling turbulence for greener transportation and energy.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Modified Phase Field Model for Mixed-mode Crack Propagation with Consistent Kinematic Modes

Eric Bryant*, WaiChing Sun**

*Columbia University, **Columbia University

ABSTRACT

Cracks in brittle, isotropic, homogeneous materials often propagate such that the pure Mode I kinematic mode is maintained at the crack tip. However, numerous geo-materials, such as sedimentary rock, shale, mudstone, concrete and gypsum, the Mode I and Mode II critical fracture energies are distinct. In such cases, it is likely that secondary Mode II and mixed-mode propagation may occur. This has previously been exhibited by experiments where wing cracks and secondary cracks develop from pre-existing flaws under a combination of shear and tensile or shear and compressive loadings. To capture the mixed-mode fracture propagations, a mixed-Mode I/II fracture model that employs multiple critical critical energy release rates based on Shen and Stephansson, IJRMMS, 1993 is adopted in a phase field framework. Within each incremental time step, an explicit-implicit operator-split scheme is used such that a local energy minimization problem is solved such that the crack propagation direction and the corresponding kinematics modes are determined. This step is followed by the update of the phase field and that of the displacement. Several numerical examples that demonstrated the Mode II and mixed mode crack propagations in brittle materials are presented. Possible extensions of the model that captures the degradation related to shear/compressive damage commonly observed in sub-surface applications and triaxial compression tests are discussed.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Numerical Analysis of Damage and Fracture Mechanisms in Ductile Metals at Different Loading Conditions

Michael Brünig*, Steffen Gerke**, Marco Schmidt***

*Bundeswehr University Munich, **Bundeswehr University Munich, ***Bundeswehr University Munich

ABSTRACT

The presentation deals with the numerical analysis of the effect of stress state on damage and fracture behavior of ductile metals. Within the general framework of continuum thermodynamics of irreversible processes a thermodynamically consistent anisotropic damage and failure model based on kinematic definition of damage tensors is discussed. The continuum model is based on free energy functions defined in fictitious undamaged and damaged configurations, respectively, leading to elastic material laws which are affected by damage. It is well known that besides stress intensity, stress triaxiality and the Lode parameter are important factors that control initiation of plastic flow, damage and fracture. In this context, a generalized hydrostatic-stress-dependent yield condition and a non-associated flow rule are used to adequately describe the plastic behavior of ductile metals. Furthermore, a damage criterion formulated in stress space is proposed based on a series of experiments and corresponding numerical simulations. Different branches of the damage criterion are taken into account corresponding to different damage and fracture mechanisms depending on stress triaxiality and Lode parameter. To validate these criteria new experiments with different two-dimensionally loaded specimens taken from aluminum alloy sheets have been developed. Specimens' geometries and loading conditions have been proposed using numerical simulations of biaxial experiments to achieve different stress states in critical regions where damage and fracture are expected to occur. These biaxially loaded specimens will allow consideration of combined shear-tension and shear-compression stress states leading to different damage and fracture mechanisms. Numerical analysis of these tests show that they cover a wide range of stress triaxialities and Lode parameters. Numerically predicted damage and fracture modes are validated by scanning electron microscopy of fracture surfaces.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Kino-Geometric Sampling Reveals Functional Molecular Motions Across Scales

Dominik Budday*, Rasmus Fonseca**, Sigrid Leyendecker***, Henry van den Bedem****

*Chair of Applied Dynamics, University of Erlangen-Nuremberg, Germany, **Department of Molecular and Cellular Physiology, Stanford University, USA; Biosciences Division, SLAC National Accelerator Laboratory, Stanford University, USA, ***Chair of Applied Dynamics, University of Erlangen-Nuremberg, Germany, ****Biosciences Division, SLAC National Accelerator Laboratory, Stanford University, USA

ABSTRACT

The function of macromolecules relies on fast, dynamic exchanges between three-dimensional conformations. Molecular dynamics (MD) simulations can reveal time-resolved, atomically detailed snapshots of these exchanges, but require sophisticated computational resources to overcome spatio-temporal barriers separating functional substates. By contrast, algorithms for randomized exploration of molecular conformational spaces can provide a fast, coarse-grained alternative, while still providing insight into molecular mechanisms. Here, we present our kino-geometric sampling (KGS) and modeling framework to study functional molecular motions across scales. KGS represents molecules as articulated multi-body complexes with dihedral angles as revolute degrees of freedom and selected non-covalent interactions such as hydrogen bonds as holonomic constraints [1]. The constraints define a lower-dimensional manifold in conformation space. KGS can rapidly explore the constraint manifold or model conformational transitions [2] using collision-free move sets proposed by sophisticated motion planners. Maintaining constraints along a sampling trajectory reduces expensive energy calculations and can bridge spatio-temporal scales out of reach for MD. Modeling the conformational transition of Adenylate Kinase between apo and holo states confirms that the KGS structural pathway passes known intermediate crystal structures as close as dynamic importance sampling molecular dynamics [2]. KGS revealed coupled motions between the functionally important M20 and FG-loops in Dehydrofolate Reductase, in qualitative agreement with MD [3]. Furthermore, our method suggests that a hydrogen bond network imparts a spatially resolved hierarchy of protein motions, analogous to eigenmodes from normal mode analysis. Enhancing our approach with a more sophisticated force-field may help access hidden excited states based off intermediate structures. Taken together, KGS is a versatile toolbox, capable of studying molecular flexibility and rigidity, and modeling. Our method is a supplementary, kinematic approach to generate hypotheses about functional dynamics of macromolecules. Subsequent detailed MD simulations can validate these hypotheses, and provide access to kinetics. [1] D. Budday, S. Leyendecker, and H. van den Bedem. Journal of the Mechanics and Physics of Solids 83, 36-47, 2015. [2] D. Budday, R. Fonseca, S. Leyendecker, and H. van den Bedem. Proteins: Structure, Function, and Bioinformatics 85(10), 1795-1807, 2017. [3] R. Fonseca, D. Budday, and H. van den Bedem. Journal of Computational Chemistry, DOI: 10.1002/jcc.25138, 2018 (in press).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Biomechanical Characterization of Brain Tissue

Silvia Budday*, Gerhard Sommer**, Paul Steinmann***, Gerhard Holzapfel****, Ellen Kuhl*****

*Friedrich-Alexander Universität Erlangen-Nürnberg, **Graz University of Technology, ***Friedrich-Alexander Universität Erlangen-Nürnberg, ****Graz University of Technology, Norwegian University of Science and Technology, *****Stanford University

ABSTRACT

Computational simulations are a powerful tool to understand the mechanical behavior of biomaterials. However, an essential prerequisite for realistic numerical predictions is the thorough experimental characterization of the material response. It is required to develop appropriate constitutive models and, equally importantly, to carefully calibrate the corresponding constitutive parameters. Biomechanical testing can be challenging for ultrasoft tissues such as brain tissue due to its high deformability and fragileness. Different test setups have led to contradictory results in the literature, not only with respect to the tissue's stiffness but also concerning directional and regional dependencies, or the influence of post-mortem time. This clearly demonstrates that the test setup has to be carefully chosen to guarantee a homogeneous deformation and to minimize boundary effects. Here, we perform finite element simulations to study effects of specimen geometry or loading modes and set the limits for maximum loadings that still allow for a homogeneous deformation state. We show that rectangular specimen dimensions can mistakenly yield a direction-dependent response. We further discuss the influence of the tissue's compressibility. Our results are valuable to design appropriate test setups and optimize testing conditions in the future.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Human Osteocyte Development during Bone Formation in a Bone-on-chip

Elisa Budyn*, Nabila Gaci**, Samantha Sanders***, Morad Bensidhoum****, Patrick Tauc*****, Bertrand Cinquin******, Eric Schmidt*******, Herve Petite********

*Ecole Normale Superieure Cachan, **Ecole Normale Superieure Cachan, ***Ecole Normale Superieure Cachan, ****University Paris-Diderot, *****Ecole Normale Superieure Cachan, ******Ecole Normale Superieure Cachan, *******University of Illinois at Chicago, ********University Paris-Diderot

ABSTRACT

Osteocytes are long-term living cells responsible for bone mineralization and characterized by a body bearing numerous processes. Osteocytes orchestrate bone homeostasis and coordinate the interactions between the osteoclasts and mesenchymal stem cells (MSCs) during remodeling. Osteoblasts differentiate into osteocytes or bone lining cells that cover non-remodeling endosteal bone surfaces that are recruited during the activation phase to seal the site of bone formation by osteoblasts, modulate the osteoclastic resorption and further differentiate into osteoblasts. However fundamental knowledge of human bone stromal cells in situ mechanobiology is challenging to quantify in particular as the mechanical properties of their environment changes as mineralization takes place. Bones-on-chip offer the opportunity to develop in situ 3D imaging and modelling of concurrent chemo-mechanical phenomena in controlled conditions and for long-term culture. Human mesenchymal stem cells were reseeded in decellularized human bone to create bone-on-chip that were cultured for over 26 months. The application of mechanical load to live systems is known to influence the cell differentiation, matrix formation and biological response. In situ measurements of the mechanical microenvironment of the cells can be quantified numerically while the cell chemical response can be observed in vitro for human native osteocytes and stem cell derived osteocytes in either native or neo-formed ECM. The cell morphology, expressed genes, and their production of proteins and minerals using PCR, immunohistochemistry, in situ immunofluorescence and the conditioned medium analysis can monitor the cell differentiation and secretome. The cytoplasmic calcium concentration variations seemed to adapt to the expected in vivo mechanical load at the successive stages of cell differentiation in agreement with studies using fluid flow stimulation. The bone-on-chip produced after 109 days an ECM of which the strength was nearly a quarter of native bone and that contained type I collagen at 256 days and calcium minerals at 39 days. The morphology of the cells displayed organized network and the newly-formed matrix were further characterized by immuno-fluorescence under confocal microscopy at 547 days and revealed the presence of E11 and sclerostin. Different cells populations were identified and one type was organized in network and connected by long processes.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Assessing the Impact of Strength Model Parameters on Simulated Cerium Flyer Plate Behavior

Joanne Budzien*, Karlene Maskaly**, JeeYeon Plohr***

*Los Alamos National Laboratory, **Los Alamos National Laboratory, ***Los Alamos National Laboratory

ABSTRACT

Cerium flyer plate experiments were simulated using the LANL Lagrangian hydrodynamics code FLAG and results were compared to experimental results. The range of experiments examined includes shocking through the cerium gamma-alpha phase transition. Several sets of parameters for the Preston-Tonks-Wallace strength model have been produced through fits to experimental Hopkinson bar data. We will present simulation results showing the effect of varying the strength parameter sets including simulations with no strength. This process may aid in differentiating the various parameter sets by testing them under conditions different from the calibration experiments.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Bone Mineral Heterogeneity as a Signature of Remodelling and Mineralisation Processes: Linking to the Cellular Scale

Pascal Buenzli*, Chloé Lerebours**, Paul Roschger***, Andreas Roschger****, Richard Weinkamer*****

*School of Mathematical Sciences, Queensland University of Technology, Brisbane, Australia, **School of Mathematical Sciences, Monash University, Clayton, Australia, ***Ludwig Boltzmann Institute of Osteology at the Hanusch Hospital of WGKK and AUVA Trauma Centre Meidling, 1st Medical Department, Hanusch Hospital, Vienna, Austria, ****Max Planck Institute of Colloids and Interfaces, Department of Biomaterials, Potsdam, Germany, *****Max Planck Institute of Colloids and Interfaces, Department of Biomaterials, Potsdam, Germany

ABSTRACT

Bone mineral density distributions (BMDDs) are frequency distributions of bone mineral density that provide measures of the mineral heterogeneity of bone samples. While BMDDs have been shown to provide signatures of bone physiology in health and disease [1], mathematical models of BMDDs are required to decrypt how dynamic parameters of bone remodelling and bone mineralisation are entangled in these measurements [2,3]. In this contribution, we will present new mathematical developments that enable us to account for the influence of microscopic resorption patterns of osteoclasts in the mineral make-up of a bone sample. We use this mathematical model to interpret differences observed in BMDD measurements of trabecular bone and femoral cortical bone [3]. Our analysis shows that it is not possible to explain these differences in BMDD measurements by accounting only for differences in turnover rate between these two skeletal sites, nor by accounting for differences in turnover rate and in osteoclast resorption patterns. We propose that the rate of mineral accumulation in bone matrix must differ as well. The BMDD properties of peak position and width in trabecular and femoral cortical BMDDs could be explained by a simple hypothesis, namely that minerals accumulate in bone matrix at a speed proportional to bone turnover rate. This suggests a primordial role of the micro-environmental availability of minerals, freed up during bone resorption, in how they become embedded in bone matrix at late stages of mineralisation. References 1. Roschger P, Paschalis EP, Fratzl P, Klaushofer K (2008) Bone 42:456 2. Ruffoni D, Fratzl P, Roschger P, Klaushofer K, Weinkamer R (2007) Bone 40:1308 3. Buenzli PR, Lerebours C, Roschger A, Roschger P, Weinkamer R (2017) Late stages of mineralisation and their signature on the bone mineral density distribution. In press, Conn. Tiss. Res.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Real-time Patient Specific Surgical Simulation using Corotational Cut Finite Element Method: Application to Needle Insertion Simulation

Huu Phuoc Bui*, Satyendra Tomar**, Franz Chouly***, Alexei Lozinski****, Stéphane P. A. Bordas*****

*University of Franche-Comté, **University of Luxembourg, ***University of Franche-Comté, ****University of Franche-Comté, *****University of Luxembourg

ABSTRACT

We present the Corotational Cut Finite Element Method for real-time surgical simulation. Users only need to provide a background mesh which is not necessarily conforming to the boundaries/interfaces of the simulated object. The details of the latter, represented by its surface or/and its internal interfaces, which can be directly obtained from binary images, are taken into account by a multilevel subelement embedding algorithm applied to elements of the background mesh that are cut by the surface/interfaces. To stabilize the system matrix when elements are cut by the surface/interfaces with very small intersections, we propose to move the background node(s) of the concerned cut elements by a distance proportional to the element size. This approach is simple but it can avoid the stability issues in such situations. Moreover, this approach does not include additional parameters as, e.g. ghost penalty method [1]. Dirichlet boundary conditions can be implicitly imposed on the surface using Lagrange multipliers, whereas traction or Neumann boundary conditions, which is/are applied on parts of the surface, can be distributed to the background nodes using shape functions. The implementation is verified by convergence studies with optimal rates. To verify the reliability of the method, it is applied to various needle insertion simulations (e.g. for biopsy or brachytherapy) into brain and liver models while considering frictional interactions between the needle and the tissue. Numerical results show that the present method can make the discretization independent from geometric description, and it can avoid the complexity of mesh generation of complex geometries while retaining the accuracy of the standard Finite Element Method. The proposed methodology is very suitable for real-time and patient specific simulations as it improves the simulation accuracy by automatically, and properly, taking the geometry of the simulated object into account. References [1] E. Burman et al, Int J Numer Meth Engg, vol. 104, no. 7, pp. 472-501, 2015.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Quantifying the Effects of Intraluminal Thrombi and Their Poroelastic Properties on Abdominal Aortic Aneurysms

Martina Bukac*, Miguel Rodriguez**, Shawn Shadden***

*University of Notre Dame, **University of California Berkeley, ***University of California Berkeley

ABSTRACT

An abdominal aortic aneurysm (AAA) occurs when weakened aortic walls bulge or dilate. Because the aorta is the primary conduit of blood to the body, a ruptured AAA can cause life-threatening bleeding. Intraluminal thrombi (ILT) are found in most of AAAs of clinically relevant size, and their influence on the wall stress and risk of rupture remains highly controversial. We will present a novel, poroelastic model for intraluminal thrombus (ILT), which captures both the flow within ILT and its deformation. The model for ILT is coupled with pulsatile blood flow and arterial wall deformation. The fully coupled model is used to study the biomechanics in a patient-specific abdominal aortic aneurysm (AAA). Using finite element analysis, numerical simulations were performed to investigate the role of ILT on the risk of AAA rupture as assessed by Peak Wall Stress (PWS). We will present a numerical study of the effects of ILT permeability on the vascular wall stress, as well as the risk of ILT embolization.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Data-driven Approach for Stability and Control of Fluid-Structure Systems

Sandeep Reddy Bukka*, Allan Ross Magee**, Rajeev K Jaiman***

*National University of Singapore, **National University of Singapore, ***National University of Singapore

ABSTRACT

A data-driven model reduction approach for fluid-structure interaction (FSI) problem of a vibrating structure in an incompressible flow is presented. The method relies on the Eigensystem Realization algorithm (ERA) to construct the reduced-order model (ROM) in a state-space format, which provides a low-order representation of the unsteady flow dynamics in the neighborhood of the equilibrium steady state. A systematic stability analysis is performed via ERA-based ROM to obtain the eigenvalue distribution and to estimate a possible lock-in region of a coupled FSI system. A series of numerical tests on canonical configurations such as single, side-by-side and tandem cylinder arrangements in both two dimensional (low Re) and three dimensional (high Re) regimes are carried out. The proposed method is shown to produce consistent results from numerical tests when compared to full order nonlinear fluid-structure simulations in terms of predicting the lock-in regions. The motivation behind choosing such diverse test cases is to demonstrate the versatility of the proposed method. From the stability analysis, two modes are found to be dominant and contribute towards the phenomenon of VIV. The mode with the frequency close to that of wake flow behind stationary structure is termed as wake mode (WM) and the one with frequency close to the natural frequency of the structure is referred to as structure mode (SM). Shifting the eigenvalues of SM from unstable to stable region essentially manifests the mitigation of the VIV of structure. This can be achieved by using active feedback control techniques such as blowing and suction or passive control techniques. Appendages such as fairings, connected-C, helical strakes on the structure can be very effective in the suppression of VIV and are considered as passive control techniques in this study. Overall, the proposed stability analysis framework is proven to be effective in designing both active and passive control techniques by shifting the unstable eigenvalues of the SM to the stable region. [1] Yao, W., and Jaiman, R., 2017. "Model reduction and mechanism for the vortex-induced vibrations of bluff bodies". Journal of Fluid Mechanics, 827 pp. 357-393 [2] Yao, W., and Jaiman, R., 2017. "Feedback control of unstable flow and vortex-induced vibration using the eigensystem realization algorithm". Journal of Fluid Mechanics, 827, pp. 394-414 [3] Reddy, S. B., Magee, A. R., & Jaiman, R., 2018. "A Data-driven approach for stability analysis of Vortex-Induced Vibrations". In ASME 2018 37th International Conference on Ocean, Offshore and Arctic Engineering, (under review)

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Numerical Investigation of Coupling Schemes for Structural Acoustics

Gregory Bunting*, Scott Miller**

*Sandia National Laboratories, **Sandia National Laboratories

ABSTRACT

Loosely coupled schemes for structural-acoustic coupling are examined that obtain the same order of accuracy as the monolithic scheme. The coupling algorithms are implemented in Sierra-SD, a massively parallel finite element application for structural dynamics and acoustics. By adapting the predictor-corrector scheme of Farhat et al. (2006), second order time accuracy is achieved with the loosely coupled approach. Node-to-face mappings allow arbitrary discretizations of the structural-acoustic interface. Convergence rates are verified with a one dimensional piston problem with known solution. Numerical results are compared to a shock induced plate experimental benchmark. Computational times for loose and strong coupling are compared for a sphere scattering problem.
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Computational Design of 2D Nano-Materials Using Two-Stage Searching Strategy Combining Molecular and Ab-initio Approaches

Tadeusz Burczynski*, Waclaw Kus**, Marcin Mazdziarz***, Adam Mrozek****

*Institute of Fundamental Technological Research of Polish Academy of Sciences, Warsaw, Poland, **Silesian Technical University, Gliwice, Poland, ***Institute of Fundamental Technological Research of Polish Academy of Sciences, Warsaw, Poland, ****AGH University of Science and Technology, Kraków, Poland

ABSTRACT

New potentially 2D graphene-like materials are generated by the two-stage searching strategy combining molecular and ab-initio approaches. The two candidates X and Y are obtained from molecular calculations and the memetic base algorithm which combines the evolutionary algorithm and the conjugate-gradient optimization technique. The main goal of the optimization is to find stable arrangements of carbon atoms under certain imposed conditions (e.g. density, shape and size of the unit cell). The fitness function is formulated as the total potential energy of an atomic system. The optimized structure is considered as a discrete atomic model and interactions between atoms are modeled using the AIREBO potential, especially developed for carbon and hydrocarbon materials. The parallel approach used in computations allows significant reduction of computation time. Validation of the obtained results and examples of the models of the new 2D materials X and Y obtained using the described algorithm are presented, along with their mechanical properties [1]. In the second stage the two candidates X and Y are then in depth analysed using first-principles Density Functional Theory from the mechanical, structural, phonon and electronic properties point of view. Both proposed polymorphs of graphene X and Y are mechanically and dynamically stable and can be metallic-like [2]. Optimal searching for the new stable atomic arrangements of two-dimensional graphene-like carbon lattices with predefined mechanical properties are also considered using the described memetic method combines the evolutionary algorithm and the conjugate-gradient optimization. The main goal of the optimization is to find stable arrangements of carbon atoms placed in the unit cell with imposed periodic boundary conditions, which reveal desired mechanical properties. Two examples of the newly obtained models of the flat, carbon materials are presented. Their mechanical properties are additionally validated during the simulation of the tensile tests using molecular dynamics [3]. At present both new 2D materials with predefined mechanical properties are analysed using first-principles DFT. References [1] Mrozek A., Kus W., Burczynski T., Nano level optimization of grapheme allotropes by means of a hybrid parallel evolutionary algorithm. Comput. Mater. Sci, 106, 2015, 161-169. [2] Mazdziarz M., Mrozek A., Ku? W., Burczynski T., First-principles study of new X-graphene and Y-graphene polymorphs generated by the two stage strategy. Materials Chemistry and Physics, 202, 2017, 7-14. [3] Mrozek A., Kus W., Burczynski T., Method for determining structures of new carbon-based 2D materials with predefined mechanical properties. Inter. J. Mulstiscale Computational Engineering, 15(5), 2017, 379-394.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Understanding the Damage Evolution of Dry Carbon Fibre Yarns in Contact with Pulleys During Textile Processing

Boris Burgarella*, Louis Laberge Lebel**, Alexandre Marcoux***

*Ecole Polytechnique de Montreal, **Ecole Polytechnique de Montreal, ***Ecole Polytechnique de Montreal

ABSTRACT

Thanks to their great specific rigidities and resistances, composite materials tends to progressively replace metal in the design of high-performance struc- tures. As an example, the last generation of airliners (Airbus A350, Boeing 787, and Bombardier CSeries) now includes up to 50% in mass of composite mate- rials. Carbon fibers are often chosen to design parts that undergo heavy loads. These fibers are usually shipped as tows, consisting of hundreds to thousands clustered single filaments. May it be for coating, storage, braiding or weaving process, carbon tows often needs to be driven through a series of pulleys. Such a process may induce strong material loss due to filament rupture and therefore induce unwanted costs. In order to understand the cause of this rupture, carbon fiber tows behavior have been investigated through experimental and numerical analyses. Filament scale explicit dynamic calculations have been conducted and compared to experimental measurements gathered on a specifically designed test bed. The experimental and numerical data obtained with different pulley and tow architectures have then been used to determine a rupture criterion.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Modelling and Application of Viscoelastic Material Behavior with Fractional Derivatives

Michael Burgwitz*, Matthias Wangenheim**

*Scientific Assistant, **Assistant Director

ABSTRACT

In structural dynamics the modelling of the material behavior is an important challenge. Some materials like steel can be well represented by linear constitutive laws but when dealing with viscoelastic components these relations become more complex. A common way to represent viscoelastic behavior is the so called prony series. A less known approach is the use of fractional derivatives. We apply a force-displacement based formulation incorporating fractional derivatives to model viscoelastic behavior to be able to simulate measured results: We recalculate a measured DMTA and compare its prony series and fractional representation. After that we utilize the fractional model to calculate the stick-slip behavior of a pneumatic seal. After giving a short overview regarding fractional derivatives and their numerical treatment in general, it is shown how we incorporated these into the material model. The detailed explanation of the model is followed by its application and comparison to measured results.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

How to Overcome the 90 Degree Uncertainty in Collagen Fibre Orientation Evaluated Using Polarized Light Microscopy

Jiri Bursa*, Stanislav Polzer**, Kamil Novak***, Anna Polisenska****, martin Hrton*****, Petr Dvorak******

*Brno University of Technology, Czech Republic, **VSB-Technical University of Ostrava, Czech Republic, ***TRW Automotive Czech s.r.o., Czech Republic, ****Brno University of Technology, Czech Republic, *****Brno University of Technology, Czech Republic, ******Brno University of Technology, Czech Republic

ABSTRACT

Although collagen fibers are responsible for distinctive mechanical response of many biological tissues such as skin, tendons, cartilages or arteries, information on their orientation and dispersion in arteries is still insufficient, ambiguous and contradictory; it is often estimated from a few manual Polarized Light Microscopy (PLM) measurements (typically n~10e1 points per image). The automated PLM algorithm we have proposed in [1] offers an amount of information on fiber orientations which is larger by orders (n~10e4 points per image) and operator-independent. The results are comparable with those obtained from quantitative polarized light microscopy requiring much more sophisticated and expensive equipment, such as confocal microscope with a quarter-wave plate and rotating analyzer [2]. Our algorithm was verified using artificial images with both sinus-like and straight lines mimicking the arrangement of collagen fibers in soft tissues and also validated using histological images of porcine tendons with more or less wavy fibers. Unfortunately, in the basic setup of PLM microscope (analyzer perpendicular to polarizer) our algorithm is limited by the 90° periodicity of polarized light intensity, i.e. it cannot distinguish between mutually perpendicular directions. The novelty of the presented approach is in a specific angle between the polarizer and analyzer which results in transmitting some colors (monochromatic light of specific wavelengths) with 180° periodicity. Exploitation of intensity of different colors enables us to transform histological images into histograms of directions in the full range between 0 and 180°. Although interpretation of these histograms is easy and straightforward only for tissues with straight collagen fibers or their regular periodical waviness, the method can make the automated analysis of preferred directions in fibrous tissues widely accessible and help to disclose preferential directions in any birefringent structures. In the field of arterial tissues, it has a potential to distinguish between dispersion and waviness of collagen fibers or between their local and global directions, as well as to answer the still opened question on the number of fiber families in different arterial tissues. It can be also advantageously used for calibration of another automated method based on nonpolarized light microscopy and Fast Fourier Transform [3]. Acknowledgement This work was supported by project of Czech Science Foundation No. 18-13663S. References [1] Novak K. et al., Microscopy and Microanalysis, 2015, doi:10.1017/S1431927615000586 [2] Massoumian F. et al., Quantitative polarized light microscopy, Journal of Microscopy, 2003, 10.1046/j.1365-2818.2003.01095.x [3] Polzer S. et al., Microscopy and Microanalysis, 2013, doi:10.1017/S1431927613013251

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Tuning Mechanical Instabilities with Magnetoelastomers

Philip Buskohl*, Vincent Chen**, Carson Wiley***, Abigail Juhl****, Stephan Rudykh*****

*AFRL, **UES, Inc, ***UES, Inc, ****AFRL, *****Technion - Israel Institute of Technology

ABSTRACT

Magnetoelastomers are an important class of hyperelastic materials that generate a large deformation and stiffness increase in respond to a magnetic field. An intrinsic mechanical response to a magnetic field is advantageous due to the fast, reversible and non-contact tuning of the material properties. Potential applications for magnetoelastomers include soft actuators, adaptive vibration dampers, mechanical filters and sensors. Previous theoretical studies have predicted that stiffness tuning of the MAE can be leveraged to tune the critical buckling strain in stiff/soft laminates of MAEs within a non-active elastomeric matrix [1,2], however experimental validation is needed. To address this issue, we fabricated the stiff/soft composite MAE laminate specimens using a commercial silicone (Sylgard 184) as the non-responsive soft matrix and a silicone loaded with carbonyl iron particles for the stiff, magnetoactive layer. The polymer matrix underwent several modifications to increase the stiffness ratio between the soft encapsulating matrix and the stiff MAE layer, including tuning of the crosslinker to polymer ratio, incorporation of hydride-terminated silicone to promote a linear network, and addition of silicone oil to further reduce crosslinking. A custom compression test jig was developed to systematically load the laminate specimen in the presence of a magnetic field. The study provides feedback on the sensitivity of the buckling strain to experimental specimen sizing/edge effects and provides broader insight on the practical integration of MAE instabilities into functional devices. [1] Rudykh, S., et al. “Multiscale instabilities in soft heterogeneous dielectric elastomers” Proceedings of the Royal Society A, Vol. 470. No. 2162, 2014 [2] Rudykh, S, and Bertoldi, K. "Stability of anisotropic magnetorheological elastomers in finite deformations: a micromechanical approach." Journal of the Mechanics and Physics of Solids, 61.4 (2013): 949-967.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Consistent Bayesian Inference with Push-Forward Measures: Surrogate Modeling and Convergence of Solutions

Troy Butler*, Tim Wildey**, John Jakeman***

*CU Denver, **Sandia National Laboratories, ***Sandia National Laboratories

ABSTRACT

Models are useful for simulating key processes and generating significant amounts of (simulated) data on quantities of interest (QoI) computed as a set of functionals from a model solution. This simulated data can be compared directly to observable data to address many important questions in scientific modeling. However, many key characteristics governing system behavior described as input parameters in the model remain hidden to direct observation. Thus, scientific inference fundamentally depends on the formulation and solution of a stochastic inverse problem (SIP) to describe sets of probable model parameters. Statistical Bayesian inference (see e.g., [1, 2]) is the most common approach solving the SIP using both data and an assumed error model on the QoI to construct posterior distributions of model inputs and model discrepancies. We have recently developed an alternative Bayesian solution to the SIP based on the measure-theoretic principles developed in [3]. We prove that this approach, which we call consistent Bayesian inference, produces a posterior distribution that is consistent in the sense that the push-forward probability density of the posterior through the QoI map will match the distribution on the observable data, i.e., the posterior is consistent with the model and the data [4]. Our approach only requires approximating the push-forward probability density of the prior, which is fundamentally a forward propagation of uncertainty. We briefly summarize the consistent Bayesian approach including existence, uniqueness, and stability of solutions. A comparison to statistical Bayesian inference is also provided. Motivated by computationally expensive models, we discuss the impact of using surrogate models to approximate the QoI on the construction of the push-forward of the prior density. We then outline the basic theoretical argument of convergence of the push-forward of the prior density using a generalized version of the Arzela-Ascoli theorem to prove a converse of Scheffe's theorem. REFERENCES [1] M. Kennedy and A. O 'Hagan, “Bayesian calibration of computer models”, Journal of the Royal Statistical Society: Series B (Statistical Methodology), Vol. 63, pp. 425-464, (2001). [2] A. M. Stuart, “Inverse problems: A Bayesian perspective”, Acta Numerica, Vol. 19, pp. 451–559, (2010). [3] J. Breidt, T. Butler, and D. Estep, “A computational measure theoretic approach to inverse sensitivity problems I: Basic method and analysis”, SIAM J. Numer. Analysis, 49, pp. 1836–1859, (2012). [4] T. Butler, J. Jakeman and T. Wildey, “A consistent Bayesian formulation for stochastic inverse problems based on push-forward measures”, arXiv:1704.00680, submitted and in review (2016)

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

On Application of the SSRVE Methodology to Phase Transformations Modelling in Steels

Krzysztof Bzowski*, Maciej Pietrzyk**, Lukasz Rauch***

*AGH University of Science and Technology, **AGH University of Science and Technology, ***AGH University of Science and Technology

ABSTRACT

Multiscale modelling of materials processing is a promising but computationally costly methodology. Therefore, an attempt to improve numerical efficiency of numerical simulation methods using material microstructures focuses mainly on two aspects: parallelization of numerical procedures and simplifying the virtual representation of the material. One of the solutions gaining popularity is the idea of statistically similar representative volume element (SSRVE) [1]. Its aim is to reduce the number of finite elements needed to discretize the volume of the microstructure. Simplification of the computational domain is achieved by transforming complex material microstructure images – often referenced as representative volume element (RVE) - into simpler, artificial cell with fewer grains and comparable statistical and rheological behaviour to its original counterpart. Application of various coefficients to design optimal SSRVE is discussed in [2]. The present paper discusses the idea of the SSRVE, material microstructures descriptions as well as generation methods of unit cell for two-phase steel microstructures. The application of the simplification procedure will be demonstrated in modelling of diffusion phase transitions in DP steels. Proposed model driven by diffusion of carbon with the moving boundary (Stefan problem) was implemented on the basis of solution of Level Set equations coupled with diffusion equation. Application of implicit method for interface evolution allow to overcome the limitations associated with the complicated shape of grains, but also in a natural way will reflect the impact of curvature of the front and influence chemical forces on the velocity of the interface. Two different phase transformations phenomena will be modeled. Austenitic – during heating, and ferritic – during cooling. Phase composition, phase volume fraction, kinetic of the process, grain size and distribution of the carbon concentration will be determined for a given parameters of a heat treatment process. Study of intercritical annealing process will be used as an example of investigation of influence of nonuniform carbon concentration to microstructure properties. Acknowledgements: Financial support of the NCN project no. 2015/17/N/ST8/01024
References 1. Scheunemann L., Schröder J., Balzani D., Brands D., Construction of Statistically Similar Representative Volume Elements – Comparative Study Regarding Different Statistical Descriptors, Procedia Engineering, Vol. 81, 2014, 1360-1365. 2. Rauch L., Pernach M., Bzowski K., Pietrzyk M., On application of shape coefficients to creation of the statistically similar representative element of DP steels, Computer Methods in Materials Science, Vol. 11, 2011, 531-541.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Towards Integration of Active Elements into Finite Element Models of Adaptive Structures

Michael Böhm*, Oliver Sawodny**

*University of Stuttgart, **University of Stuttgart

ABSTRACT

Adaptive structures present a completely new approach in structural engineering. Actuators are included between two nodes each to control the structure's state. Different actuation principles are possible, some unknown yet. Examples for state of the art actuators include hydraulic cylinders, pneumatic actuators and even electric motors. The control input has to be modeled depending on the actuation principle. While passive structures are commonly studied using FE-analysis, where mass and stiffness matrices are calculated in the usual way that is largely automated, the input has to be included manually. Some FE-tools offer the possibility to include simple actuators, such as the LINK11 element in ANSYS. However, it is not possible to define forces depending on the actual state of the structure, i.e. including the control algorithm in the analysis. Overall, this only allows for a limited analysis of adaptive structures with active structural elements. Commonly, when working with adaptive structures, other analysis tools have to be used to manually integrate the active elements in the analysis afterwards. As a first step towards a better integration of these elements and towards a more user-friendly and seamless analysis of adaptive structures, we present here a methodology to calculate an additional input matrix automatically for active elements, simplifying the subsequent analysis. In order to do this, we present possible actuation principles and compare them with respect to their suitability for different tasks, revealing fundamental pros and cons leading to different use cases for each principle. Specifically, we will study parallel actuation and serial actuation. The former means integrating the actuator in parallel to an existing passive support element, while the latter describes an in-series-integration of the actuator into a passive support element. Combinations of these principles are also possible and considered. As a third actuation principle, we briefly discuss changing a structural element's stiffness, as well.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

On the Phenomenological Modelling of History Effects in Skeletal Muscles

Markus Böl*, Robert Seydewitz**, Tobias Siebert***

*Institute of Solid Mechanics, Braunschweig, Germany, **Institute of Solid Mechanics, Braunschweig, Germany, ***Institute of Sport and Motion Science, Stuttgart, Germany

ABSTRACT

Among the different types of soft tissue, skeletal muscles are able to contract and to generate active forces. A well-established experimental procedure to obtain active mechanical properties is to measure the force during isometric contraction while the positions of the muscle ends are fixed. Experimental observations revealed, however, that the amount of forces strongly depends on the elongation history. A muscle, which undergoes isometric contraction, isokinetic elongation and again isometric contraction, generates higher active forces than for pure isometric contraction at final length. This force difference is often described as force enhancement. Contrary, considering isokinetic contraction between first and second isometric contraction, forces are lower in comparison to pure isometric contraction. The drop of the active force at same length is designated as force depression. Although, experimental data about history effects such as force enhancement and depression are available and well documented, the underlying mechanism behind those effects still remains not fully understood. In that sense we present a phenomenological three-dimensional continuum-based approach to simulate the above mentioned history effects. For the identification of the model parameters experimental data of the soleus muscle were used. Further, the model was implemented in a finite element framework to analyse stress distribution in the muscle architecture during contraction.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Design of Fixed-Geometry Fluid Diodes Considering 2D-Swirl by Using Topology Optimization

Bruno C Souza*, Emílio C N Silva**

*University of Sao Paulo, **University of Sao Paulo

ABSTRACT

The scope of this article is to propose a new methodology of designing fixed-geometry fluid diodes using Topology Optimization considering a 2d-swirl system in order to maximize its efficiency. In several applications, such as mechanical and labyrinth seals in compressors and in hydraulic systems, it is necessary to inhibit the fluid flow in one direction. For such cases, a classic labyrinth seal or a simple one-way check-valve can be applied due to the simplicity, size and cheapness, however the rotating axis in many equipment may need a 2D axisymmetric system and complex geometries obtained nowadays from topology optimization method with the 3D printing technology can produce more efficient devices. Nikola Tesla has proposed in 1920 a patent of an intuitive geometry of passive valves and Sen Lin et al (2015) has proposed another geometry using topology optimization of a 2D geometry that can be used for example in flat-plate oscillating heat pipe (Thompson et al, 2011), however not considering any rotation of inner components. Thus this work explores how the topology optimization can help designing passive valves for systems with rotating parts which is relevant for example in the design of sealing for compressors and turbines. The topology optimization is implemented, considering the energy dissipation in both direction and the rotation of rotor in respect to the stator. Different parameters of Reynolds and rotational speed has been tested and the new geometries of fixed-geometry fluid diodes are offered. Bibliography Lin, Sen, et al. "Topology optimization of fixed-geometry fluid diodes." Journal of Mechanical Design 137.8 (2015): 081402. Thompson, S. M., H. B. Ma, and C. Wilson. "Investigation of a flat-plate oscillating heat pipe with Tesla-type check valves." Experimental Thermal and Fluid Science 35.7 (2011): 1265-1273.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Generalized Gradient Phase-field Theories

VICTOR CALO*, Luis Espath**, Eliot Fried***

*Curitn University, **KAUST, ***OIST

ABSTRACT

We postulate a virtual power principle for second-grade materials described by phase fields. We a priori assume a lack of smoothness in arbitrary parts of the domain, by explicitly accounting for corner and edge microtractions. Subject to thermodynamic constraints, we develop a general set of balance equations, constitutive relations, and boundary conditions for a phase-field model where its free-energy includes second gradients. The resulting balance equations are general and independent of constitutive equations. The thermodynamics of the process constrain the constitutive relations through the free-energy imbalance. We then show the equivalence between the principle of virtual power for second-grade phase fields and the balance of microforces and microtorques. This framework allows us to generalize the second-grade phase-field (Swift–Hohenberg) equation and the conserved second-grade phase-field (Phase-Field Crystal) equations. Finally, we depict the configurational traction (Eshelby traction) involved in both theories.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Numerical Computation of the Forces Previously Measured in a Rigid Tube Bundle Under Turbulent Cross Flow

Jerome CARDOLACCIA*, Sofiane HOUBAR**, Ulrich BIEDER***, Philippe PITEAU****

*Den-Service d'études mécaniques et thermiques (SEMT), CEA, Université Paris-Saclay, F-91191, Gif-sur-Yvette, France, **Den-Service de thermo-hydraulique et de mécanique des fluides (STMF), CEA, Université Paris-Saclay, F-91191, Gif-sur-Yvette, France, ***Den-Service de thermo-hydraulique et de mécanique des fluides (STMF), CEA, Université Paris-Saclay, F-91191, Gif-sur-Yvette, France, ****Den-Service d'études mécaniques et thermiques (SEMT), CEA, Université Paris-Saclay, F-91191, Gif-sur-Yvette, France

ABSTRACT

In Pressurized Water Reactors (PWR), the turbo-alternator producing electric current is fed by several Steam Generators (SG). These consist of long vessels in which secondary water vaporizes throughout thousands of U-tubes containing the hot water of the primary circuit. Maintaining the integrity of the U-tubes is a top priority in order to prevent loss of coolant and contamination of the secondary flow. The Fluidelastic Instability (FEI) is a major threat in that respect : under certain conditions, some tubes may enter into uncontrollable vibrations involving wear or fatigue and thus potential failure in the long-term. Despite decades of joint effort, researchers have failed so far to provide a thorough explanation of this phenomenon. The lack of insight into how the fluid behaves in such complex systems has long been, in our very own opinion, one of the main hurdle standing in the way of a breakthrough. Indeed, while a fair quantity of experimental data has been gathered (most often on simplified bundles made of short portions of straight cylinders submitted to a cross flow), it essentially depicts tubes displacements or efforts exerted on them. It is only since the last years that numerical simulations have started to flourish, giving us more detailed knowledge about the fluid behavior. The present work is about building a numerical simulation reproducing our in-house experimental facility and trying to compare measured versus computational data. As for now, all of the 3x5 tubes will be fixed so that there is no fluid-structure interaction per se. The major obstacles concern the rather high Reynolds number (66K based on the gap velocity) combined with the extent of the domain (span-to-diameter ratio equal to 10) and the time duration required for appropriate statistics. Other difficulties arise from the treatment and confrontation of 2D versus 3D data. The TrioCFD code has been used for the resolution of the single-phase incompressible Navier-Stokes equations. In the end, we offer our humble answers to repeated questions like "Is a tube length of one diameter sufficient for the 3D simulations ? " or "How many rows of cylinders are required to get a fully turbulent flow ?".

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Random Choice Method for Modelling the Rubinstein and Stefan-like Problems

sabrina CARPY*, hélène MATHIS**, Teodor Burghelea***, Cathy CASTELAIN****, Gael CHOBLET*****, Anais CRESTETTO******, Caroline DUMOULIN*******, Olivier GRASSET********, Guy MOEBS*********, Erwan LE MENN**********, Gabriel TOBIE**********

*Planetology and Geodynamics, LPG-CNRS, Université de Nantes, France., **Mathematics, LMJL-CNRS, Université de Nantes, France., ***Thermics and Energy, LTEN-CNRS, Université de Nantes, France., ****Thermics and Energy, LTEN-CNRS, Université de Nantes, France., *****Planetology and Geodynamics, LPG-CNRS, Université de Nantes, France, ******Mathematics, LMJL-CNRS, Université de Nantes, France., *******Planetology and Geodynamics, LPG-CNRS, Université de Nantes, France, ********Planetology and Geodynamics, LPG-CNRS, Université de Nantes, France, *********Planetology and Geodynamics, LPG-CNRS, Université de Nantes, France, **********Planetology and Geodynamics, LPG-CNRS, Université de Nantes, France, **********Planetology and Geodynamics, LPG-CNRS, Université de Nantes, France

ABSTRACT

Simulations of liquid-solid phase change are of major importance both for industrial applications (i.e. solidification of a binary alloy in metallurgical engineering), but also for investigating complex natural phenomena from microscopic to planetary scales. This work is part of a research project aimed at studying the Exchange Processes between the deep icy layers and the ocean of the giant moons around Jupiter and Saturn. By studying the properties of the moving interfaces separating the liquid and the solid phases at melting temperature, new insights into the characteristics of the deep internal structures of the giant moons might be gained. When the material is pure, the interface is at a constant melting temperature; this is the well-known two-phase Stefan problem. When a solute is present in the material, the melting temperature is no longer constant but depends on the concentration of the solute in the liquid and the solid phases that can coexist at thermodynamical equilibrium. Coupled heat and mass transfer process drive the phase transition by a jump in concentration at the melting front while the temperature remains continuous. Far from the melting front, the phase transition is modelled by phasic heat and mass diffusion equations given by the Fourier and the Fick laws [1]. In our study, we propose to define the moving interface by a Rankine-Hugoniot type jump relation of the heat fluxes at the melting free boundary. In order to capture the moving melting front, we introduce a Lagrange projection scheme based on a random sampling projection. Using a finite volume formulation, we define accurate numerical fluxes for the temperature and concentration fields that guarantee the sharp treatment of the boundary conditions at the moving front, especially the jump of the concentration according to the liquidus solidus diagram. We compare our Random Choice Method with exact solution [2] and level set method developed in [3] and provide some numerical illustrations that assess the good behavior of our method. [1] L. I. Rubinstein. The Stefan problem. American Mathematical Society, Providence, R.I., 1971. Translated from the Russian by A. D. Solomon, Translations of Mathematical Monographs, Vol. 27. [2] F. J. Vermolen Javierre, C. Vuik and S. van der Zwaag. A comparison of numerical models for one-dimensional stefan problems. J. Comput. Appl. Math., 2006 [3] S. Chen, B. Merriman, S. Osher, and P. Smereka. A simple level set method for solving stefan problems. J. Comp. Phys., 1997.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Effects of Breakaway Oxidation on the Stress Evolution and Degradation of Thermal Barrier Coatings

Yijun CHAI*, Yueming LI**, Kazuhiro OGAWA***

*Xi'an Jiaotong University, Tohoku University, **Xi'an Jiaotong University, ***Tohoku University

ABSTRACT

As an inevitable process of alloy in high-temperature service, oxidation changes the composition and induces extreme large stress in the alloy, resulting in alloy degradation in such aggressive environments. The NiCrAlY BC (bond coat) of TBCs (thermal barrier coatings) is a typical alloy used in aerospace and land-based gas turbines, which functions as an oxidation and corrosion-resistance layer adhered to the superalloy component. Experiments [1-2] showed that the oxidation process of BC can be divided into several stages for how breakaway oxidation occurs, and some researches [3-4] were conducted to model the breakaway oxides growth. However, the relationship between the breakaway oxidation and stress evolution as well as the degradation mode of TBCs has not been reported. This work studies the oxide scale (including the alumina and the breakaway oxide) growth upon high-temperature oxidation, by developing an ABAQUS User-Defend Element code. The results reveal distribution and volume fraction of the evolved oxide at any given time. The stress evolutions induced by the mixed oxide growth and the non-linear behavior (combined creep-plastic) of the BC and TGO (thermally grown oxide) are investigated. The degradation mode of TBCs is finally analyzed. This work provides a convenient strategy for the understanding of how the breakaway oxidation evolves and its effects on the TBCs failure.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A New Hybrid Particle-Mesh Approach for Incompressible Fluid Dynamics

CHRIS CHARTRAND*, Blair Perot**

*Sandia National Laboratories, **University of Massachusetts Amherst

ABSTRACT

The Navier Stokes equations can be naturally divided into two parts. On the left-hand side of the equations there are the time evolution and the advection terms. These two terms make up the material derivative. On the right-hand side, there are the pressure, viscous, and other force terms. In this work, we propose using a hybrid numerical solution approach to compute incompressible fluid dynamics. The method shown here will use a static mesh to represent continuum variables, such as pressure and viscous stresses, and use particles to represent extrinsic variables such as mass and momentum. The particles are accelerated by the Eulerian pressure and viscous stress fields, and similarly particle motion is used as the sources for the viscous stress tensor and for the discrete Poisson equation that solves for the pressure. The proposed method solves for pressure and viscous forces directly at each particle location via the mesh based continuum representation. The method strives to be a mimetic particle method with attributes similar to dual mesh methods. In this formulation, the dual mesh is the particle locations. The complexity of the mimetic particle dual mesh method arises because the particle dual mesh contains no connectivity or geometric information like a classical dual mesh does. The talk explores what is required to obtain local conservation of mass, momentum, angular momentum, and kinetic energy, and second order spatial convergence for the velocity and pressure. The method has some commonality with classic PIC [1][2] and FLIP [3] methods with some notable differences. [1] D. Burgess, D. Sulsky, and J. Brackbill, “Mass matrix formulation of the flip particle-in-cell method,” Journal of Computational Physics, vol. 103, no. 1, pp. 1–15, 1992. [2] C. Jiang, C. Schroeder, and J. Teran, “An angular momentum conserving affine-particle-in-cell method,” Journal of Computational Physics, vol. 338, pp. 137–164, 2017. [3] J. Brackbill and H. Ruppel, “Flip: A method for adaptively zoned, particle-in-cell calculations of fluid flows in two dimensions,” Journal of Computational Physics, vol. 65, no. 2, pp. 314–343, 1986.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Calculation of Exact Potential Energy Hessians Based on FEM

STAVROS CHATZIELEFTHERIOU*, NIKOS LAGAROS**

*Institute of Structural Analysis & Antiseismic Research, School of Civil Engineering, National Technical University of Athens, **Institute of Structural Analysis & Antiseismic Research, School of Civil Engineering, National Technical University of Athens

ABSTRACT

The potential energy of nanostructures within the molecular mechanics (dynamics) framework is usually calculated by adding bonded and nonbonded atomic energy contributions, i.e. bonds between 2 atoms, bond angles involving 3 atoms, dihedral angles involving four atoms, nonbonded terms expressing the Coulomb and Lennard-Jones interactions, etc. In this work a novel, a FE-based procedure is presented for studying the mechanical behavior of 3D nanostructures at the atomic scale. The energy gradient and Hessian matrix of such assemblies are commonly computed numerically; a potential energy FE model is proposed herein where these two components are expressed analytically. In particular, generalized finite elements are developed that express the interactions among atoms in a manner equivalent to that invoked in simulations performed based on the molecular dynamics method. Thus, the global tangent stiffness matrix for any nanostructure is formed as an assembly of the generalized finite elements and is directly equivalent to the Hessian matrix of the potential energy. The advantages of the proposed model are identified in terms of both accuracy and computational efficiency.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Recent Results in Improving the Material Point Method for Model-Based Simulation and Evaluation of the Additive Manufacturing Process

ZHEN CHEN*, Jun Tao**, Yu-Chen Su***, Yonggang Zheng****, Yong Gan*****

*Dalian University of Technology / University of Missouri, **Dalian University of Technology, ***University of Missouri, ****Dalian University of Technology, *****Zhejiang University

ABSTRACT

The multiphase (solid-fluid-gas) and multiscale (from nano to continuum) interactions in the mushy zone of additive manufacturing (AM) of metallic parts play a key role in determining the long-term performance of AM products. Based on the conservation laws of mass, momentum and energy, the generalized interpolation material point (GIMP) method is being developed for simulating and evaluating the fully coupled thermomechanical responses in the AM process. The fully coupled thermomechanical GIMP method (CTGIMP) considers the effects of both the temperature on deformation and the deformation on temperature [Tao et al., 2017]. A staggered solution scheme is designed to solve the coupled governing equations with explicit time integration. To improve the solution accuracy for multiphase interactions, the recent results [Gan et al., 2017; Lu et al., 2018] will be integrated into the CTGIMP. The improved CTGIMP representing the spatial discretization of a continuum will then be combined with molecular dynamics representing physical particles at nanoscale in order to effectively perform concurrent multiscale simulation of the AM process. Representative examples will be presented to demonstrate the proposed model-based simulation and evaluation procedure. References Gan, Y., Sun, Z., Chen, Z., Zhang, X., and Liu, Y., “Enhancement of the Material Point Method Using B-spline Basis Functions,” International Journal for Numerical Methods in Engineering, https://doi.org/10.1002/nme.5620, 2017. Lu, M., Zhang, J., Zhang, H., Zheng, Y., and Chen, Z., “Time-discontinuous Material Point Method for Transient Problems,” Computer Methods in Applied Mechanics and Engineering, Vol. 328, pp. 663-685, 2018. Tao, J., Zhang, H., Zheng, Y., and Chen, Z., “Development of Generalized Interpolation Material Point Method for Simulating Fully Coupled Thermomechanical Failure Evolution,” submitted for publication in Computer Methods in Applied Mechanics and Engineering, 2017.

13th World Congress on Computational Mechanics (WCCM XIII) and 2nd Pan American Congress on Computational Mechanics (PANACM II), July 22-27, 2018, New York City, NY, USA

NON LINEAR ANALYSIS OF BEAMS AND FRAMES BY MEANS OF A NEW SMART DISPLACEMENT BASED (SDB) BEAM ELEMENT

B. PANTO'*, D. RAPICAVOLI†, S. CADDEMI‡ AND I. CALIO'◊

Department of Civil Engineering and Architecture, University of Catania
Via Santa Sofia 64, 95125 - Catania, Italy
*bpanto@dica.unict.it
†daviderapicavoli@hotmail.it
‡scaddemi@dica.unict.it
◊icalio@dica.unict.it

Key words: Beam element, Diffused plasticity, Fibre approach, Displacement based approach, Displacement shape functions.

Abstract. In this paper a new displacement based beam finite element within the framework of diffused plasticity models is proposed. The proposed element is based on the formulation of enriched adaptive displacement shape functions which, contrarily to standard approaches, are able to update in accordance to the diffusion of the plastic deformations during the analysis. In view the adaptive character of the presented displacement shape functions the element is named Smart Displacement Based (SDB) beam element. The stiffness matrix of the SDB element is provided explicitly and shown to be dependent on the displacement shape functions updating. The axial force-bending moment interaction is approached by means of a fibre discretisation suitable for the analysis of r/c frame members. The SDB element is shown to be accurate and further improved by the proposal of a procedure to verify strong equilibrium of the axial force along the beam element which is not usually accomplished by classical displacement based beam elements.

1 INTRODUCTION

The standard displacement based inelastic beam element suffers of approximations related to the inability of the cubic polynomial interpolation functions to properly describe the displacement response of the beam when exhibiting inelastic behaviour[1]. The increase of the number of finite elements, or the use of higher order functions with additional internal degrees of freedom, are common remedies suggested to improve the approximation leading to an unavoidable reduction of the computational efficiency[2]. Improvements in mesh refinement procedures of displacement based elements have been achieved in[3,4] where each structural member (upgraded with quartic shape functions) is checked upon occurrences of plastic deformations and, when necessary, subjected to restricted automatic re-meshing.

Alternatively, it has been shown that the development of force based finite elements, based on the adoption of exact force shape functions, lead to more accurate results, although requiring different and more complicated iterative solution strategies[5-8]. On the other hand, since force based beam finite elements do not rely on displacement shape functions, they are not for their nature dedicated to the reconstruction of the displacement field during the analysis which requires a double integration procedure for the above purpose[9]. Moreover, the force based approach is not able to reproduce the linear curvature distribution appearing in the plastic zones as shown by detailed experimental analysis[10]. A comprehensive analysis and critical discussion of the two approaches is reported in[11] together with an extensive literature therein contained.

Within this scenario, this work proposes a new displacement beam element aiming at avoiding a re-meshing of each structural member however providing an accuracy competitive with force based procedures. Precisely, this paper proposes a new inelastic beam element, within the context of the displacement based approach, employing variable displacement shape functions denoted as Smart Displacement Shape Functions (SDSFs). The analytic expressions of the SDSFs are provided explicitly as related to the plastic deformation evolution in the beam element. The latter expressions are obtained by identifying, at each step, an equivalent tangent beam, characterised by abrupt variations of flexural stiffness, as a suitable representation of the current inelastic state of the beam. The presented approach leads to the formulation of a Smart Displacement Based (SDB) beam element whose accuracy appears to be comparable to those obtained through a force based approach but requiring a reduced implementation effort and a more straightforward approach. The term “smart” aims at emphasizing the ability of the element to upgrade the displacement field according to the current inelastic state. The proposed SDB beam element is able to incorporate a fibre approach for non linear analysis of r/c sections and it is formulated to account for the axial load-bending moment interaction. Finally, a procedure to impose strong equilibrium of the axial force along the beam element, which is not usually accomplished by classical displacement based beam elements is proposed. Precisely, within the Newton-Raphson predictor-corrector type iterative incremental procedure, a inner iteration scheme is started, after each corrector phase, by imposing a fictitious axial strain field and terminated when the axial force over the integration Gauss points is constant.

2 THE STEPPED BEAM MODEL

In the usual non linear beam elements undergoing diffused plasticity, where control cross sections are chosen at the Gauss integration points, stiffness decay due to the occurrence of plastic strains is usually supposed to be uniform over pre-defined segments of the beam. The beam element during the iterative step-by-step integration procedure develops according to a stepped beam model where both axial and flexural stiffness undergo abrupt variations along the beam axis. In this section the closed form solution of the non-uniform Euler-Bernoulli (E-B) beam model according to stepped variations of axial and flexural stiffness is proposed to lay the bases for an accurate description of the state of the beam during the evolution of the plastic strains.

The governing equations in x,z plane of a beam with abscissa x, $0 \le x \le L$, and with abrupt axial $\beta_{x,i}$ and flexural $\beta_{z,i}$ stiffness changes at x_i, $i = 1,\ldots,n$, subjected to a static axial $p_x(x)$ and transversal $p_z(x)$ load distribution, can be written as follows:

$$
\begin{aligned}
E_o A_o \left\{ \left[1 - \sum_{i=1}^{n} (\beta_{x,i} - \beta_{x,i-1}) U(x - x_i) \right] u_x^{I}(x) \right\}^{I} &= -p_x(x) \\
E_o I_o \left\{ \left[1 - \sum_{i=1}^{n} (\beta_{z,i} - \beta_{z,i-1}) U(x - x_i) \right] u_z^{II}(x) \right\}^{II} &= p_z(x)
\end{aligned}
\tag{1}
$$

where the apex indicates derivative with respect to x, while E_o, A_o, I_o represent the reference values of the Young modulus, the area and the moment of inertia of the cross section, respectively, and $U(x - x_i)$ is the well know Heaviside (unit step) generalised function. Integration of Eq. (1) according to the generalised function integration rules[12] leads to the following explicit expressions for the axial displacement and the transversal deflection functions $u_x(x), u_z(x)$, respectively:

$$
\begin{aligned}
u_x(x) &= a_1 + a_2 g_2(x) + g_3(x) \\
u_z(x) &= c_1 + c_2 x + c_3 f_3(x) + c_4 f_4(x) + f_5(x)
\end{aligned}
\tag{2}
$$

where $a_1, a_2, c_1, c_2, c_3, c_4$ are integration constants and $p_x^{[k]}(x), p_z^{[k]}(x)$ indicate the *k*-th primitive functions of the relevant external load distributions $p_x(x), p_z(x)$, respectively. The functions $g_2(x), g_3(x), f_3(x), f_4(x), f_5(x)$ appearing in Eq. (2) are defined as follows:

$$
\begin{aligned}
g_2(x;\beta_{x,i}^*) &= -x - \sum_{i=1}^{n} \beta_{x,i}^* (x - x_i) U(x - x_i) \\
g_3(x;\beta_{x,i}^*) &= -\frac{p_x^{[2]}(x)}{E_o A_o} - \sum_{i=1}^{n} \frac{\beta_{x,i}^*}{E_o A_o} \left[p_x^{[2]}(x) - p_x^{[2]}(x_i) \right] U(x - x_i) \\
f_3(x;\beta_{z,i}^*) &= \left[x^2 + \sum_{j=1}^{n} \beta_{z,i}^* (x - x_i)^2 U(x - x_i) \right] \\
f_4(x;\beta_{z,i}^*) &= x^3 + \sum_{j=1}^{n} \beta_{z,i}^* (x^3 - 3x_i^2 x + 2x_i^3) U(x - x_i) \\
f_5(x;\beta_{z,i}^*) &= \frac{p_z^{[4]}(x)}{E_o I_o} + \sum_{i=1}^{n} \frac{\beta_{z,i}^*}{E_o I_o} \left[p_z^{[4]}(x) - p_z^{[4]}(x_i) \right] U(x - x_i) - \sum_{i=1}^{n} \beta_{z,i}^* p_z^{[3]}(x_i)(x - x_i) U(x - x_i)
\end{aligned}
\tag{3}
$$

where the following new parameters $\beta_{x,i}^*, \beta_{z,i}^*$ have been defined:

$$
\beta_{x,i}^* = \frac{\beta_{x,i}}{1 - \beta_{x,i}} - \frac{\beta_{x,i-1}}{1 - \beta_{x,i-1}} \quad , \quad \beta_{z,i}^* = \frac{\beta_{z,i}}{1 - \beta_{z,i}} - \frac{\beta_{z,i-1}}{1 - \beta_{z,i-1}}
\tag{4}
$$

The solution in Eqs. (2)-(4) represents an explicit closed-form expression of axial and transversal displacement of an E-B beam in presence of an arbitrary number of abrupt cross-section which does not require the imposition of any continuity conditions where the discontinuities occur. The latter explicit closed-form solution is adopted in the next sections to formulate a two node non linear beam finite element able to account for diffusion of plasticity along the beam axis.

For convenience of notation the positions of the abrupt cross section variations are collected in the vector $\mathbf{x}^{EI} = \{x_1, x_2, \ldots, x_i, \ldots, x_n\}^T$, while the intensity of the axial and flexural stiffness are collected in the vectors $\boldsymbol{\beta}_x^* = \{\beta_{x,1}^*, \beta_{x,2}^*, ..., \beta_{x,n}^*\}^T$, $\boldsymbol{\beta}_z^* = \{\beta_{z,1}^*, \beta_{z,2}^*, ..., \beta_{z,n}^*\}^T$.

3 THE SMART DISPLACEMENT SHAPE FUNCTIONS

Based on the solution of the stepped beam model proposed in the previous section a beam element with nodal degrees of freedom as in Fig.1 can be conveniently introduced by formulating the shape functions of the axial $u_x(x)$ and transversal $u_z(x)$ displacements by imposing the following conditions:

$$\begin{aligned} &u_x(0) = q_1; \quad u_z(0) = q_2; \quad \varphi(0) = -u_z^I(0) = -q_3; \\ &u_x(L) = q_4; \quad u_z(L) = q_5; \quad \varphi(L) = -u_z^I(L) = -q_6 \end{aligned} \tag{5}$$

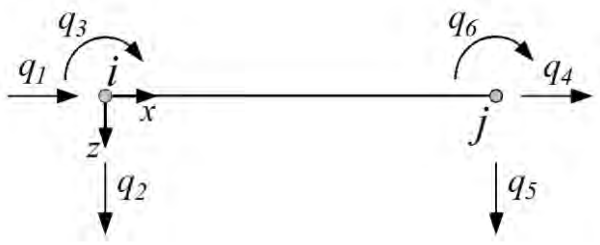


Fig. 1. The nodal degrees of freedom of the beam element.

Enforcement of Eq. (5) by using the solution in Eqs. (2)-(4) leads to to the expressions of the axial and transversal deflection, collected in the vector $\mathbf{u}^T\left(x; \mathbf{x}^{EI}, \boldsymbol{\beta}^*\right) = \left[u_x(x; \mathbf{x}^{EI}, \boldsymbol{\beta}^*) \quad u_z(x; \mathbf{x}^{EI}, \boldsymbol{\beta}^*)\right]$, in terms of nodal displacement vector $\mathbf{q}_e = \{q_1, q_2, q_3, q_4, q_5, q_6\}^T$ and the external load function as follows:

$$\mathbf{u}\left(x; \mathbf{x}^{EI}, \boldsymbol{\beta}^*\right) = \mathbf{N}(x; \mathbf{x}^{EI}, \boldsymbol{\beta}^*) \cdot \mathbf{q}_e + \mathbf{u}_p\left(x; \mathbf{x}^{EI}, \boldsymbol{\beta}^*\right) \tag{6}$$

where $\mathbf{N}(x; \mathbf{x}^{EI}, \boldsymbol{\beta}^*)$ collects the relevant displacement shape functions as follows:

$$\mathbf{N}\left(x; \mathbf{x}^{EI}, \boldsymbol{\beta}^*\right) = \begin{bmatrix} N_{x,1} & 0 & 0 & N_{x,2} & 0 & 0 \\ 0 & N_{z,1} & N_{z,2} & 0 & N_{z,3} & N_{z,4} \end{bmatrix} \tag{7}$$

with

$$
\begin{aligned}
&N_{x,k}(x;\boldsymbol{x}^{EI},\boldsymbol{\beta}^*) = {}^{k}A_1 + {}^{k}A_2 g_2(x;\beta^*_{x,i}), \quad k=1,2\\
&N_{z,j}(x;\boldsymbol{x}^{EI},\boldsymbol{\beta}^*) = {}^{j}C_1 + {}^{j}C_2 x + {}^{j}C_3 f_3(x;\beta^*_{z,i}) + {}^{j}C_4 f_4(x;\beta^*_{z,i}), \quad j=1,\ldots,4\\
&{}^{1}A_1 = 1; \quad {}^{1}A_2 = -\frac{1}{g_2(L)}; \quad {}^{2}A_1 = 0; \qquad {}^{2}A_2 = \frac{1}{g_2(L)}\\
&{}^{1}C_1 = 1; \quad {}^{1}C_2 = 0; \quad {}^{1}C_3 = -\frac{f_4^{I}(L)}{w}; \qquad {}^{1}C_4 = \frac{f_3^{I}(L)}{w};\\
&{}^{2}C_1 = 0; \quad {}^{2}C_2 = 1; \quad {}^{2}C_3 = \frac{-f_4^{I}(L)+f_4(L)f_2^{I}(L)}{w}; \qquad {}^{2}C_4 = \frac{-f_3(L)+f_3^{I}(L)}{w};\\
&{}^{3}C_1 = 0; \quad {}^{3}C_2 = 0; \quad C_3^3 = \frac{f_4^{I}(L)}{w}; \qquad {}^{3}C_4 = -\frac{f_3^{I}(L)}{w};\\
&{}^{4}C_1 = 0; \quad {}^{4}C_2 = 0; \quad {}^{4}C_3 = -\frac{f_4(L)}{w}; \qquad {}^{4}C_4 = \frac{f_3(L)}{w};\\
&w = f_3(L)f_4^{I}(L) - f_4(L)f_3^{I}(L)
\end{aligned}
\tag{8}
$$

Finally, the last vector in Eq. (6), defined as $\mathbf{u}_p^T\left(x;\mathbf{x}^{EI},\boldsymbol{\beta}^*\right)=\left[u_{p_x}\left(x;\mathbf{x}^{EI},\boldsymbol{\beta}^*\right) \quad u_{p_z}\left(x;\mathbf{x}^{EI},\boldsymbol{\beta}^*\right)\right]$, providing the additional contributions of the external load distributions $p_x(x), p_z(x)$ to the axial and transversal displacements, is given as follows:

$$
\begin{aligned}
&u_{p_x}\left(x;\mathbf{x}^{EI},\boldsymbol{\beta}^*\right) = -\frac{g_3(L)}{g_2(L)}g_2(x) + g_3(x)\\
&u_{p_z}\left(x;\mathbf{x}^{EI},\boldsymbol{\beta}^*\right) = \frac{f_4(L)f_5^{I}(L)-f_5(L)f_4^{I}(L)}{w}f_3(x) + \frac{f_5(L)f_3^{I}(L)-f_3(L)f_5^{I}(L)}{w}f_4(x) + f_5(x)
\end{aligned}
\tag{9}
$$

It has to be noted that the shape function matrix $\mathbf{N}\left(x;\mathbf{x}^{EI},\boldsymbol{\beta}^*\right)$, in Eqs. (7),(8), and the load vector contribution $\mathbf{u}_p\left(x;\mathbf{x}^{EI},\boldsymbol{\beta}^*\right)$ in Eq. (9), allow the reconstruction of the element deformed configuration once the nodal displacements are evaluated. The displacement shape functions proposed in Eqs. (7),(8) differ from the classical polynomials in view of additional distributional terms able to account for the abrupt cross section variations. For the latter reason their dependence on the vectors $\mathbf{x}^{EI},\boldsymbol{\beta}^*$, has been highlighted throughout Eqs. (6)-(9). The distributional terms appearing in the functions $g_2(x), g_3(x), f_3\left(x\right), f_4\left(x\right), f_5\left(x\right)$, as formulated in Eq. (3), are those subjected to update at the Gauss integration points during the inelastic analysis conducted by means of a Newton-Raphson type of procedure. In fact, the parameters in the vector $\boldsymbol{\beta}^*$ change with the axial and flexural stiffness according to the chosen inelastic constitutive model. In view of the adaptive character of the proposed displacement shape function with the occurrence of plastic deformations the latter are here addressed to as Smart Displacement Shape Functions (SDSFs).

Once the SDSFs, to be updated during the evolution of non linear events, have been defined it is now possible to evaluate the vector of generalised deformation components $\mathbf{d}(x)=\left[\varepsilon_o(x) \quad \chi_y(x)\right]^T$, collecting the axial deformation $\varepsilon_o(x)$ of the beam geometrical axis

and the curvature $\chi_y(x)$ of the proposed beam element, expressed in terms of nodal displacements and distributed external forces, by accounting for the standard Euler-Bernoulli model relationships, as follows:

$$\mathbf{d}(x;\mathbf{x}^{EI},\boldsymbol{\beta}^*)=\mathbf{B}(x;\mathbf{x}^{EI},\boldsymbol{\beta}^*)\cdot\mathbf{q}_e+\tilde{\mathbf{u}}_p\left(x;\mathbf{x}^{EI},\boldsymbol{\beta}^*\right) \tag{10}$$

where the matrix $\mathbf{B}(x;\mathbf{x}^{EI},\boldsymbol{\beta}^*)$ and the vector $\tilde{\mathbf{u}}_p\left(x;\mathbf{x}^{EI},\boldsymbol{\beta}^*\right)$, also subject to updating during the iterative step-by-step inelastic analysis, contain the first and second derivatives of the SDSFs and the load dependent terms $u_{p_x}\left(x;\mathbf{x}^{EI},\boldsymbol{\beta}^*\right), u_{p_z}\left(x;\mathbf{x}^{EI},\boldsymbol{\beta}^*\right)$, respectively.

4 THE SMART DISPLACEMENT BASED BEAM ELEMENT STIFFNESS MATRIX

The formulation of the SDSFs presented in the previous sections is adopted to define a Smart Displacement Based (SDB) beam element by providing the expression of the element stiffness matrix according to the application of the principle of virtual work.

By exploiting a fibre approach[5,6], the cross section area is discretised into n_f fibres, as depicted in Fig.4 in the form of stripes, each of them is characterised by an area A_f and a uni-axial non linear normal stress-axial strain elastic-plastic behaviour (since shear deformations and the consequent interaction with axial deformations is not taken into account). By assuming the principle of planar section conservation, the axial strain $\varepsilon_x(x)$ of each fibre is written as:

$$\varepsilon_x(x;z_f)=\varepsilon_o(x)+\chi_y(x)z_f=\begin{bmatrix}1 & z_f\end{bmatrix}\begin{bmatrix}\varepsilon_o(x)\\ \chi_y(x)\end{bmatrix}=\boldsymbol{\alpha}(z_f)\cdot\mathbf{d}(x) \tag{11}$$

where the row vector $\boldsymbol{\alpha}(z_f)=\begin{bmatrix}1 & z_f\end{bmatrix}$, depending on the distance z_f of the *f*-th fibre from the beam axis, has been introduced. The axial deformation of the *f*-th fibre of the cross section can be expressed in terms of nodal displacements $\mathbf{q}_e$ for the proposed SDB beam element by replacing Eq. (10), purged of the external load contribution $\tilde{\mathbf{u}}_p\left(x;\mathbf{x}^{EI},\boldsymbol{\beta}^*\right)$, into Eq. (11) as follows:

$$\varepsilon_x(x;z_f)=\boldsymbol{\alpha}(z_f)\cdot\mathbf{B}(x;\mathbf{x}^{EI},\boldsymbol{\beta}^*)\cdot\mathbf{q}_e \tag{12}$$

The non linear uni-axial constitutive relation between the axial strain $\varepsilon_x(x;z_f)$ and the normal stress $\sigma_x(x;z_f)$ can written as $\sigma_x(x;z_f)=E_T(x;z_f)\varepsilon_x(x;z_f)$ in terms of the tangent modulus $E_T(x;z_f)$ of the *f*-th fibre at cross section with abscissa x, to be evaluated according to the uni-axial constitutive model chosen for the applications.

Application of the principle of virtual displacements for the SDB beam element, in view of the fibre approach introduced in Eq. (12), writes:

$$\mathbf{Q}_e^T \cdot \delta\mathbf{q}_e = \mathbf{q}_e^T \int_0^1 \mathbf{B}^T(x;\mathbf{x}^{EI},\boldsymbol{\beta}^*) \sum_{f=1}^{n_f} \boldsymbol{\alpha}^T(z_f) E_T(x;z_f) A_f \boldsymbol{\alpha}(z_f)\, \mathbf{B}(x;\mathbf{x}^{EI},\boldsymbol{\beta}^*) dx\, \delta\mathbf{q}_e(x;z_f) \quad \forall \delta\mathbf{q}_e \tag{13}$$

where $\delta\mathbf{q}_e$ indicates virtual nodal displacements. Eq. (13) implies the following element stiffness matrix $\mathbf{K}_e(\mathbf{x}^{EI},\boldsymbol{\beta}^*)$, dependent on the current state of the element by means of the plastic intensity parameter vectors $\boldsymbol{\beta}^*$ and the plastic segment extension vector $\mathbf{x}^{EI}$, defined as follows:

$$\mathbf{K}_e(\mathbf{x}^{EI},\boldsymbol{\beta}^*) = \int_0^1 \mathbf{B}^T(x;\mathbf{x}^{EI},\boldsymbol{\beta}^*)\mathbf{k}(x)\mathbf{B}(x;\mathbf{x}^{EI},\boldsymbol{\beta}^*)\, dx \tag{14}$$

The inner matrix $\mathbf{k}(x)$ appearing in the integral in Eq. (14) represents the cross section stiffness matrix obtained by the adopted fibre discretisation as follows:

$$\mathbf{k}(x) = \sum_{f=1}^{n_f} \boldsymbol{\alpha}^T(z_f) E_T(x;z_f) A_f \boldsymbol{\alpha}(z_f) = \begin{bmatrix} \sum_{f=1}^{n_f} E_T(x;z_f) A_f & \sum_{f=1}^{n_f} E_T(x;z_f) A_f z_f \\ \sum_{f=1}^{n_f} E_T(x;z_f) A_f z_f & \sum_{f=1}^{n_f} E_T(x;z_f) A_f z_f^2 \end{bmatrix} \tag{15}$$

The cross section stiffness matrix given in Eq. (30) is used to retrieve the values of the discontinuity parameters collected in the vector $\boldsymbol{\beta}^*$ during the non linear analysis once the integration of the non linear constitutive equations is performed for each fibre of the cross sections. Furthermore, the expression reported in Eq. (14) shows clearly how the element stiffness matrix $\mathbf{K}_e$, differently from the classical displacement based approach commonly adopted in the literature, depends on the variation of the shape functions which are updated in accordance to the discontinuity parameter vector $\boldsymbol{\beta}^*$.

According to the Gauss integration scheme, the element stiffness matrix in Eq. (14) can be evaluated as follows:

$$\mathbf{K}_e(\mathbf{x}^{EI},\boldsymbol{\beta},\boldsymbol{\beta}^*) \approx \sum_{r=1}^{n} \mathbf{B}^T(x_r^G;\mathbf{x}^{EI},\boldsymbol{\beta}^*)\mathbf{k}(x_r^G)\mathbf{B}(x_r^G;\mathbf{x}^{EI},\boldsymbol{\beta}^*)\, w_r \tag{16}$$

where the matrix $\mathbf{B}(x_r^G;\mathbf{x}^{EI},\boldsymbol{\beta}^*)$, collecting the derivatives of the displacement shape functions formulated explicitly in Eqs. (12)-(14), are evaluated at the Gauss integration cross sections (the positions of the Gauss points are indicated as x_i^G, $i=1,\ldots,n$) and updated at each iteration as plastic deformations occur. The inner matrix $\mathbf{k}(x_r^G)$ in the product appearing in Eq. (16) represents the tangent stiffness matrix of the Gauss cross sections to be evaluated by means of integration of the fibre constitutive equations through the cross section according to Eq. (15).

6 AXIALLY EQUILIBRATED SDB BEAM ELEMENT

One of the problems encountered in the formulation of classical DB beam element is due to the assumption of the linear axial shape functions implying a constant axial force distribution during the analysis which does not reflect the variation of the internal axial force at the Gauss cross sections obtained by integration of the non linear constitutive laws. As a result axial equilibrium is not strictly enforced along the beam axis and it is rather verified in a weak form. The latter issue, clearly discussed in[2], implies a low performance of the DB element and requires a dense mesh to reach an accuracy comparable to the FB approach against experimental results. The concept of DB beam element strictly satisfying axial equilibrium along the beam axis was originally introduced by Izzudin et al.[13] for non-linear elastic problems while an interesting and appealing approach to achieve strong axially equilibrium for DB beam elements was recently proposed by Tarquini et al.[14] with an internal iterative procedure to correct the axial strains at each Gauss point requiring the solution of a linear system of equations.

In this section the SDSFs proposed in section 3 are employed to formulate an axially equilibrated SDB beam element (SDB/ae) in a strong form. Precisely, in order to reach a constant axial load along the Gauss integration points, a point load distributions, generated by the axial force difference $N(x_i^G)-N(x_{i-1}^G)$, $i=1,\dots,n$, between each two successive Gauss points will be exploited, defined as follows:

$$\tilde{p}_x(x)=\sum_{i=1}^{n-1}\left[N(x_i^G)-N(x_{i-1}^G)\right]\delta(x-x_i) \tag{17}$$

where $\delta(x-x_i)$ is the well know Dirac's delta distribution adopted in Eq. (17) to model a sequence of axial point loads concentrated at cross sections $x_i, i=1,\dots,n$. The axial load distribution $\tilde{p}_x(x)$, as defined in Eq. (17), is responsible for the onset of the axial displacement increment field $\Delta u_{\tilde{p}_x}\left(x;\boldsymbol{x}^{EI},\boldsymbol{\beta}^*\right)$ straightforwardly provided by the first expression in Eq. (9) as follows:

$$\Delta u_{\tilde{p}_x}\left(x;\boldsymbol{x}^{EI},\boldsymbol{\beta}^*\right)=-\frac{g_3(L)}{g_2(L)}g_2(x)+g_3(x) \tag{18}$$

where $g_2(x), g_3(x)$ are evaluated by means of Eq. (3) for the axial load distribution $\tilde{p}_x(x)$ in Eq. (17).

The axial displacement increment field $\Delta u_{\tilde{p}_x}\left(x;\boldsymbol{x}^{EI},\boldsymbol{\beta}^*\right)$, due to the axial point distribution $\tilde{p}_x(x)$ in Eq. (17), gives rise to a fictitious axial deformation increment $\Delta\varepsilon_{\tilde{p}_x}(x;\boldsymbol{x}^{EI},\boldsymbol{\beta}^*)=\dfrac{d}{dx}\Delta u_{\tilde{p}_x}(x;\boldsymbol{x}^{EI},\boldsymbol{\beta}^*)$ responsible of an inner iterative correction of the trial axial deformation until a constant axial force is obtained over the element delivering an axially equilibrated element.

In other words, within the standard predictor-corrector Newton-Raphson procedure, after the element state determination an internal iterative procedure is triggered by the superimposition of the axial deformation increment $\Delta\varepsilon_{\tilde{p}_x}(x;\boldsymbol{x}^{EI},\boldsymbol{\beta}^*)$ due to the lack of axial force equilibrium in strong form. When the increment $\Delta\varepsilon_{\tilde{p}_x}(x;\boldsymbol{x}^{EI},\boldsymbol{\beta}^*)$ is applied a new element state determination is performed to determine the updated axial force unbalance. The inner iterations are stopped when the difference of axial forces $N(x_i^G)-N(x_{i-1}^G)$, $i=1,\ldots,n$, is null, delivering a strongly axially equilibrated element.

5 APPLICATION

The reinforced concrete cantilever beam studied in[14] by means of standard and axial equilibrated displacement elements, as well as the forced based approach is analysed in this section. The beam length is L = 300cm with rectangular cross section 30x40cm and 20mm of cover concrete. Twelve $\phi 16$ reinforcing steel bars are symmetrically disposed along the section, as reported in Fig.2a. The analyses are conducted applying a shear force F at the free end of the beam. A constant axial force N = 75kN, corresponding to 1,25% of the axial-compression capacity of the section, is applied to the beam.

In the numerical simulations the modified Kent and Park constitutive law, according to Yassin model[15], is adopted in compression while a linear softening behaviour is adopted in traction. The compression strength of the confined concrete is f_{cc}=42Mpa, while the strength of the unconfined concrete is f_c=37Mpa. The concrete strain at the peak-stress are respectively $\varepsilon_c = 0,24\%$ and $\varepsilon_{cc} = 0,28\%$ for unconfined and confined concrete which correspond to an initial Young modulus E_c=30Gpa of the Kent and Park model. The tensile strength of the concrete is assumed equal to 10% of the compression strength and the softening slope equal to $2/3E_c$. The steel bars are modelled by the Menegotto and Pinto constitutive law[16] with Young modulus E_s=200Gpa, f_y =480Mpa, hardening 0.5%, initial value of the curvature parameter 15 and curvature degradation parameters respectively 0,925 and 0,15.

The proposed SDB/ae model is compared to the standard DB model, the DB/ae model[14] and the FB model. In particular, the analyses employing the SDB/ae model and the DB/ae model are performed through the software HISTRA[17], where both models have been implemented, while the analyses on the standard DB model and the FB model are performed in OPENSEES[18] environment employing the "Concrete02" and "Steel02" uniaxial materials. All the analyses are performed considering a single finite element, 10 Gauss-Lobatto integration points and discretising the cross section by means of 40 fibres. Figure 2b reports the capacity curves in terms of external force F versus the lateral deflection of the free end of the column $u_z(L)$.

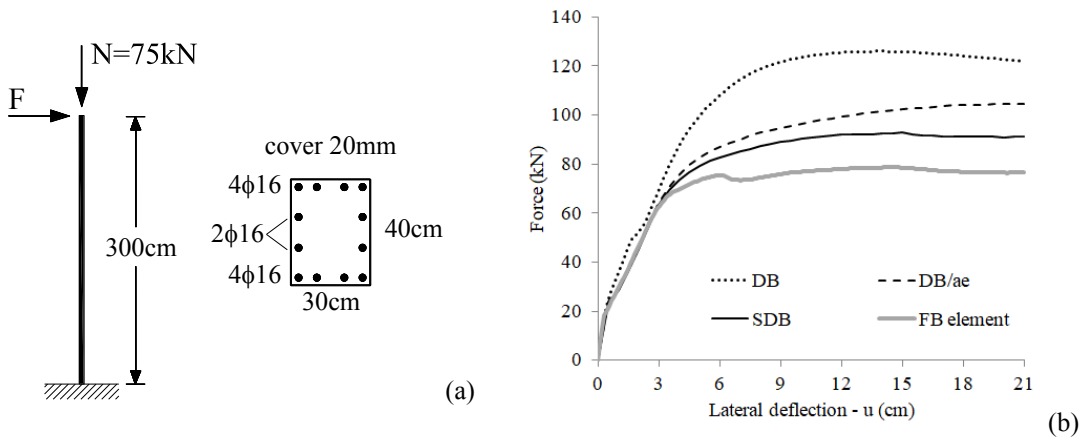


Fig.2. Cantilever geometrical layout (a) and comparison of the monotonic lateral capacity curves (b).

The maximum lateral force registered by the FB model is 78,6 kN. The standard DB model overestimates the beam lateral strength of 60,1% (126,0kN), while the error decreases to 33,2% and 18,1% by using the DB/ae model and the SDB/ae model, respectively, providing a reliable prediction of the load-caring capacity of the beam, even though a mesh refinement of the beam is not introduced.

0 shows sensitivity of the SDB/ae model to the number of the integration points (0a) and the number of elements adopted for the beam discretisation (0b). In the same Figure 3 the lines representative of the FB and standard DB responses are also reported. A low influence on the response is observed by increasing the integration points from 5 to 20, while by increasing the number of elements the SDB/ae response converges to the FB curve.

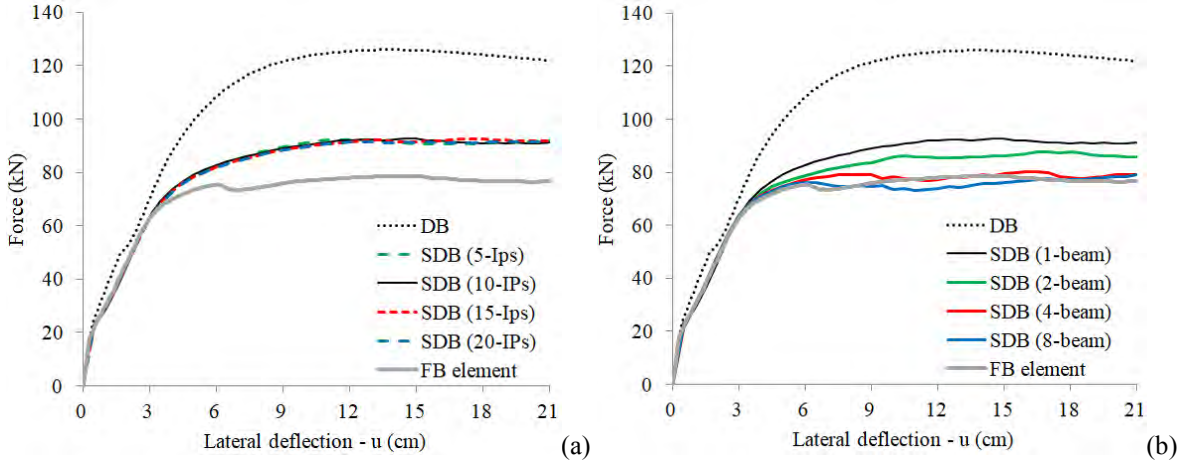


Fig.3. Influence of the number of the integration points (a), and the number of elements with 10 IPs (b) on the capacity curves for the system in Fig.2.

6 CONCLUSIONS

The shape functions, adopted by classical displacement based finite formulations for the discretisation of the beam element displacement field, are based on the adoption of Hermite polynomials which, however, are not able to capture the curvature variations due to along axis plastic deformation occurrences. The latter circumstance results in the inadequacy of such shape functions to properly represent the displacement field in presence of flexural stiffness variations implied by plastic constitutive behaviour. As a result a great computational disadvantage is related to the need of adopting refined meshes in order to converge towards a more accurate solutions which are, on the contrary, provided by force based finite elements procedures.

In order to improve the performance of displacement based beam finite elements for inelastic analysis of beam-like and frame structures in this work the concept of Smart Displacement Shape Functions (SDSFs) capable of updating during the diffusion of plastic deformations along the beam axis has been proposed. The SDSFs change during the iterative step-by-step analysis following the stiffness decay of the control cross sections according to a model of non uniform beam with stepped variations of both axial and flexural stiffness. The SDSFs updating is transferred to additional distributional terms explicitly introduced by closed form integration of the fourth order integration of the Euler-Bernoulli stepped beam.

The stiffness decay during the plastic incremental analysis is evaluated according to a fibre approach very convenient for r/c cross sections in order to account for the interaction of axial force –bending moment. The proposed beam element is formulated with six degrees of freedom at the element nodes and its smart character provides a better accuracy with respect to classical displacement based beam elements which is comparable with the alternative force based approach.

REFERENCES

[1] Crisfield, M.A. Non-linear finite element analysis of solids and structures, John Wiley & Sons, Chichester, UK, Vol. I, (1991), Vol. II, (1997).

[2] Calabrese, A., Ameida, J.P., Pinho, R. Numerical issues in distributed inelasticity modeling of rc frame elements for seismic analysis. Journal of Earthquake Engineering (2010) 14: 38-68.

[3] Izzudin, B.A., Elnashai, A.S. Adaptive space frame analysis: part I, a plastic hinge approach. Structures & Buildings (1993) 99(3): 303-316.

[4] Izzudin, B.A., Elnashai, A.S., Adaptive space frame analysis: part II, a distributed plasticity approach. Structures & Buildings (1993) 99(3): 317–326.

[5] Spacone, E., Filippou, F.C., Taucer, F.F. Fiber beam-column model for non-linear analysis of r/c frames: Part I. Formulation. Earthquake Engineering and Structural Dynamics (1996) 25: 711–725.

[6] Spacone, E., Filippou, F.C., Taucer, F.F. Fiber beam-column model for non-linear analysis of r/c frames: Part II. Applications. Earthquake Engineering and Structural Dynamics (1996) 25: 727–742.

[7] Spacone, E., Ciampi, V., Filippou, F.C. Mixed formulation of nonlinear beam finite element. Computers and Structures (1996) 58(1): 71–83.

[8] Neuenhofer, A., Filippou, F.C. Evaluation of nonlinear frame finite element models. Journal of Structural Engineering (ASCE) (1997) 123(7): 958–956.

[9] Neuenhofer, A., Filippou, F.C. Geometrically nonlinear flexibility-based frame finite element. Journal of Structural Engineering (ASCE) (1998) 124(6): 704–711.

[10] Goodnight, J.C., Kowalsky, M.J., Nau, J.M. Effect of load history on performance limit states of circular bridge columns. Journal of Bridge Engineering (ASCE) (2013) 18(12): 1383-1396.

[11] Almeida, J.P., Tarquini, D., Beyer, K. Modelling approaches for inelastic behaviour of rc walls: Multi-level assessment and dependability of results. Archive of Computational Methods in Engineering (2016) 23: 69-100.

[12] Pantò, B., Rapicavoli, D., Caddemi, S., Caliò, I. A smart displacement based (SDB) beam element with distributed plasticity. Applied Mathematical Modelling (2017) 44: 336–356.

[13] Izzudin, B.A., Karayannis, C.G., Elnashai, A.S. Advanced nonlinear formulation for reinforced concrete beam-columns. Journal of Structural Engineering (ASCE) (1994) 120(10): 2913–2934.

[14] Tarquini, D., Almeida, J. P., Beyer, K. Axially equilibrated displacement based beam element for simulating the cyclic inelastic behaviour of RC members. Earthquake Engng Struct. Dyn., (2017) 46: 1471–1492.

[15] Yassin, M. Nonlinear analysis of prestressed concrete structures under monotonic and cyclic loads. Ph.D. dissertation, University of California (Berkeley) (1994).

[16] Menegotto, M., Pinto, P.E. Method of analysis of cyclically loaded RC plane frames including changes in geometry and non-elastic behavior of elements under normal force and bending. Preliminary Report IABSE (1973) vol. 13.

[17] HiStrA (Historical Structure Analysis). HISTRA s.r.l, Catania, Italy. Release 17.2.3, April 2015. http://www.histra.it.

[18] McKenna, F. OpenSees: a framework for earthquake engineering simulation. Computing in Science & Engineering, (2011) 13(4): 58-66.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Study of a Vibroacoustic Interior Problem with Viscoelastic Sandwich Structure Using the Asymptotic Numerical Method

jean-marc Cadou*, Bertille Claude**, Laetitia Duigou***, Gregory Girault****

*IRDL - Université de Bretagne Sud - France, **IRDL - Université de Bretagne Sud - France, ***IRDL - Université de Bretagne Sud - France, ****IRDL - Université de Bretagne Sud - France

ABSTRACT

The aim of this study is to compute the eigenvalues of a vibroacoustic interior problem with fluid-structure coupling. A displacement-pressure formulation is chosen to modelize the problem. Then, the spatial discretisation with the finite element method leads to a non symmetric and poorly conditioned matrix system. It is proposed to solve this discretized system with the Asymptotic Numerical Method (ANM). This method associates a high order perturbation method to a continuation technique [1]. Thus, the initial nonlinear problem is linearized and a set of linear algebraic systems easier to solve is obtained. The proposed method is validated with numerical tests on a conservative problem (that is to say for an elastic structure).These tests show that the computational times required with this method are lower than those needed with an Arnoldi-based method. Moreover our method is not sensitive to poorly conditioned matrix, so there is no need to add a preconditioning step [2]. Once the conservative problem is solved, the corresponding solutions are used as initial values to solve the associated dissipative problem (that is to say a viscoelastic sandwich structure [3]). Numerical developments are ongoing to evaluate the method coupling the homotopy to the ANM, and results are expected for the conference. REFERENCES [1] L. Duigou, E. M Daya and M. Potier-Ferry, Iterative algorithms for non-linear eigenvalue problems. Application to vibrations of viscoelastic shells, Computer Methods in Applied Mechanics and Engineering, Vol. 192, pp. 1323-1335, 2003. [2] B. Claude, L. Duigou, G. Girault and J.M. Cadou, Eigensolutions to a vibroacoustic interior coupled problem with a perturbation method, Comptes Rendus Mécanique, Vol. 345, 2, pp. 130-136, 2017. [3] L. Rouleau, J.F. Deu, A. Legay and J.F. Sigrist, Vibro-acoustic study of a viscoelastic sandwich ring immersed in water, Journal of Sound and Vibration, Vol. 331, pp. 522-539, 2012.

13th World Congress on Computational Mechanics (WCCM XIII) and 2nd Pan American Congress on Computational Mechanics (PANACM II), July 22-27, 2018, New York City, NY, USA

MICRO-SCALE THERMAL SIMULATIONS OF CEMENT PASTES CONTAINING MICROENCAPSULATED PHASE CHANGE MATERIALS (MPCM)

ANTONIO CAGGIANO*,†, CHRISTOPH MANKEL*, AND EDUARDUS A.B. KOENDERS*

* Institute of Construction and Building Materials, TU-Darmstadt, Germany
Franziska-Braun-Straße 3 (vorm. Petersenstr. 12)
Darmstadt, Germany
caggiano@wib.tu-darmstadt.de, mankel@wib.tu-darmstadt.de, koenders@wib.tu-darmstadt.de
www.wib.tu-darmstadt.de

†LMNI, INTECIN, CONICET, Universidad de Buenos Aires
Av. Las Heras 2214
Ciudad Autónoma de Buenos Aires, Argentina
acaggiano@fi.uba.ar

Keywords: Thermal-energy storage, Enthalpy-based method, MPCMs, Porous cementitious containers, Microscale, Hydration.

Abstract. In the last decades, the use of smart components embedded inside cementitious composites, called Phase Change Materials (PCMs), has become a more and more attractive solution for saving energy and to provide a more efficient thermal comfortability to modern buildings and constructions. This work presents the current research activities running at the Institute of Construction and Building Materials (WiB) of TU Darmstadt, and deals with the investigation of advanced coupling of two physical mechanisms represented by a heat problem and microstructural heterogeneities in cement-based composites. Particularly, the thermal response of cement pastes, along with occurring phase change phenomena, will be simulated at the microscale level. A virtual 3D porous microstructure with embedded Microencapsulated-(M)PCMs, which are created with an available hydration model, provide a fundamental basis for the analysis of the morphological influence on the effective thermal energy diffusion parameters. The current work is based on investigating the influence of the morphological effect on the thermal properties of hydrating cement paste systems by using the cement hydration and microstructure development model Hymostruc, combined with MPCMs. Laboratory characterization of MPCM-pastes were also performed using several test methods which are here briefly reported. Test thermal performances in terms of heat capacity, conductivity and temperature evolutions of cement paste systems with and without MPCMs were experimentally evaluated, and are used as benchmark for calibration purposes.

1 INTRODUCTION

Building energy consumption could be easily reduced by employing smart materials that passively control the heat flow and temperature fluctuations in residential and commercial buildings [1]. Cementitious composites containing Phase Change Materials (PCMs) have been employed in the last years as a way to enhance the energy efficiency and saving of new construction [2]. A huge Thermal Energy Storage (TES) in PCMs is available in form of latent heat by reversibly changing phase between solid-liquid and vice versa. Therefore, the inclusion of PCMs in concrete could significantly improve the thermal properties of such a material, making it greener and more eco-friendly in construction and building applications [3].

Experimental activities available in literature, at several scales of observation, aimed at reporting the main benefits in terms of thermal properties of cementitious materials containing PCMs [4]. Some contributions reviewed the effect of the PCMs on the resulting mechanical capacities of concrete [5]. Other works demonstrated that by employing PCMs in concrete allows to have a certain beneficially reduction in terms of hydration heat during the hardening process of the fresh concrete [6].

Plenty of theoretical and numerical formulations have been proposed for analyzing TESs in porous cement pastes, mortar and/or concretes containing phase change materials. The majority of these models arise from an extension of the so-called Stefan problem [7]. The solution of this latter has been classically treated in literature by means of three main methods: (i) the fixed grid method [8], (ii) the deformed grid method [9] and (ii) a combination of these two latter [10]. Simulation examples related to cementitious composites are those related to the use of the so-called Enthalpy-based Method (EM), which moves into the fixed grid solution. Then, the Apparent Calorific Capacity Method (ACCM) [11-12] and the Heat Source Method (HSM) [13-14] represent two main alternatives used for solving the EM.

Concrete and other cementitious materials are multiphase (composite) materials and, for this reason, they can be considered and modelled as homogeneous continuums at the macroscale and/or structural practice-oriented one, while, at lower levels (meso-, micro- or even nano-scale) multi-phase composite approaches can be considered. Available models can be thus categorized in this matter by means of those scales of observation. Structural-scale models allow to capture the essence of heat storage phenomena at the structural (building physics) scale level [15]. Macro-scale models are based on the assumption that the schematized material acts as a continuum and homogenous medium [16]. By considering lower scales of analysis (i.e., meso- and microscale behavior of PCM composite materials), the mechanism of PCMs, affected by external thermal fluctuations, can be better understood. At these lower scales the material can be idealized by considering different phases which together constitute the composite. Thereby, the interaction among the different phases (i.e., matrix, aggregates, PCMs, hydrated products, voids, water and possible interfaces between them) is explicitly considered in these approaches [17].

This work proposes a theoretical model for simulating the thermal behavior in hardened cement pastes produced with and without Microencapsulated-PCMs. An Enthalpy-based approach formulated in the framework of the Apparent Calorific Capacity Method (ACCM) is solved to accurately analyze the above mentioned phenomena. The model has been validated at macroscale

by means of temperature curves, measured from three different cement pastes without MPCMs and with 10% and 20% in MPCM volume fraction contents. Then, microscale analysis are performed on 3D virtual PCM-cement paste microstructures. The study of Representative Element Volume (REV) of heterogeneous PCM-cement paste microstructures will be performed with the aim of defining the minimum size of a sample that must be employed for determining the corresponding effective properties of a homogenized macroscopic model.

2 EXPERIMENTAL DATA

This section briefly reports the employed materials, the considered tests and results considered as reference for the numerical activities. DSC, conductivity and temperature evolution tests were done for investigating the thermal properties of plain and MPCM-cement pastes.

2.1 Materials and Methods

Nine mixtures, made with three different w/c ratios and three amount of MPCM volume fractions, were considered. A commercial ordinary Portland cement (CEM I 42,5 R) and microencapsulated paraffin waxes (namely, Micronal® DS 5038 X by BASF [18]), in form of powder MPCM, were mixed with different volume fractions. All mixtures were prepared according to EN 196-1 [19] and following the recipes highlighted in Table 1 (the first row of the Table identifies the mixture type by reporting the corresponding label which helps to provide the key information about the amount of MPCM and the considered w/c ratio).

Table 1: Mix overview of the nine paste systems.

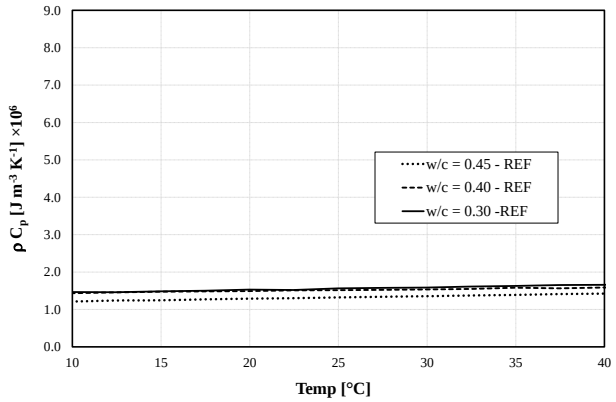
Labels	**c-45-ref** [kg/m^3]	**c-45-10%** [kg/m^3]	**c-45-20%** [kg/m^3]	**c-40-ref** [kg/m^3]	**c-40-10%** [kg/m^3]	**c-40-20%** [kg/m^3]	**c-30-ref** [kg/m^3]	**c-30-10%** [kg/m^3]	**c-30-20%** [kg/m^3]
Cement	1294.4	1129.9	977.2	1383.9	1208.2	1044.9	1606.2	1402.2	1212.7
Water	582.5	508.5	39.8	553.6	483.3	417.9	481.9	420.7	363.8
MPCM	-	90.0	80	-	90.0	180.0	-	90.0	180.0
Air content [V.-%]	1.5	2.7	4.5	1.5	2.7	4.5	1.5	2.7	4.5
w/c ratio	0.45			0.40			0.30		

After one day of casting, all specimens were removed from the formwork and stored in a water bath at 20° C and during 28 days. Then, after the maturation, the specimens were completely dried for 42 days at 50° C until they reached a constant mass.

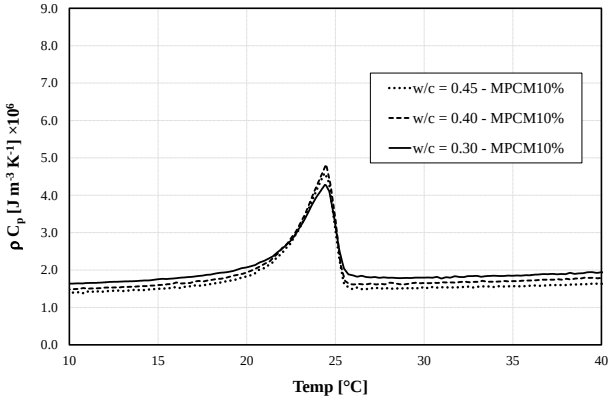
2.2 DSC test data

Differential scanning calorimetry (DSC) measures were performed for each one of the mixtures. Solid samples (3 per MPCM mixtures and 2 for the reference cement pastes) were prepared in aluminum DSC pans and tested (Figure 1a).

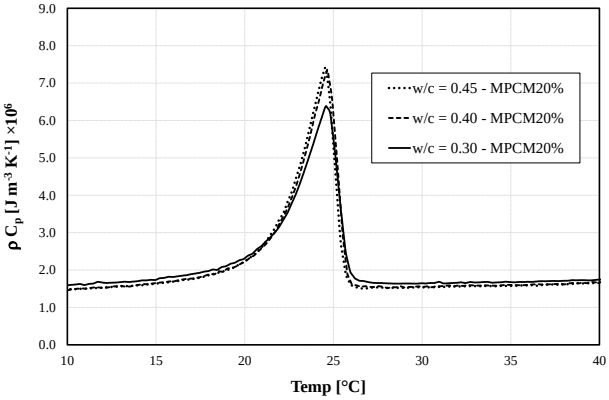
(a)



(b)



(c)



(d)

Figure 1: Results of DSC tests (obtained with a heating rate of 1 K×min^{-1}) in terms of $\rho \times C_p$: (a) the used 0.6 *mm* pan and results with cement pastes having (b) 0%, (c) 10% and (d) 20% MPCM volume fraction.

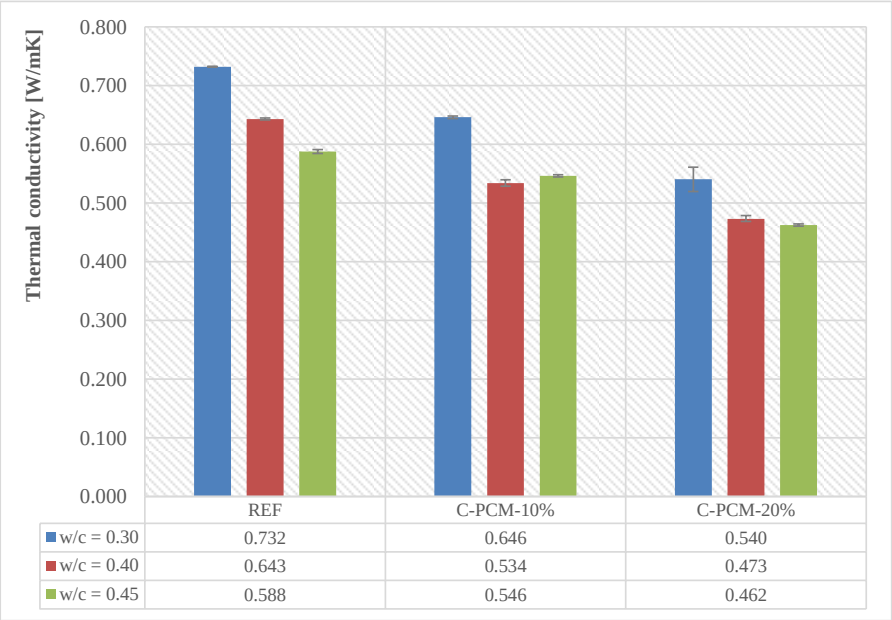
DSC results for the reference cement pastes are shown in Figure 1b. The response of the three cement pastes is characterized by the same kind of sensible behavior, analyzed in the temperature ranges between 10 and 40 °C. As expected, the almost similar behavior characterizes each one of the cement pastes. The results also remark an almost temperature independent behavior of the $\rho \times C_p$ response.

Then, DSC thermograms of Figure 1c-d show the $\rho \times Cp\text{-}T$ response for the cases of 10% and 20% of MPCM volume fractions, respectively. They are characterized by an almost sensible behavior in the temperature ranges far from the melting point and an evident latent peak in that region close to the temperature of phase changes. Particularly, all curves are characterized by a remarkable peak which mainly represent the solid–liquid melting phase change of the MPCM stored in the

porous structure of the paste. It can be easily recognized that the latent storage capacity of the cement pastes with 20% MPCM volume fraction is strongly higher (as imaged) than the corresponding one with 10% volume fraction.

2.3 Conductivity tests

Thermal conductivity tests were performed by means of the Hot-Disk transient heat source method and using 40 mm × 40 mm × 160 mm beams. The complete test procedure is omitted in this work for the sake of brevity. However further details are available here [20].



	REF	C-PCM-10%	C-PCM-20%
w/c = 0.30	0.732	0.646	0.540
w/c = 0.40	0.643	0.534	0.473
w/c = 0.45	0.588	0.546	0.462

Figure 2: Thermal conductivity of the REF, C-PCM-10% and C-PCM-20% mixtures with different w/c ratios.

Figure 2 reports the results of the conductivity tests for the analyzed MPCM cement pastes. It can be observed that the thermal conductivity generally decreases when higher water-to-cement ratios are considered. Moreover, when comparing the results by focusing on the effect of MPCM replacements it can be also shown that the thermal conductivity is generally affected by the presence of MPCMs. In particularly the thermal conductivity reduces when higher MPCM volume fractions are substituted in the considered matrix.

2.4 Thermal tests and mechanical tests

Temperature measurements and mechanical tests, for the complete characterization of the materials under investigation, were also done. Particularly, three spheres characterized to have a diameter of about 70 mm and produced with embedded thermocouples were cast to investigate the structural and microscale behavior of such shapes and through studying temperature evolutions under certain heating environmental conditions. The thermal experiments were accompanied by mechanical tests to observe the effect MPCMs have on the resulting strengths in both compression and bending. These results are omitted herein for the sake of the brevity, however they are fully documented in [20].

3 FIRST LAW OF THERMODYNAMICS AND ENTHALPY-BASED METHOD

The basic equations, employed for predicting phase transformation phenomena in PCM cement-based systems, are described in this section.

3.1 Thermodynamics principles

The basic equation describing a heat conduction problem can written as follows:

$$\frac{\partial Q}{\partial t} = \nabla.\left(\lambda \nabla T\right) + \dot{q}_v \qquad \forall \mathbf{x} \in \Omega \tag{1}$$

where Q is the heat of the system, t the time, λ the thermal conductivity of the material (depending on temperature T and position vector $\mathbf{x}$ of the considered body Ω), $\dot{q}_v$ is the possible source term while $\nabla.$ and ∇ are the divergence and gradient tensorial operators.

In thermodynamics a small amount of heat added to a system (dQ) is defined by means of the *first law of thermodynamics* as:

$$dU = dQ - p\,dV \tag{2}$$

where dU is a variation of the internal energy of the system and pdV the rate of the work spent, indicated as dW (under the simplified hypothesis that $dW=pdV$).

By introducing the definition of the enthalpy of a homogenous system, $H = U + p\,dV$, and by combining Eqs. (1) and (2), and adopting the hypothesis of a constant pressure process, the following enthalpy-based equation can be reached:

$$\frac{\partial H}{\partial t} = \nabla.\left(\lambda \nabla T\right) + \dot{q}_v \qquad \forall \mathbf{x} \in \Omega \tag{3}$$

which is the mostly used equation for solving phase changes in construction and building material applications, and is commonly addressed as the enthalpy-based method.

3.2 Enthalpy-based and Apparent Calorific Capacity Method

The Apparent Calorific Capacity Method (ACCM) allows for describing the enthalpy evolution of a system in terms of an apparent (or sometime called effective) heat capacity during the thermal phase change.

The approach is based on following chain rule:

$$\frac{\partial H}{\partial t} = \frac{\partial H}{\partial T}\frac{\partial T}{\partial t}, \tag{4}$$

then, by introducing the so-called temperature-dependent apparent (effective) heat capacity, defined as follows:

$$\frac{\partial H}{\partial T} = \rho C_{eff}(T) \tag{5}$$

Eq. (3) modifies into the following non-linear transient heat equation:

$$\rho C_{eff}(T)\frac{dT}{dt} = \nabla.(\lambda \nabla T) + \dot{q}_v \qquad \forall \mathbf{x} \in \Omega \tag{6}$$

To complete the above problem statement of the ACCM approach outlined in Eq. (6), Initial Conditions (ICs) and Boundary Conditions (BCs) need to be employed.

4 MICROSCALE POROUS STRUCTURE

3D virtual PCM-cement paste microstructures were generated through the Hymostruc hydration model [24]. The generation of the microgeometries, numerically performed with the simulated hydration processes, are based on several input parameters which aim at reproducing the microscale geometries of the 9 cement pastes (with and without MPCMs) investigated in the experimental campaign (Section 2).

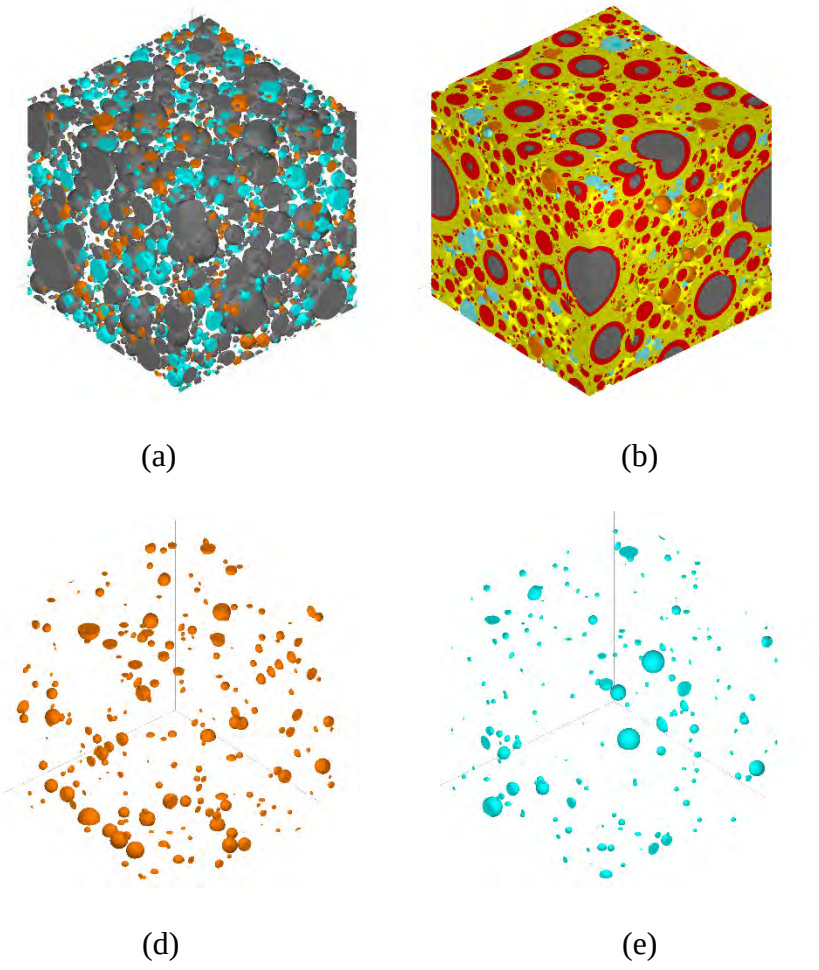
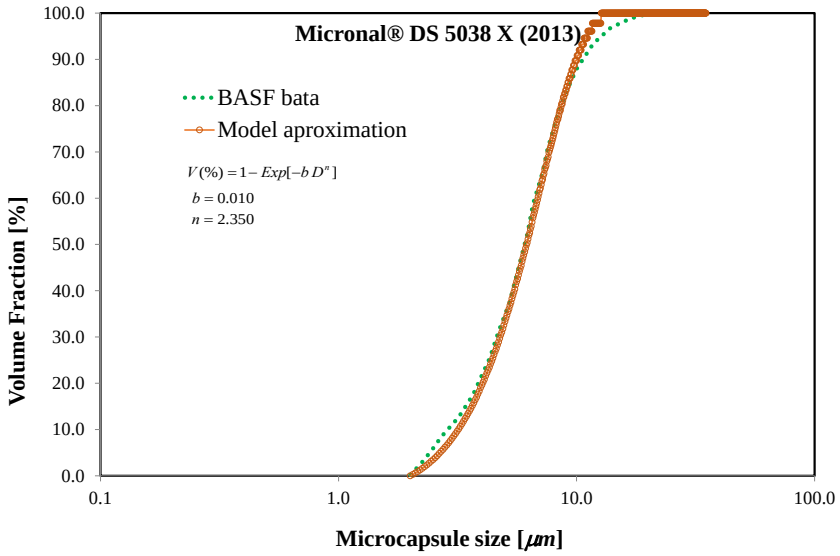


Figure 3: (a) 3D microstructure with initial anhydrated cement, (b) hydrated microstructure, (c) detail of the MPCMs and (d) air bubbles distribution. For color figures the reader could refer to the digital version of the paper.

Particle size distribution of the (anhydrated) cement, type of cement/binder, water/cement ratio, hydration age, initial mix temperature, air bubbles and MPCM particles distribution are the key input parameters which affect the final hydrated structure. They were selected following the information and measured data of the experimental campaign (i.e., cement type, water-to-cement ratio, air bubbles, MPMCs).

As example, a 3D generated geometry has been shown in Figure 3 which is characterized by a 3D virtual structure with a cubic shape with a rib size of 100 µm, a regular Portland cement with a specific surface of 400 m^2kg^{-1}, w/c = 0.45, isothermal reaction at 20°C, MPCM volume fraction of 20% with a particle distribution as highlighted in Figure 4 and air bubble contents according to Table 1. It is worth to mention that the w/c ratio is one of the key parameter that controls the morphology of the obtainable porous microstructure [25].



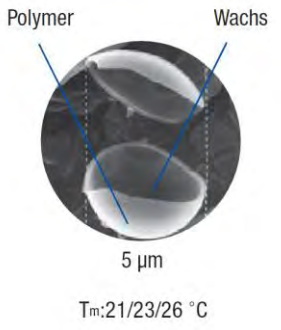


Figure 4: Grain size distribution of the employed MPCMs vs. BASF-data [18].

The initial cement particles and MPCMs are stacked based on a random selection of locations with an equal probability of occurrence. Particles allocation starts from the largest particles down to the smaller ones and the process continues until all particles in the smallest fractions have been stacked. Volume fraction and particle-size distribution follow the rule $V(\%) = 1 - Exp[-b\,D^n]$ which was opportunely calibrated for predicting the sheet data finished by BASF [18]. After having generated this initial particle structures, hydration algorithms are invoked for forming the 3D virtual microstructure.

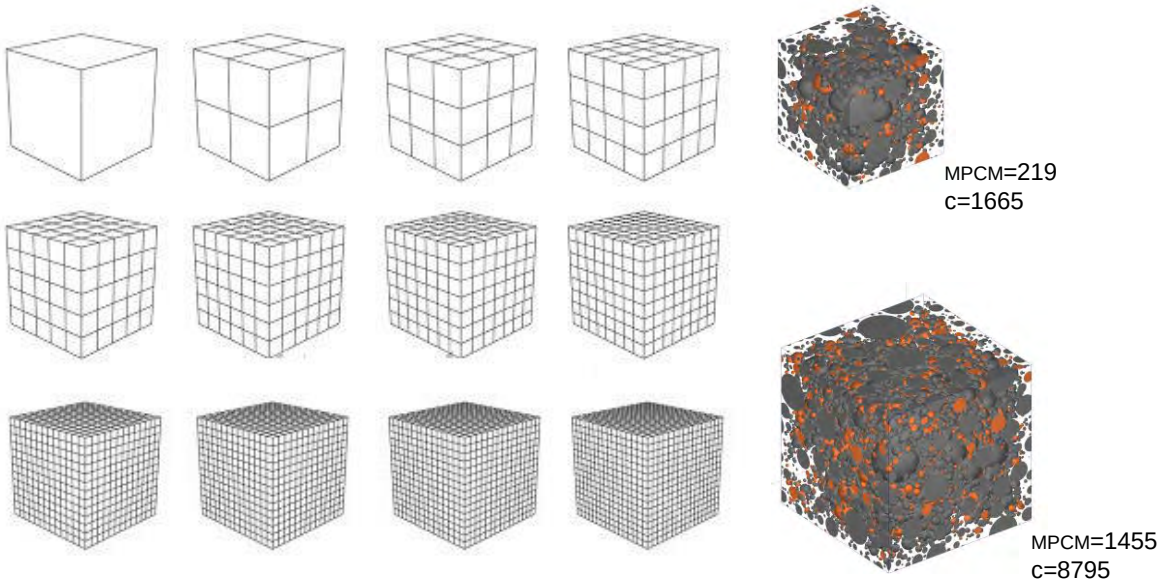


Figure 5: 3D REV microstructures with different discretization size (left) and two specimen sizes as example (e.g., 50 and 100 μm^3 on the right).

The study of the most appropriate Representative Element Volume (REV) of heterogeneous PCM-cement paste microstructures is currently ongoing and will be aimed at defining the minimum size of a sample that must be employed for determining the corresponding effective properties of the dual homogenized macroscopic model. The REV dimension should be large enough to contain the necessary information about the microstructure, thus to be representative.

An indicator proposed by Guittman et al. [23] can be estimated for each 3D microstructure to find out the most appropriate REV size and particularly to quantify the change of the calculated homogenized (effective) thermal property based on the mean value calculated for the different numerical realizations. More specifically, six different generations of the initial cement particle locations needs to be generated and used for the hydration simulation and for each different mixture type.

The following expression was proposed by Guittman et al. [23]:

$$\chi^2 = \sum_{i=1}^{m} \left(R_{\text{energy,i}} - R_{\text{energy,a}} \right)^2 / R_{\text{energy,a}}{}^2 \tag{7}$$

where $R_{\text{energy,i}}$ is the investigated effective thermal energy parameter (e.g., the thermal conductivity, specific heat capacity, enthalpy), $R_{\text{energy,a}}$ is the average of the investigated $R_{\text{energy,i}}$, and m=6 the total number of numerical realizations performed with different initial cement particle and MPCM locations.

The variability of the results can be estimated with χ^2, indicating that for smaller values of χ-*square*, the closer the volume of the sample under consideration represents the expected REV. In fact, the true REV may only be obtained for a sample with an infinite volume. Nonetheless, a size of a sample can normally be used if the value of χ^2 is acceptably low. Generally, 0.1 is regarded to be an acceptable value [24].

5 CONCLUSIONS

This paper proposes the theoretical basis for simulating the thermal behavior of cement paste systems made with and without M-PCMs. A micro-scale based approach formulated through the use of the so-called Apparent Calorific Capacity Method (ACCM) was solved to accurately analyze the above mentioned phenomena. The model considered the experimental data measured from three different cement pastes without MPCMs and with 10% and 20% of MPCM volume fraction contents. The model validation of the proposed method dealt with simulating the experimental tests for given boundary and initial conditions and based on the adopted experimentally-based $\rho C_{eff}(T)$ curves. The proposed study was developed within the framework of the "2CENENRGY" project and will be further extended on investigating the 3D thermal-mechanical response in micro and mesoscopic structural specimens.

It may be worth to mention that although a significant research effort has already been done in the field of numerical modelling for heat transfer processes with PCM accumulations, further efforts in the field of cementitious composites embedding PCMs are certainly needed. Unambiguous knowledge on how porous microstructures, like cementitious composites or aggregates, should be built up and/or what are the critical demands that allow empty pores to serve as "closed" encapsulation cavities, is still lacking. A novel approach, combining a micro- to mesoscale poro-analysis model with a multiscale/multiphysics approach, along with a microstructural response, moisture diffusivity, phase change and thermal analysis, will be developed as next step of the current research.

ACKNOWLEDGEMENTS

The authors are grateful to the Hochschulrechenzentrum (HRZ) of TU-Darmstadt for its important support on performing calculations for this research which were partially conducted on the Lichtenberg high performance computer. The first author wishes to acknowledge the Alexander von Humboldt-Foundation for funding his position at the WiB – TU Darmstadt under the research grant ITA-1185040-HFST-P (2CENENRGY project). Finally, the support to networking activities provided by the SUPERCONCRETE Project (H2020-MSCA-RISE-2014 n 645704; http://www.superconcrete-h2020.unisa.it/) funded by the EU is gratefully acknowledged.

REFERENCES

[1] Aidan, R. and Kinnane, O. The impact of thermal mass on building energy consumption, Applied Energy (2017) 198:108-121.

[2] Ricklefs, A., Thiele, A. M., Falzone, G., Sant, G. and Pilon, L. Thermal conductivity of cementitious composites containing microencapsulated phase change materials. International journal of heat and mass transfer, (2017) 104:71-82.

[3] Devaux, P. and Farid, M.M. Benefits of PCM underfloor heating with PCM wallboards for space heating in winter., Applied energy, (2017) 191:593-602.

[4] Shadnia, R., Zhang, L. and Li, P. Experimental study of geopolymer mortar with incorporated PCM., Construction and building materials, (2015) 84:95-102.

[5] Niall, D., Kinnane, O., West, R. P. and McCormack, S. Mechanical and thermal evaluation of different types of PCM–concrete composite panels., Journal of Structural Integrity and Maintenance, (2017) 2(2):100-108.

[6] Kim, Y. R., Khil, B. S., Jang, S. J., Choi, W. C. and Yun, H. D. Effect of barium-based phase change material (PCM) to control the heat of hydration on the mechanical properties of mass concrete., Thermochimica Acta, (2015) 613:100-107.

[7] Crank, J, Free and Moving Boundary Problems, (Clarendon, Oxford, 1984).

[8] Eyres, N. R., Hartree, D. R., Ingham, J., Jackson, R., Sarjant, R. J. and Wagstaff, J. B. The calculation of variable heat flow in solids., Philosophical Transactions of the Royal Society of London. Series A, Mathematical and Physical Sciences, (1946) 240(813):1-57.

[9] Lynch, D. R. and O'Neill, K. Continuously deforming finite elements for the solution of parabolic problems, with and without phase change., International Journal for Numerical Methods in Engineering, (1981) 17(1):81-96.

[10] Udaykumar, H. S., Mittal, R. and Shyy, W. Computation of solid–liquid phase fronts in the sharp interface limit on fixed grids. Journal of computational physics, (1999) 153(2):535-574.

[11] Šavija, B. and Schlangen, E. Use of phase change materials (PCMs) to mitigate early age thermal cracking in concrete: Theoretical considerations., Construction and Building Materials, (2016) 126:332-344.

[12] Thiele, A. M., Wei, Z., Falzone, G., Young, B. A., Neithalath, N., Sant, G. and Pilon, L. Figure of merit for the thermal performance of cementitious composites containing phase change materials., Cement and Concrete Composites, (2016) 65:214-226.

[13] Rostamizadeh, M., Khanlarkhani, M. and Sadrameli, S. M. Simulation of energy storage system with phase change material (PCM)., Energy and Buildings, (2012) 49:419-422.

[14] Fachinotti, V. D., Cardona, A. and Huespe, A. E. A fast convergent and accurate temperature model for phase-change heat conduction., International Journal for Numerical Methods in Engineering, (1999) 44(12):1863-1884.

[15] Heim, D. and Clarke, J. A. Numerical modelling and thermal simulation of PCM–gypsum composites with ESP-r., Energy and buildings, (2004) 36(8):795-805.

[16] Tittelein, P., Gibout, S., Franquet, E., Johannes, K., Zalewski, L., Kuznik, F., ... and David, D. Simulation of the thermal and energy behaviour of a composite material containing encapsulated-PCM: Influence of the thermodynamical modelling., Applied Energy, (2015) 140:269-274.

[17] Aguayo, M., Das, S., Castro, C., Kabay, N., Sant, G. and Neithalath, N. Porous inclusions as hosts for phase change materials in cementitious composites: Characterization, thermal performance, and analytical models., Construction and Building Materials, (2017) 134:574-584.

[18] BASF, Datenblatt Micronal PCM DS 5038 X, (11/2013).

[19] EN 196-1, Methods of Testing Cement – Part 1: Determination of Strength, (2005).

[20] Mankel, C., Caggiano, A., Stolze, J., Guardia, C. and Koenders, E.A.B., Thermal Characterization of Porous Cement Paste Systems Containing Microencapsulated Phase Change Materials (MPCM), In RILEM-week 2018, 26-29 August 2018, Delft, the Netherlands.

[21] Van Breugel, K. Simulation of hydration and formation of structure in hardening cement-based materials, PhD-thesis, Delft University of Technology, Delft, The Netherlands (1991).

[22] Ukrainczyk, N. and Koenders, E.A.B., Representative elementary volumes for 3D modeling of mass transport in cementitious materials, Modelling and Simulation in Materials Science and Engineering, (2014) 22(3):035001.

[23] Gitman, I.M., Gitman, M.B., and Askes H. Quantification of stochastically stable representative volumes for random heterogeneous materials. Arch. Appl. Mech., (2006) 75:79-92.

[24] Zhang, M.Z., Ye G., and van Breugel K. A numerical–statistical approach to determining the representative elementary volume (REV) of cement paste for measuring diffusivity, Mater. de Construcc. (2010) 300:7-20.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Analysis of Multi-crack Problems by FEM-SFBEM Coupling Method

Keming Cai*, Cheng Su**, Zhi Xu***, Xueming Fan****

*South China University of Technology, **South China University of Technology, ***South China University of Technology, ****South China University of Technology

ABSTRACT

The computational efficiency for analysis of stress intensity factors of multi-crack problems is still an important issue in fracture mechanics. The formulation of a super element with a single crack embedded in is first developed using the spline fictitious boundary element method (SFBEM) based on the Erdogan's solutions corresponding to an infinite plane with a single crack. The super elements are then incorporated into the finite element mesh to simulate the behaviour of the multiple crack zones in a plate structure, while the other zones without cracks are modelled using the traditional finite elements. The proposed FEM-SFBEM coupling method is further applied to the analysis of stress intensity factors of multi-crack problems, in which the computational accuracy and efficiency of the present approach is demonstrated.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Hermite Spectral Method for the Homogeneous Boltzmann Equation

Zhenning Cai*, Yanli Wang**

*National University of Singapore, **Peking University

ABSTRACT

The Boltzmann equation is the fundamental mathematical model in the gas kinetic theory. However, solving Boltzmann equation numerically is expensive due to its high dimensionality and its complicated collision term. In this work, we focus on the numerical discretization of the collision term, especially for the inverse-power-law model, and we propose a Hermite spectral method to approximate it. This method can also be generalized to a modeling tool for the collision operator. Using this tool, we can generate affordable models which are much more accurate than the BGK-type models. The new models and the numerical methods keep the conservation of mass, momentum and energy exactly, and they are very efficient in capturing the lower order moments. Even for discontinuous distribution functions, the evolution of the stress tensor and the heat flux can be accurately approximated. A number of numerical experiments are carried out to verify the efficiency of this method.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Quantifying Incertitude in Astrophysical Simulation Codes

Alan Calder*, Melissa Hoffman**, Donald Donald***, Maximilian Katz****, Douglas Swesty*****, Scott Ferson******

*Stony Brook University, **NRAO, ***Stony Brook University, ****NVIDIA Corporation, *****Stony Brook University, ******University of Liverpool

ABSTRACT

We present a study addressing the treatment of incertitude, that is, epistemic uncertainty, in input parameters in astrophysical simulations. We look at the propagation of incertitude in control parameters for stellar winds in simulations performed with the MESA stellar evolution code. We apply two methods of incertitude propagation, the Cauchy Deviates method and the Quadratic Response Surface method, to quantify the output uncertainty in white dwarf stars, the endpoint of stellar evolution for low-mass stars. The methodology we apply is applicable to the problem of propagating input incertitudes through any simulation code treated as a ``black box," i.e. a code for which the algorithmic details are either inaccessible or prohibitively complicated. We have made the tools developed for this study freely available to the research community. This work was supported in part by the US Department of Energy under grant DE-FG02-87ER40317.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Modelling the Biomechanics of the Eye after Strabismus Surgery

Begoña Calvo*, Jorge Grasa**

*University of Zaragoza, **University of Zaragoza

ABSTRACT

In this work, a finite element model is presented to reach a better understanding of the eye biomechanics when subjected to strabismus surgery. During this procedure, the point of action of the extraocular muscle is changed using and adjustable suture to align properly the eyeball. Using MRI images from an animal model (New Zeland rabbit) the contours of the eyeball and muscles were segmented semi-automatically using a software application. After certain manipulation of the volumes, a 3D finite element mesh was developed and based on animal dissections, the approximate size of tendons was determined for the extraocular muscles. Active and passive behaviour of these tissues were considered using a previous muscle model with a transversely isotropic formulation in finite strains. The direction of muscle fibres that was required for the hyperelastic constitutive law was also determined from the muscle samples. The parameters needed to define both active and passive behaviour were determined experimentally using a custom made experimental protocol previously developed. Computational simulations showed how the relative position of the muscles modifies the biomechanical behaviour of the eye ball and also muscle activation levels to perform certain movements. The computational simulation could provide assistance to surgeons to decide the appropriate location of insertion points before surgery.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

3D Modeling of Amoeboid Motility through Complex Environment

Eric Campbell*, Prosenjit Bagchi**

*Rutgers University, **Rutgers University

ABSTRACT

Amoeboid motility refers to a specific form of motility in which cells move by extending finger-like membrane-protrusions that are generally known as pseudopods. This form of motility is commonly observed in single-celled organisms known as amoeba. It is also observed in neutrophils, epithelial cells, embryonic cells, and in certain types of metastatic cancer cells. Amoeboid motility is a complex and multiscale process with a strong coupling between nano-scale protein biochemistry, cell deformation, and cytoplasmic and extra-cellular fluid motion. For metastatic cells, migration occurs in a 3D environment through the extra-cellular matrix (ECM) resulting in a strong interaction with the surrounding tissue. Amoeboid migration of metastatic cells, however, does not require a strong adhesion, and ECM degradation or remodeling. Instead, cells squeeze through the existing pores of the ECM. The microstructural details of the ECM as well as the deformability of the cells are expected to affect the migration behavior. To understand the coupling between cell deformability and ECM microstructure during 3D cell motility, we have developed a multiscale fully 3D computational model of amoeboid motility through complex tissue scaffolds. The methodology couples a coarse-grain model for biochemistry with cell deformation, pseudopod dynamics, cytoplasmic and extracellular flows, and ECM microstructure. We follow a continuum approach wherein the cell is modeled as a viscous liquid surrounded by viscoelastic membrane. The membrane resists deformation against area dilation, bending and shearing deformation, and the membrane stresses are obtained using a finite-element model. The intra- and extra-cellular flows are obtained following the Stokes equations that are solved by finite-volume methods. The protein biochemistry leading to the protrusive force causing pseudopod generation is coarse-grained using a dynamic pattern formation model wherein nonlinear reaction-diffusion equations are solved for activator and inhibitors using a finite-element method. The different components of the model are seamlessly integrated using the continuous forcing immersed boundary method (IBM). The microstructures of the ECM are also modeled as immersed objects, but using a sharp-interface (ghost-node) IBM. The predicted shapes of the migrating cells in unbounded medium show remarkable similarity with experimentally observed shapes of Dicty. Our simulations predict that the cell speed increases with increasing deformability, but decreases with increasing confinement. We find that the number of pseudopods increases and the pseudopods become more increasingly confined at the front of the cells with increasing deformability. This mechanism allows the cell to achieve a persistent unidirectional motion even in absence of any external cues.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Mechanics and Applications of Soft Materials -from Tunable Surfaces to Emerging Electronics to Medical Devices

Changyong Cao*

*Michigan State University

ABSTRACT

Soft materials, such as polymers, foams and hydrogels, can deform easily and to very large strains. Their shapes and sizes can vary greatly even if the applied forces are small. Different from the “hard materials” like steel and concrete, soft materials have very different and unique properties, which may have potential applications in various fields but have been much less explored. This offers people great opportunities for making breakthrough discoveries and inventions in engineering and medicine. The mechanical instabilities of hybrid (soft and hard) materials result in self-organized patterns and drastic changes in morphology, which may lead to unprecedented functions of materials, structures and devices. I will first describe how to use numerical and experimental methods to identify the instability modes and the scaling laws for generating desired tunable surface patterns. Then, I will demonstrate how to harness mechanical instabilities and large deformations from soft materials to develop stretchable supercapacitors and novel medical devices. Also, I will demonstrate how we combine the mechanics principle with additive manufacturing to fabricate robust electronics and energy-storage devices.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Smooth Finite Element Method Based on Bivariate Simplex Splines on Triangle Configurations

Juan Cao*, Zhonggui Chen**, Xiaodong Wei***, Yongjie (Jessica) Zhang****

*Xiamen University, China, **Xiamen University, China, ***Carnegie Mellon University, USA, ****Carnegie Mellon University, USA

ABSTRACT

Recently, a new bivariate simplex spline scheme based on triangle configurations has been introduced into the geometric computing community. It defines a complete bivariate spline space that retains many attractive theoretic properties of classical B-splines, e.g., it provides inbuilt C^{n-1} continuity across the triangle edges. In this study, we propose a framework for finite element analysis using bivariate simplex splines defined on triangle configurations and investigate its performances by conducting numerical tests on well-known benchmark cases. Within the present framework, the centroidal Voronoi tessellation method is used to generate knots on the domain. Then, knot subsets are carefully selected by a locally computed triangulation, on which shape functions are recursively computed. To achieve high-precision numerical integration, triangle faces served as background integration cells in weak formulations are obtained by triangulating the entire domain restricted to all knot-lines. Various numerical examples are carried out to numerically demonstrate the efficacy/stability and optimal convergence of the proposed method.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Stochastic Multiscale Modeling of Heterogeneous Materials

Le Cao*

*Ph.D. Student, Department of Civil Engineering, College of Engineering, University of Kentucky

ABSTRACT

Mechanical properties are varied with material heterogeneity at multiple length scales. The research aims to investigate the stochastic heterogeneous material response and progressive failure of the functionally graded lattice truss microstructures, associated with topological optimization of the fabricated architecture. Lattice truss microstructures are designed with large degrees of static indeterminacy, which may have little reserve capacity to tolerate abnormal loading conditions. Progressive failure mechanism can be triggered by the loss or reduction of the load-carrying capacity of a small portion of the entire material structure due to an applied abnormal load. Following the initial local damage, a propagation of disproportionate collapse could be spread. The colossal computation was needed traditionally to discretize the domain in finite element method, to study the heterogeneous material behavior. In multiscale modeling, the representative volume elements (RVE) at the microscale and their assembly construct the heterogeneity of a functionally graded material at the macro scale. Stochastic analysis is developed with varied microstructural member sizes and the optimal topology. The optimization is attempted in a two-dimensional domain for the cross-sections of a representative volume element (RVE). Material structure is optimized against the instability, which includes the nonlinear structural behavior. Homogenization evolution is investigated to analyze a large variety of the heterogeneous lattice truss microstructures. The results are examined with the complete structural modeling in finite element simulation. Constitutive behavior of RVE is investigated with some oscillation in both elastic and inelastic regimes. In the stochastic multiscale analysis, a probabilistic-based approach is developed in the inelastic regime, whereas the material response in the elastic regime is expected to be deterministic based on the literature in previous studies ([1], [2]). The results are mapped into a spectrum with respect to the parameters in topology optimization. Furthermore, a functionally graded material with lattice truss microstructures also likely fails due to the fracture of microstructural members. The progressive failure mechanism develops associated with internal force redistribution. The modeling technique is discussed to simulate the material failure. The effect on the failure mechanism by the uncertainty of material parameters is investigated as well.
References: [1] Graham-Brady, Lori (2017). Inelastic Homogenization of Heterogeneous Media: Case Studies for Probabilistic Analysis, Engineering Mechanics Institute (EMI) Conference 2017, ASCE, San Diego, California, June 2017 [2] Blandford, George (1996). Large Deformation Analysis of Inelastic Space Truss Structure, Journal of Structural Engineering, ASCE, vol.122, no.4, pp.407-415

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Understanding the Mechanisms of Amorphous Plasticity through Molecular Simulation: Shear Flow, Slip Avalanches, and Creep

Penghui Cao*, Michael Short**, Sidney Yip***

*MIT, **MIT, ***MIT

ABSTRACT

Using a meta-dynamics method of sampling activated state pathways we study three related rheological responses of a model metallic glass at experimental strain-rate levels beyond the reach of traditional molecular dynamics simulations. The problems are (1) transition from Newtonian (homogeneous) to inhomogeneous (shear localized) flow, (2) discrete stress relaxation (slip avalanches) in the onset of yielding and subsequent strain evolution, and (3) stress effects on creep rate [1]. In (1) we find an intermediate regime with characteristically strong spatial and temporal fluctuations. This points to a strain-rate mediated mechanism that acts to bridge the regime of homogeneous flow observed experimentally at low strain rates and high temperature [2] with the regime of shear-band flow probed by molecular dynamics simulation at high strain rates and low temperature [3]. In (2) we quantify the yielding response and the role of major and minor avalanches in sustaining serrated plastic deformation. In the case of deformation under a constant stress, problem (3), we demonstrate a nonlinear interplay between non-affine atomic displacement and cooperative shear transformation distortion of local atomic clusters that provides a molecular explanation of the familiar behavior of creep-rate upturn beyond a stress threshold, as well as a mechanism map delineating the effects of stress and temperature [1]. Collectively these findings lead to an understanding of the elementary processes governing deformation and flow of disordered materials and the effects of thermal and stress activations. In an overall interpretation based on the concept of potential-energy landscape, we discuss the relevance of the mechanism models of F. Spaepen and A. S. Argon, and how the present simulation results can inform and thus help unify various existing theoretical descriptions, such as the theory of shear transformation zone (STZ), extended mode-coupling theory (e-MCT), mean-field theory with weakening mechanism, and concepts of self-organized criticality for slowly driven, interaction dominated threshold systems. References: [1] P. Cao, M. P. Short, S. Yip, Proc. National Acad. Sci. 114, 13631 (2017). [2] J. Lu, G. Ravichandran, W. L. Johnson, Acta Met. 51, 3429 (2003). [3] J. Chattoraj, C. Caroli, A. Lemaitre, Phys. Rev. Lett. 105, 266001 (2010).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Coupling Effects on Cylindrical Fuel Bundles Under Axial Flow: Theory and Experiments

Roberto Capanna*, Guillaume Ricciardi**, Christophe Eloy***, Emmanuelle Sarrouy****

*CEA Cadarache, St Paul les Durance, France, **CEA Cadarache, St Paul les Durance, France;, ***Institute de Recherche sur les Phénomènes Hors Equilibre (IRPHE), Marseille, France, ****Laboratoire de Mécanique et d'Acoustique (LMA), Marseille, France

ABSTRACT

The safety of a nuclear power plant subjected to earthquakes is a major concern of the nuclear industry. Efficient modelling and accurate knowledge of the mechanical behaviour of the reactor core is therefore needed to estimate the effects of seismic excitation on a nuclear power plant. Fuel assemblies (in the reactor core) are subjected to an axial water flow, which strongly modifies the dynamical behaviour of the fuel assemblies; therefore the identification of the fluid forces is very important. In this work is presented a model for the fluid-structure interaction forces developed using the potential flow theory and considering the structure as an Euler Bernoulli beam. The flow is thus described only using one scalar function (velocity potential) instead of a vector field. This assumption strongly simplifies the fluid mechanics equations, avoiding the necessity to solve Navier-Stokes equations. The model is implemented in a Finite Element Software and pressure distribution around cylinders is solved. The empirical model is compared to reference works in literature for validation. Several simulations are run for multi-cylinder geometries in order to evaluate the influence of different parameters like the distance between cylinder, the excitation mode and the presence of symmetries in the geometry. Furthermore, in this work an experimental approach is considered. Tests are performed on an experimental mock-up made of 4 fuel assemblies (half scale) under an axial water flow. One of the fuel assemblies is excited with a hydraulic jack and the displacements on all of them are then measured. On this work we focus on the effects induced on non-excited assemblies due to the presence of water between the cylinder. The water, in fact, creates coupling between different assemblies which are not in contact each other. In the final part of this paper experimental results and numerical simulations based on the model presented before will be compared. We will outline the capability of this simple model to describe added mass effects and we will present the differences between the theoretical model and experimental results. The analysis of the discrepancies will be useful for understanding the limits of this model and to look for further improvement, as for instance adding a viscosity empirical factor into the model.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Patient-specific Simulations for Planning Treatment of Congenital Heart Diseases: A Single Centre Translational Experience

Claudio Capelli*, Emilie Sauvage**, Giorgia Maria Bosi***, Stephane Couvreur****, Benedetta Biffi*****, Silvia Schievano******, Andrew Taylor*******

*UCL Institute of Cardiovascular Science & Great Ormond Street Hospital for Children, NHS Foundation Trust, London, UK, **UCL Institute of Cardiovascular Science & Great Ormond Street Hospital for Children, NHS Foundation Trust, London, UK, ***UCL Mechanical Engineering, ****UCL Institute of Cardiovascular Science & Great Ormond Street Hospital for Children, NHS Foundation Trust, London, UK, *****UCL Dept of Med Phys & Biomedical Eng, ******UCL Institute of Cardiovascular Science & Great Ormond Street Hospital for Children, NHS Foundation Trust, London, UK, *******UCL Institute of Cardiovascular Science & Great Ormond Street Hospital for Children, NHS Foundation Trust, London, UK

ABSTRACT

Patient-specific computational models have been extensively developed over the last decade and applied to investigate a wide range of the cardiovascular mechanics. Modelling can also offer support to personalized and predictive medicine. Such vision could be particularly suitable to face the wide variety of congenital heart disease (CHD). The translation of these technologies into clinical applications, however, is still far from becoming a standard of care in clinical practice and currently limited to few single cases. This study reports the experience of a single clinical and engineering centre, based in the main UK children hospital, which has been involved in the development of a modelling framework that allows the use of realistic simulations to prospectively support clinical decisions. A cohort of CHD patients (n=18) who were referred for percutaneous pulmonary valve implantation (PPVI), stenting of aortic coarctation (CoA) and repair of double outlet right ventricle (DORV) was included in this study. Image data routinely acquired for clinical assessment (MRI, CT, echocardiography, x-ray) were postprocessed to set up patient-specific models. Finite element analyses (FEA) and computational fluid-dynamics (CFD) were performed to predict structural and haemodynamic changes following the procedures. Simulations were carried out to: select the best-matching device for each anatomy; address the risks of spatial interference with surrounding structures; optimize size and positions of device; design a surgical patch. The results were presented during clinical unit's multidisciplinary meeting. Measurable clinical outcomes from the real procedures were compared with the computer model predictions. The numerical results of FEA and CFD analyses were in accordance with the delivered treatment in all cases except in one case of PPVI. When devices were implanted, the post-procedural fluoroscopy images confirmed correct sizing and positioning of the stent in PPVI and CoA cases with an average difference in the stent sizes of 1.2 and 0.8 mm, respectively. Pressure and velocity data acquired by transthoracic echocardiography showed agreement with the results calculated with CFD analyses for CoA stenting and DORV repairs with a max error less than 3 mmHg. Each computational framework process was completed within a week with no requirements for additional clinical data. The early results of using computer simulations in clinics seem to be promising in terms of reliability of the simulations, response time, and usefulness in clinical practice. The translation of these technologies is crucial as it can limit the procedural risks for treatment of CHD cases.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Uncertain Quantification for Nonlinear Structural Dynamical Systems

Evangeline Capiez-Lernout*

*Université Paris-Est

ABSTRACT

This work is devoted to a research synthesis regarding advanced computational methodologies for structural and elasto-acoustic dynamical systems. It is about improving the modeling by considering two realistic phenomena that are the nonlinear geometrical effects and the uncertainty propagation on the dynamical response. The nonlinear geometrical effects are linked to the possibility for the mechanical system to be subjected to high-amplitude vibrational motion. In this context, it is relevant to consider exceptional operating regime as out of linear range regime. Moreover, the structural complexity of industrial systems put in evidence quantified uncertainties for input parameters and also a lack of knowledge in the nature of uncertainties. A special care in the probabilistic modeling has to be taken for analyzing how uncertainty propagates through the dynamical response of the system. The consideration of both phenomena is of particular importance because the nonlinear geometrical effects act as an internal excitation outside of the excitation range, yielding unexpected resonances that can potentially be sensitive to uncertainties. Then, a supplementary methodological constraint is required. It consists in adapting the computational strategy for the case of large-scale computational models, representing complex sensitive systems that can be found in the aeronautic or aerospace context. Consequently, efficient nonlinear reduced-order models have to be constructed in order to limit the computational costs. The main theoretical steps of the present strategy are first summarized, from the construction of the stochastic nonlinear reduced-order model to its numerical resolution [1]. The nonparametric probabilistic approach is used for implementing the uncertainties [2]. Note that the explicit construction of each linear, quadratic and cubic term operators issued fro the mean nonlinear reduced-order model has to be considered when uncertainty is implemented from these reduced operators. On the contrary, the stochastic nonlinear reduced internal efforts are directly constructed when uncertainty is implemented from a chosen reduced-order basis. A large panel of computational applications resulting from several academic, military and industrial collaborations is then presented. It concerns as well as the uncertain post-buckling behavior of cylindrical shells, as the intentional and unintentional turbomachinery mistuning, as the sloshing instability of the liquid surface of an aerospace tank. [1] Capiez-Lernout, E., Soize, C., Mignolet, M.-P., Computational stochastic statics of an uncertain curved structure with geometrical nonlinearity in three-dimensional elasticity, Computational Mechanics, 49(1), 87-97, 2012. [2] Soize, C., Stochastic Models of Uncertainties in Computational Mechanics, Lecture Notes in Engineering Mechanics 2, American Society of Civil Engineers, 2012.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Improving the Diffusive and Dispersive Properties of a Finite-Volume Cartesian Method in Presence of Adaptive Mesh Refinements

Francesco Capizzano*

*CIRA – Italian Aerospace Research Center 81043 Capua (CE), ITALY.

ABSTRACT

Key Words: Fluids; Finite-Volume; Cartesian method; Mesh refinement; Skew-symmetric operator. ABSTRACT The on-going effort aimed at developing a finite-volume Cartesian method for scale-resolving turbulent flows is described. In particular, the dissipative and dispersive properties of a discrete convective operator are investigated when applied on meshes with cell-based refinements. A skew-symmetric formulation [1, 2] is used to low the influence of numerical dissipation on the physical one especially when solving highly separated flows. The main objective is to conserve not only momentum and energy but also their quadratic forms as well as mass. In principle, this should enhance the correct evolution of the turbulent kinetic energy in the wake of bluff-bodies. Airframe noise and aero-elastic loads are typical examples in which massively separated flows play an important role. In particular, strong turbulent flows involve a wide range of spatial and temporal scales whose estimate represent a prohibitive task for methods based on Reynolds-Averaged Navier-Stokes (RANS) equations. Indeed, the latter mimic the presence of turbulent scales inside the flow field but do not resolve them. On the contrary, Large Eddy simulations (LES) resolve a significant range of turbulent scales leaving modelled only the smallest ones. The computational effort for LES simulations is, on the other hand, very high and too demanding for complex three-dimensional flows especially at high Reynolds numbers. Here, a hybrid RANS-LES Cartesian method is proposed as a reliable and robust tool for time-accurate simulations of complex flows around three-dimensional bluff-body configurations. A fully automatic and adaptive mesh refinement (AMR) strategy allows the saving of computational resources. An immersed boundary technique is coupled with a wall-model [3] in order to make affordable the study of high Reynolds number flows. Basic one- and two-dimensional studies are carried out in order to test the performance of the scheme at the interface between cells of different size. Indeed, the refined Cartesian meshes are characterized by a fixed cell-size ratio of two and accuracy issues can locally occur. A backward-facing step benchmark is carried out and the results are compared with solutions from body-conforming methods and experimental data.
REFERENCES [1] R. Verstappen, A. Veldman, Symmetry-preserving discretization of turbulent flow, Journal of Computational Physics, 187 (2003), 343-368. [2] J. C. Kok, A high-order low-dispersion symmetry-preserving finite-volume method for compressible flow on curvilinear grids, Flow Turbulence Combustion, 228 (7) (2009), 6811-6832. [3] F. Capizzano, Coupling a wall diffusion model with an immersed boundary technique, AIAA Journal, 54 (2) (2016), 2367-2381.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Simulation of Fretting Problems through an Enrichment-Based Approach

Raphael Cardoso*, David Néron**, Sylvie Pommier***, José Araújo****

*ENS Paris-Saclay / University of Brasilia, **ENS Paris-Saclay, ***ENS Paris-Saclay, ****University of Brasilia

ABSTRACT

The aim of this work, in collaboration with SAFRAN Aircraft Engines, is to use an enrichment-based approach to perform fretting simulations on coarse meshes. Indeed, contact problems subjected to fretting conditions give rise to high levels of stress concentration nearby the contact surfaces, and most of the times, it requires numerical simulations carried out on relatively fine meshes in the standard FE framework, which makes some industrial applications prohibitive. The main purpose of the present work is to enrich fretting simulations performed on cylinder-on-plane contact configurations (typical use-case in the study of the fretting phenomenon) in an attempt to reduce the computational costs in such cases. The enrichment functions considered in the analysis comes from the fact that the mechanical fields distribution in the neighbourhood of the contact edges in the fretting problems analysed are similar to the ones present close to the crack tip in LEFM problems. Simulations were enriched through the X-FEM. Besides plain fretting and fretting fatigue simulations, the proposed methodology was also tested when gross slip takes place. The first results were encouraging showing that, without considerably loss of accuracy, one can work with meshes up to 10 times coarser than it should be regarding the standard FEM. The use of nonlocal intensity factors, also coming from the crack analogy approach assumed in this study, demonstrated to be good indicators of the contact status (partial/gross slip conditions), with the advantage that those intensity factors can be obtained cheaply and are not strongly sensitive to the mesh refinement. Experimental fretting fatigue tests where analytical solutions are not available were conducted in order to test the applicability of the enrichment technique proposed. In this setting, the stress solutions extracted from the enriched simulations were applied to multiaxial fatigue models in order to predict experimental observations by means of fatigue limit.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Coupling Three-Dimensional Sperm Motility and Calcium Dynamics in a Kirchhoff-Rod Model

Lucia Carichino*, Sarah Olson**

*Worcester Polytechnic Institute, **Worcester Polytechnic Institute

ABSTRACT

Sperm are navigating in a complex three-dimensional fluid environment in order to achieve egg fertilization. Observed sperm trajectories can vary form planar to quasi-planar, and to helical, depending on the species, on the external fluid properties and on the proximity to oviductal walls. Changes in calcium concentration along the sperm flagellum regulate sperm motility and hyperactivation, characterized by an increased flagellar bend amplitude and beat asymmetry, enabling the sperm to reach and to penetrate the egg. However, the exact mechanisms of how calcium regulates the flagellar beat form are yet unknown and under investigation. We propose a fluid-structure interaction model that couples the three-dimensional motion of the flagellum in a viscous fluid with the calcium dynamics in the flagellum. The flagellum is modeled as a Kirchhoff-rod: an elastic rod where preferred intrinsic curvature and twist are imposed weakly by penalizing the energy functional. Given the low Reynolds number associated with sperm motility, the fluid surrounding the flagellum is modeled as a viscous and incompressible Newtonian fluid using Stokes equations. This fluid-structure interaction problem is solved using the method of regularized Stokeslets. The calcium dynamics are represented as a one-dimensional reaction-diffusion model on the moving flagellum, that accounts for calcium CatSper channels and calcium ATP-ase pumps in the principal piece of the sperm tail, and for a calcium store in the neck. The sperm motility and calcium dynamics are coupled assuming that the sperm flagellum preferred curvature depends on the evolving calcium concentration in time. The model is used to investigate the emergent three-dimensional waveforms and trajectories when coupling calcium and curvature, comparing three cases of preferred trajectories: planar, helical (spiral with equal amplitude in both directions), and quasi-planar (helical with smaller amplitude in one direction). The model results suggest that, given the same material properties of the sperm flagellum, the planar swimmer is faster than the three-dimensional swimmer, and clearly shows a turning motion when calcium coupling is accounted for in the model. Moreover, quasi-planar trajectories case exhibit flagelloid curves, defined as the paths followed by a fixed point on the flagellum, similar to hypotrochoid roulette with four or three singular points, depending on calcium coupling. Similar flagelloid curves have been observed experimentally.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Conservative Model Reduction for Finite-volume Models in CFD

Kevin Carlberg*, Youngsoo Choi**, Syuzanna Sargsyan***

*Sandia National Laboratories, **Lawrence Livermore National Laboratory, ***HERE Technologies

ABSTRACT

We present a method for model reduction of finite-volume models that guarantees the resulting reduced-order model is conservative, thereby preserving the structure intrinsic to finite-volume discretizations [1]. The proposed reduced-order models associate with optimization problems characterized by (1) a minimum-residual objective function and (2) nonlinear equality constraints that explicitly enforce conservation over subdomains. Conservative Galerkin projection arises from formulating this optimization problem at the time-continuous level, while conservative least-squares Petrov–Galerkin (LSPG) projection associates with a time-discrete formulation. We note that other recent works have also considered ROMs that associate with constrained optimization problems [3, 2], although none are conservative. We equip these approaches with hyper-reduction techniques in the case of nonlinear flux and source terms, and also provide approaches for handling infeasibility. In addition, we perform analyses that include deriving conditions under which conservative Galerkin and conservative LSPG are equivalent, as well as deriving a posteriori error bounds. On a parameterized quasi-1D Euler equation problem, the proposed method not only conserves mass, momentum, and energy globally, but also has significantly lower state-space errors than nonconservative reduced-order models such as standard Galerkin and LSPG projection. References [1] K. Carlberg, Y. Choi, and S. Sargsyan. Conservative model reduction for finite-volume models. arXiv e-print, (1711.11550), 2017. [2] L. Fick, Y. Maday, A. T. Patera, and T. Taddei. A reduced basis technique for long-time unsteady turbulent flows. arXiv preprint arXiv:1710.03569, 2017. [3] R. Zimmermann, A. Vendl, and S. Görtz. Reduced-order modeling of steady flows subject to aero- dynamic constraints. AIAA Journal, 52(2), 2014.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Proper Generalized Decomposition in Electrocardiology

Michele Giuliano Carlino*, Simona Perotto**, Alessandro Veneziani***

*University School for Advanced Studies IUSS, **MOX - Politecnico di Milano, ***Emory University

ABSTRACT

Among model reduction techniques available in the literature, Proper Generalized Decomposition (PGD) [1] seems to be particularly suited to approximate parametric differential problems. In contrast to more popular model reduction techniques, such as the Reduced Basis approach, PGD builds an approximate solution without any a priori knowledge of the full solution.??The basic idea of PGD is to consider the parameters of interest as additional independent variables. The consequent augmentation of the problem dimensionality is formally tackled via a classical separation of variables, that is eventually solved by an alternating direction algorithm. This approach guarantees a linear dependence of the computational complexity on the dimension of the problem, with a clear advantage for the efficiency of the procedure. In this presentation, after introducing the basics for a PGD approximation, we explore its application to the Inverse Conductivity Problem (ICP) in cardiac electrophysiology [2]. After introducing the Monodomain equations to model the polarization of the cardiac tissue cells at a macro-scale level, we show how PGD can be employed to estimate the conductivity parameters of the transmembrane electrical potential by minimizing a mismatch functional between sparse potential measures and the numerical solution. The efficient solution of the ICP is critical in clinical settings, for a factual use of computational patient-specific models. Results show that PGD is a promising option also in realistic geometries. References: [1] F. Chinesta, R. Keunings, A. Leygue, The Proper Generalized Decomposition For Advanced Numerical Simulations: A Primer. Springer Science & Business Media, 2013. [2] H. Yang, A. Veneziani, “Estimation of cardiac conductivities in ventricular tissue by a variational approach”. In: Inverse Problems 31.11 (2015), p. 115001.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Simulation of Fatigue Crack Growth and Failure Using a Variational Phase-Field Model

Pietro Carrara*, Marreddy Ambati**, Roberto Alessi***, Stefano Vidoli****, Laura De Lorenzis*****

*Technische Universität Braunschweig, Institute of Applied Mechanics, Germany, **Technische Universität Braunschweig, Institute of Applied Mechanics, Germany, ***Department of Structural and Geotechnical Engineering, SAPIENZA Università di Roma, Italy, ****Department of Structural and Geotechnical Engineering, SAPIENZA Università di Roma, Italy, *****Technische Universität Braunschweig, Institute of Applied Mechanics, Germany

ABSTRACT

Fatigue is a key phenomenon in mechanics, and is largely responsible for most of structural. Despite the significance of the problem, most existing fatigue theories are based on empirical laws that lack of generality and predictive capabilities. Hence, the development of mathematically sound and reliable fatigue models is still an open issue. Recently, Alessi et al. [1] proposed a new variational fatigue phase-field model based on the idea that the fracture toughness is degraded as a suitable internal history variable is accumulated. Such degradation, on turn, is ruled by a suitable dissipation potential which explicitly depends on the strain history. Therein the analysis is limited to a simple case, namely: one-dimensional, linear elasticity, brittle material behavior and symmetric response in tension and compression. This work aims at extending this model to higher dimensions including the unsymmetric response in tension and compression for the evolution of both phase-field and internal history variable, on which the fatigue relies on. The tension-compression splits proposed by Amor et al. [2] and Miehe et al. [3] are adopted. Also, the use of alternative internal history variables is explored highlighting advantages and drawbacks. To show the capability of the proposed model, classical benchmark problems, such as single edge tension/shear test and compact tension (CT) specimen for cyclic loadings are investigated. The effects of load amplitude and fatigue material parameters on the fatigue life are studied. Also, for the CT specimen, the Paris' law curves relating the fatigue crack growth rate obtained numerically (da/dN) vs. the stress intensity factor (dK) deduced by available semi-empirical relationships are presented. It is shown that the model is able to describe all three typical fatigue fracture regimes, namely the fatigue fracture initiation, the stable fatigue crack propagation and the final abrupt fracture stages. [1] R. Alessi, S. Vidoli L. De Lorenzis, A phenomenological approach to fatigue with a variational phase-field model: The one-dimensional case, Engineering Fracture Mechanics, in press (2017). [2] H. Amor, J.J Marigo, C. Maurini, Regularized formulation of the variational brittle fracture with unilateral contact: Numerical experiments, Journal of the Mechanics and Physics of Solids 57 (2009) 1209-1229. [3] C. Miehe C, F. Welschinger, M. Hofacker, Thermodynamically consistent phase-field models of fracture: variational principles and multi-field FE implementations, International Journal of Numerical Methods in Engineering 83 (2010) 1273-1311.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Thermal Simulation of Additive Manufacturing Processes Using Immersed Multi-level Isogeometric Analysis

Massimo Carraturo*, Ernst Rank**, Stefan Kollmannsberger***, Ferdinando Auricchio****, Alessandro Reali*****

*University Of Pavia, **Technical University of Munich, ***Technical University of Munich, ****University Of Pavia, *****University Of Pavia

ABSTRACT

We present the application of an advanced numerical framework, combining isogeometric analysis (IGA) and the finite cell method (FCM) [1] to the simulation of additive manufacturing (AM) processes. The different physics involved in the transient processes (phase transition from powder to liquid and solid) are treated with FCM, an immersed boundary method employing high order shape functions. The idea is to embed the solidified region within a fictitious domain which can be easily discretized by a cartesian grid, whereas the transient geometry of the physical problem is reconstructed only in the integration phase. This approach avoids the generation of a conforming mesh for the evolving domain with very complex shape. In order to exploit the local nature of the problem, in the present work FCM is combined with a multi-level implementation of IGA [2] based on the multi-level Bézier extraction technique and truncated hierarchical B-Splines (THB-splines). This method combines an efficient high order and higher continuous discretization with accurate refinement and coarsening schemes, allowing to localize the computational effort in a small region around the heat affected zone (HAZ). In fact, as shown in [3], it is favourable to choose a spatial discretization of high order together with refinement and de-refinement schemes towards the HAZ. While refinement is rather straightforward, the de-refinement procedure for high order polynomial basis is not trivial. It requires to locally project the solution from a source (fine) mesh onto a target (coarsened) mesh and, furthermore, the target discretization has to address some admissibility requirements to avoid numerical instabilities which can arise during projection. Verification and comparison with standard FEM technologies are obtained by means of analytical reference results, showing the higher approximation capabilities of the presented technology with respect to classical methodologies. Finally, validation results for the presented method are carried out using experimental data. References [1] Parvizian, J., Düster, A. and Rank, E., ”Finite Cell Method” in Computational Mechanics, 41(1):121–133, (2007). [2] D’Angella, D., Kollmannsberger, S., Rank, E. and Reali, A., Multi-level Bézier extraction for hierarchical local refinement of Isogeometric Analysis, Computer Methods in Applied Mechanics and Engineering, (2017), http://dx.doi.org/10.1016/j.cma.2017.08.017. [3] Kollmannsberger, S., Özcan, A., Carraturo, M., Zander, N. and Rank, E., A hierarchical computational model for moving thermal loads and phase changes with applications to Selective Laser Melting, Computers & Mathematics with Applications, (2017), https://doi.org/10.1016/j.camwa.2017.11.014.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Understanding Spatial Adaptation in Cortical Bone and the Driving Mechanical Stimuli

Alessandra Carriero*, Andre Pereira**, Amanda Wilson***, Simone Castagno****, Behzad Javaheri*****, Andrew Pitsillides******, Massimo Marenzana*******, Sandra Shefelbine********

*The City College of New York, **Imperial College London, ***Imperial College London, ****Imperial College London, *****Royal Veterinary College, ******Royal Veterinary College, *******Imperial College London, ********Northeastern University

ABSTRACT

Bone is a dynamic tissue and adapts its architecture in response to biological and mechanical factors. However, we still do not understand how the process of bone adaptation is regulated. Particularly, it is still unclear how bone spatially adapts to the applied loads, and what is the mechanical stimulus for adaptation. Spatial regulation of bone mechanoadaption has been difficult to understand for 1) the challenges to accurately investigate a spatially and temporally varying mechanical filed in the bone during loading, and for 2) the difficulty to indetify regions of adaptation throughout the bone, when the amount of bone formation was in the order of 10 ?m or less. Here, we use the murine tibial loading model to determine spatial relationships between the mechanical environment and bone formation in the entire tibial cortical bone. We examine both strain and fluid flow dependent stimuli in an experimentally validated finite element model. Regions of bone formation are detected with three-dimensional imaging of fluorochrome labels in a novel slice-and-view technique for cortical bone histomorphometry at high resolution (1.59 ?m). The mechanical stimuli (strain energy density or fluid velocity) are compared visually and quantitatively to regions of bone formation on the tibial endosteal and periosteal surface along the entire cortical bone lenght. Our results show that (i) in adult (22 weeks old) C57BL6 mouse, bone adapts to loads along its entire length on both the endosteal and periosteal surface, and that (ii) high fluid flow is able to predict formation of bone on both these surfaces, while high strain energy density can predict bone formation only periosteally. Providing clues to the biophysical stimuli to which bone responds, future studies can use this knowledge to develop loading protocols that direct bone adaptation to a specific site in osteopenic bone.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

An Immersed Boundary Method and Dynamic LES Finite Element Method for Modeling Internal Combustion Engines

David Carrington*, Jiajia Waters**

*Los Alamos National Laboratory, **Los Alamos National Laboratory

ABSTRACT

A stabilized finite element mass consistent projection method has been developed for modeling turbulent reactive flow in machines with immersed moving parts. The method employs a dynamic Vreman LES where the turbulent or eddy viscosity becomes zero for laminar or fully resolved flow regions; flow regimes and regions where eddy viscosity is expected to vanish. This feature of the Vreman dynamic LES make it ideal for modeling highly unsteady wall-bounded flow. Immersed moving boundaries or moving parts either are actuated through the fluid (valves) or moving the fluid (pistons). The effect of these immersed moving boundaries on the flow is determined with immersed boundary method. A moving marker system determines the location of the immersed boundaries. The effects of these boundary motions are determined through a series of projections along the normal to a surface from the marker's location. The primitive values are determined at element nodes. On the non-fluid side of the intersected element, the primitive values are viewed as no-slip boundary values. On the fluid side of the intersected element, a normal vector is created to the moving surface from the marker's location. Then where that normal intersects neighboring fluid elements, the nearest nodal value in those neighbor fluid elements are projected orthogonally onto the normal vector and a distance to the marker is determined. With this projected value and the value on the moving surface boundary (at its current state) interpolation then provides primitive values at the intersected elements fluid nodes. A 2nd order differencing supplies the properties at these nodes. The immersed boundary method allows for an Eulerian frame for solving the physical model equations, that is, a fixed domain is being used throughout the entire simulation. Many moving boundaries surfaces can easily be simulated at once. Gridding complex systems with many parts is greatly simplified because the moving boundaries are simply represented by triangulated surfaces, in stl format. These surfaces overlay the fluid grid. Therefore, grid generation proceeds without considering the parts making a simply a convex grid for the combustion chamber and ports, something can easily be created automatically. The developed code is the 5th generation of LANL's KIVA software going by the name of KIVA-hpFE. Specifics of these methods as they pertain to the engine modeling along with their application and validation are provided.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Characterizing Slip Network Formation within a Polycrystalline Aggregate during Cyclic Loading Utilizing a Novel Formulation for Representing and Evolving Smooth Lattice Orientation Fields

Robert Carson*, Paul Dawson**

*Cornell University, **Cornell University

ABSTRACT

Cyclic loading of polycrystalline metals result in complex states of intragrain heterogeneous deformation. In cyclic loading, persistent slip bands (PSBs) have been studied since the late 1950s as a mechanism for void and crack formation in fatigued single crystals. Several models exist that offer an explanation for the formation of persistent slip bands. Of these, only a few potentially extend to polycrystalline aggregates, where the manner in which PSBs manifest is unclear [1]. From these models, however, is a recurrent ingredient which is the presence of localized slip. In this presentation, we explore how networks of localized multislip are able to traverse and evolve over a crystal and the aggregate during the first few cyclic loads of a sample. A smooth crystal lattice orientation assumption is imposed upon each crystal in order to allow for these networks to form and cross grain boundaries. First, we present the degree to which these networks are able to form not only across a crystal but also the aggregate. Next, we present how these networks can differ between an equiaxed sample and a sample instantiated from near-field high energy x-ray diffraction data. Finally, we present how various kinematic and diffraction intragrain-heterogeneous metrics [2] can present signs of network formation for a combined near-field and far-field high energy x-ray experiment. [1] J. Man, K. Obrtlík, and J. Polák. Extrusions and intrusions in fatigued metals. Part 1. State of the art and history. Philosophical Magazine, 89(16):1295–1336, Jun 2009. [2] Robert Carson, Mark Obstalecki, Matthew Miller, and Paul Dawson. Characterizing heterogeneous intragranular deformations in polycrystalline solids using diffraction-based and mechanics-based metrics. Modelling and Simulation in Materials Science and Engineering, 25(5):055008, May 2017.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Topology-Optimized Design of Ceramic Structural Elements for Civil Applications

Josephine Carstensen*, Michal Ganobjak**, Jackson Jewett***

*Massachusetts Institute of Technology, **Massachusetts Institute of Technology, ***Massachusetts Institute of Technology

ABSTRACT

Topology optimization design algorithms have in recent years become increasingly popular for mechanical engineering design; it is especially used in the automotive and aerospace industries. However, the number of gradient based algorithms for civil engineering design applications remain limited. The few existing examples include using topology optimization for conceptional structural design, outrigger-placement in dynamically loaded tall buildings and a handful of algorithms specifically for reinforced concrete design. Most of the world's civil construction makes used of concrete and other ceramic materials. These types of materials can be highly heterogeneous and typically exhibits different strength properties in tension and compression. Topology optimization algorithms have been proposed for both conventional and fiber reinforced concrete design. However, currently no designs have been fabricated and experimentally examined. In this work, we focus on numerically and experimentally examining the performance of plain concrete structures designed with existing topology optimization algorithms. The heterogeneous nature of concrete is simplified as isotropic and the strength difference in tension and compression is accounted for by (i) stress constraints [1] and (ii) neglecting the tensile capacity [2]. For civil applications, there exist many types of conventional low weight structural elements of ceramic materials, such as hollow decks, bricks or cinderblocks. With an increased focus on the energy performance of the built environment, there is renewed interest in design algorithms that can produce novel composite construction elements with combined stiffness and thermal performance. In this work, we suggest a topology optimization algorithm to design climate specific construction modules. In the algorithm, the minimum length scale is controlled through the Heaviside projection method and MMA [3] is used as the gradient-based optimizer. [1] Gaynor, A.T., Guest, J.K. and Moen, C.D. (2013), "Reinforced concrete force visualization and design using bi-linear truss-continua topology optimization", J Struct Eng, 139, pp 607-618. [2] Le, C., Norato, J., Bruns, T., Ha, C. and Tortorelli, D. (2010) "Stress-based topology optimization for continua", Struct Multidisc Optim, 41, pp 605-620. [3] Svanberg, K. (1987), "The method of moving asymptotes – A new method for structural optimization", Int J for Numer Meth in Engrg, 24, pp 359-373.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Non-linear Finite Volume (NLFV) Method Coupled to a Multidimensional Optimal Order Detection Method (MOOD) for the Numerical Simulation of Oil-water Flows in Petroleum Reservoirs

Darlan Carvalho*, Fernando Licapa**, Marcio Souza***, Paulo Lyra****

*Federal University of Pernambuco, UFPE, **Federal University of Pernambuco, UFPE, ***Federal University of Paraiba, UFPB, ****Federal University of Pernambuco, UFPE

ABSTRACT

In this work, we propose a full finite volume approach to simulate two-phase flows of oil and water in heterogeneous and anisotropic petroleum reservoirs in 2-D. The pressure equation has an elliptic operator with a diffusion coefficient, which is, in general, a heterogeneous full tensor. In the context of petroleum reservoir simulation, failure to satisfy the Discrete Maximum Principle (DMP) or at least failure to produce monotone solutions leads to spurious oscillations in the pressure field that can, for instance, lead to the appearance of spurious gas in regions of the reservoir where the pressure falls erroneously below the bubble point. To solve the pressure equation, we have devised a Non-Linear Finite Volume (NLFV) method. This method provides monotone solutions and it reproduces piecewise linear solutions exactly, even for very distorted polygonal meshes and arbitrary anisotropic permeability tensors [3]. To solve the non-linear hyperbolic saturation equation, we adapt a novel method proposed by [1] called Multidimensional Optimal Order Detection (MOOD). This scheme is radically different from classical high order methods, since it is based on an “a-posteriori” limitation procedure. In short, the MOOD scheme consists in determining an optimal polynomial degree reconstruction for each control volume (CV) at each time step, satisfying some physical restriction, e.g., monotonicity. Then, the candidate solution in all control volumes are rigorously analyzed by the physical criteria. Whenever the physical criteria is violated in the control volume, the latter is marked and this solution is automatically discarded and the degree of the polynomial is decreased until the physical restriction is satisfied in the CV. The performance of the proposed full finite volume formulation is verified by solving some relevant benchmark problems. References [1] Clain, S., Diot, S., & Loubere, R., 2011. A high-order finite volume method for systems of conservation laws Multi-dimensional Optimal Order Detection (MOOD). Journal of computational Physics 230.10: 4028-4050. [2] Contreras, F. R. L., Lyra, P. R. M., Souza, M. R. A., & Carvalho, D. K. E., 2016. A cell-centered multipoint flux approximation method with a diamond stencil coupled with a higher order finite volume method for the simulation of oil–water displacements in heterogeneous and anisotropic petroleum reservoirs. Computers & Fluids 127: 1-16. [3] Queiroz, LES., Souza, MRA., Contreras, FRL., Lyra, PRM. & Carvalho, DKE. 2014. On the accuracy of a nonlinear finite volume method for the solution of diffusion problems using different interpolations strategies. Int J Numer Meth Fl, 74(4):270-291.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Discontinuous Skeletal Method for Bingham Fluids

Karol Cascavita*, Jérémy Bleyer**, Xavier Chateau***, Alexandre Ern****

*Université Paris-Est, CERMICS (ENPC) and INRIA Paris., **NAVIER, UMR 8205, École des Ponts, IFSTTAR, CNRS, UPE., ***NAVIER, UMR 8205, École des Ponts, IFSTTAR, CNRS, UPE., ****Université Paris-Est, CERMICS (ENPC) and INRIA Paris.

ABSTRACT

Keywords: Discontinuous Skeletal methods, Viscoplastic flows, Augmented Lagrangian methods This work is motivated by the growing interest in the simulation of yield stress fluids for civil engineering materials, blood, foams, etc. To this aim, we propose a Discontinuous Skeletal (DiSk) method for the antiplane Bingham model, inspired by the Hybrid-High Order method introduced in [1] for linear elasticity. In particular, we focus on the lowest order case, where discrete velocity unknowns are constant polynomials: one per cell and one per face, and the cells unknowns are eliminated by static condensation. The main advantages are local conservativity and the possibility to use general meshes. We consider the Augmented Lagrangian method to solve the variational inequalities resulting from the discrete Bingham problem. We introduce constant Lagrange multipliers for the velocity gradient in each cell and for its jumps at each face. In comparison to Finite Element Methods, such as the use of Taylor-Hood elements [2], a crucial advantage of DiSk methods is that polytopal meshes are supported. We can exploit their use in performing local mesh adaptation, either locally refining around liquid-solid interfaces or coarsening in the solid regions. Numerical results are presented for circular and square domains and for different Bingham numbers. We show local adaptation can be exploited and the method is shown to capture regions of sharp transition between solid- and fluid-like regimes. References [1] D.A. Di Pietro and A. Ern. A hybrid high-order locking-free method for linear elasticity on general meshes. Comput. Methods Appl. Mech. Engrg., Vol. 283, pp 1-21, 2015. [2] P. Saramito and N. Roquet. An adaptive finite element method for viscoplastic fluid flows in pipes. Comput. Meth. Appl. Mech. Eng., Vol. 190, pp 5391 -5412, 2001.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Some Model Order Reduction Developments at Safran

Fabien Casenave*, Nissrine Akkari**, Christian Rey***

*Safran, **Safran, ***Safran

ABSTRACT

For the last two years, reduced order models have been developed at Safran on various applications. The nonlinear transient heat equation has been reduced in a context of directional solidification of turbine blades in monocrystalline alloy. The change of phase is modelled by a local maximum of the heat capacity with respect of the temperature, located around the temperature of fusion. The nonlinearity is hyperreduced using the Empirical Interpolation Method (EIM). The translation of the blade out of the oven induces an advection phenomenon in the frame of the blade, known to be poorly reducible. Local (in space) POD basis are used to recover a good speedup, and are observed to improve the stability of the EIM. Life calculation of elasto-visco-plastic materials is critical in design phases to prevent fatigue-induced deterioration of certain parts of aircraft engines. Such computations require the simulation of a large number of cycle loads on large meshes, which is currently a challenge. The POD and the EIM are used to extrapolate the behavior of the material, after some cycles have been computed using the high fidelity model. A nonintrusive model reduction platform is in development for the reduction of solid mechanics computations: starting from displacement snapshots, a mesh of the domain and the knowledge of the loading and the behavior, an in house finite element engine in python and the Zmat behavior law solver are used to carry-out the hyperreduction part of the procedure, instead of modifying the source code of the solver used to generate the snapshots. In some parts of the turbofan, the Large Eddy Simulation (LES) is computed by aircraft engine manufacturers to assess the effects of the turbulence, in particular in the combustion chamber and the injectors. The incompressible Navier-Stokes equations have been reduced using an original stabilization for the POD, based on the construction of modes for the velocity and the gradient of the velocity. To explore different local designs of injectors without recomputing the whole domain, an original procedure based on the computation of local LES and a POD correction on the rest of the domain is proposed. Finally, an original method has been proposed for the nonlinear regression of the solution of parametrized linear systems, making use of the knowledge of the (assumed affine) parametric dependence. This works aimed to add information of the underlying physics to black-box-like regression procedures.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Residual Strength Analysis of Aircraft Structures with a High Performance Computing Code

Eva Casoni*, Adrià Quintanas-Corominas**, Gerard Guillamet***, Jose Reinoso****

*CASE, Barcelona Supercomputing Center, **AMADE, University of Girona, ***CASE, Barcelona Supercomputing Center, ****Elasticity and Strength Material group, University of Sevilla

ABSTRACT

The use of laminated composite materials in the aircraft industry increases due to their excel- lent stiffness-to-weight ratios. Over the time of its service life, some parts of the aircraft are prone to damage up to the final failure. The failure from these materials involves different damage mechanisms and it is complex to predict due to anisotropy of the material. These damage mechanisms can be studied, at different length scales or even from a multi-scale point of view. In general, the mesoscale level is the most suitable and reliable for the prediction of the structural behaviour and the material degradation, but can be prohibitive for large scale structures. A 3D consistent damage model for composite laminates at the mesoscopic length scale is proposed [1]. The onset and growth of damage is based on experimental phenomenology iNcorporating energetic considerations into the progressive damage evolution. Additionally, the current damage model is used with continuum shell elements, that are specially formulated with the aim of reproducing the full stress state and avoid the locking pathologies inherent in solid elements [2]. The overall framework is implemented in a high-performance multi-physic parallel tool, Alya, a mechanics FE code specifically developed for large-scale massively parallel simulations [3]. The combination of continuum shell elements and the 3D damage model has been demonstrated in a simulation of stringer-stiffened composite panel test and a complex barrel fuselage, which are prone to buckle. The selected examples are a good representation of Alya applicability, because they are highly non-linear and require refined meshes in order to obtain accurate results, thus increasing the computational cost. The numerical predictions are compared to experimental results and the computational efficiency is also analysed. References [1] A.Quintanas-Corominas,P.Maimi?,E.Casoni,J.A.Mayugo,A.Turon,M.Va?zquez(2017). A 3D transversally isotropic constitutive model for advanced composites implemented in a high-performance computation code. European Journal of Mechanics A/solids, (submitted) [2] J. Reinoso and A. Bla?zquez (2016) Application and finite element implementation of 7- parameter shell element for geometrically nonlinear analysis of layered CFRP composites. Composite Structures, 139, 263-276. [3] E. Casoni, A. Je?rusalem, C. Samaniego, B. Eguzkitza, P. Lafortune, D. Tjahjanto, X. Sa?ez, G. Houzeaux and M. Va?zquez (2015) Alya: computational solid mechanics for supercom- puters. Archives of Computational methods in Engineering, 22 (4), 557-576.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Node-Based Form Finding with Shape-Dependent Target Definition

Michael Caspari*, Paul Steinmann**, Philipp Landkammer***

*Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), **Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU), ***Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)

ABSTRACT

Metal forming processes are distinguished into sheet and bulk metal forming. This classification results from the prevailing stress state of the respective forming operation. The recent sheet-bulk metal forming (SBMF) process, presented in [1], combines the two basic processes into a single more complex process. Within this studies in particular tailored blanks are considered, i.e. semi-finished products are a priorily adapted to the intended SBMF process. For this purpose, our form finding algorithm is designed to optimize the shape of the semi-finished product, i.e. the material configuration in a forming process. The geometry of the semi-finished product is adapted so that the computed spatial configuration corresponds to a prescribed target spatial configuration. Differences between these two configurations are iteratively minimized. The algorithm works non-invasively, thus there is a strict separation between the form update of the finite element (FE) forming simulation. This separation allows the use of arbitrary commercial FE-solvers. Furthermore, it is possible to optimize structures of high complexity with nonlinear material behavior, contact constraints and large deformations. The basic optimization approach was first introduced by Landkammer and Steinmann [2] and various enhancements have been presented in [3]. The focus of our current work is on the further improvement of the stability and robustness of the optimization algorithm. The latest developments include two major modifications in order to enhance its applicability to real processes. The dependency of the optimized material position of individual nodes on the respective nodes in the target spatial configuration is entirely bypassed by releasing the mesh of the target spatial configuration from that of the FE forming simulation. This is realized by changing the computation of the differences between the computed spatial configuration and the target spatial configuration. In addition, a first step is made to consider manufacturability of the optimization result when manufacturing constraints must be taken into account. The constraint considered here is the available design space for the semi-finished product, which is limited by the material pre-distribution process.
References: 1. Merklein, M., Allwood, J., Behrens, B.-A., Brosius, A., Hagenah, H., Kuzman, K., Mori, K., Tekkaya, A., and Weckenmann, A. (2012), „Bulk forming of sheet metal", CIRP Annals - Manufacturing Technology, 61(2):725-745 2. Landkammer, P. and Steinmann, P. (2016), „A non-invasive heuristic approach to shape optimization in forming", Computational Mechanics, 57(2):169-191 3. Landkammer, P., Caspari, M., and Steinmann, P. (2017), „Improvements on a non-invasive, parameter-free approach to inverse form finding", Computational Mechanics, doi:10.1007/s00466-017-1468-2

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

The Divergence-Conforming Immersed Boundary Method

Hugo Casquero*, Yongjie Jessica Zhang**, Carles Bona-Casas***, Hector Gomez****

*Carnegie Mellon University, **Carnegie Mellon University, ***Universitat de les Illes Balears, ****Purdue University

ABSTRACT

The divergence-conforming immersed boundary (DCIB) method is presented to tackle a long-standing issue of immersed boundary (IB) numerical methods for fluid-structure interaction, namely, the challenge of accurately imposing the incompressibility constraint at the discrete level [1]. IB methods deal with incompressible visco-elastic solids interacting with incompressible viscous fluids. The DCIB method follows up on our previous works [2-3], where we developed discretizations of the mathematical model proposed by the IB method based on non-uniform rational B-splines (NURBS) and T-splines, respectively. In the DCIB method, the Eulerian velocity-pressure pair is discretized using divergence-conforming B-splines, which leads to inf-sup stable, H^1-conforming, and pointwise divergence-free Eulerian solutions. The Lagrangian displacement is discretized using NURBS, which enables to robustly handle large mesh distortions. The data transfer needed between Eulerian and Lagrangian descriptions is performed at the quadrature level by using the same spline basis functions that define the computational meshes, conducing to a fully variational formulation, sharper treatment of the fluid-solid interface, and a 0.5 increase in the convergence rate of the Eulerian velocity and the Lagrangian displacement measured in L^2 norm. By combining the generalized-alpha method and a block-iterative solution strategy, the DCIB method results in a fully-implicit discretization, which is key to impose accurately the no-penetration and no-slip conditions at the fluid-solid interface. Various two- and three-dimensional problems are solved to show all the above-mentioned properties of the DCIB method together with mesh-independence studies, comparisons with other methods from the literature, and measurement of convergence rates. The DCIB method leads to completely negligible incompressibility errors at the Eulerian level and various orders of magnitude of increased accuracy at the Lagrangian level compared to other IB methods. Finally, we use the DCIB method to answer open questions in cell-scale blood flow.
REFERENCES 1. H. Casquero, Y. J. Zhang, C. Bona-Casas, L. Dalcin, H. Gomez, Non-body-fitted fluid-structure interaction: Divergence-conforming B-splines, fully-implicit dynamics, and variational formulation, under review, 2018. 2. H. Casquero, C. Bona-Casas, H. Gomez, A NURBS-based immersed methodology for fluid-structure interaction. Computer Methods in Applied Mechanics and Engineering, 284, 943-970, 2015. 3. H. Casquero, L. Liu, C. Bona-Casas, Y. J. Zhang, H. Gomez, A hybrid variational-collocation immersed method for fluid-structure interaction using unstructured T-splines. International Journal for Numerical Methods and Engineering, 105, 855-888, 2016.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

An Off-Lattice Hybrid Model for Tissue-Engineered Articular Cartilage

Simone Cassani*, Sarah Olson**

*Worcester Polytechnic Institute, **Worcester Polytechnic Institute

ABSTRACT

Articular cartilage is an avascular connective tissue that covers articular joints in the body to provide: (i) a lubricated smooth surface that allows bones to slide over each other during motion, and (ii) a shock absorbing surface that keeps bones from colliding during moderate and vigorous physical activities. Articular cartilage has a complex structure composed of a dense extracellular matrix (ECM), which includes fluid, a collagen network, and other proteins. Distributed in the matrix there are chondrocytes (cells) that synthesize the building blocks of the ECM. Nutrients and oxygen are provided via diffusion through the gel-like structure of the ECM. Pathologies such as osteoarthritis, injuries and normal wear and tear can cause the erosion and damage of articular cartilage. Due to the limited ability of cartilage to self-repair, tissue engineering represents a promising path towards the treatment of damaged cartilage. Tissue-engineered cartilage is produced in vitro to be implanted at the site of the damaged cartilage to restore its normal functionality. To guarantee a successful outcome, tissue-engineered cartilage must have specific structural and mechanical properties. In this work, a hybrid mathematical model is used to investigate the phenomena of cartilage growth in a tissue-engineered construct to elucidate and clarify the influence of different biological factors and conditions, such as scaffold porosity, nutrient distribution and cell velocity. This hybrid model couples a discrete modeling approach for the chondrocytes, with a continuous approach for the remaining components of the matrix. The chondrocytes are described using an off-lattice cellular automata model that accounts for cell movement, cell division, cell-to-cell contact inhibition and cell death. The cellular movement follows a random motion biased by the local nutrient concentration and the local porosity surrounding the cells. Cell division is modulated by the cellular cycle, and by the availability of nutrient and the level of porosity surrounding the cell. The continuous components of the model, nutrient concentration, scaffold porosity and ECM volume fraction are modeled based on physiological behaviors consistent with the literature. We use the model to investigate the influence of different scaffold properties and cell seeding on the synthesis of new ECM. The insight provided by the model will be used to elucidate some of the outcomes of laboratory experiments involving tissue-engineered articular cartilage.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Grounding System Analysis for Underground Electrical Substations Based on Boundary Element Method

Manuel Casteleiro*, Raquel Guizán**, Fermín Navarrina***, José París****, Ignasi Colominas*****

*Universidade da Coruña, **Universidade da Coruña, ***Universidade da Coruña, ****Universidade da Coruña, *****Universidade da Coruña

ABSTRACT

Electrical substations are essential elements in the electricity supply system. Traditionally, they are industrial units located above ground that require large areas of land for their electrical equipment. However, nowadays, the electricity supply system have experienced an increasing demand for power and power supply and the need to transmit electricity at high voltage levels to the bustling urban centers, since most of electricity customers live and work at cities. Consequently, the construction of new electrical substations located in urban areas, where the free surface is limited and the environmental requirements are more severe, is needed. Thus, the engineers developed the underground electrical substations, which are compact solutions where all electrical equipment is placed underground inside precast concrete enclosures. An essential element in the design of electrical substations is safety. During a fault condition, grounding systems are the devices in charge to ensure the proper functioning of the electrical equipment and the safety of people in the vicinity areas. Since the beginning of electrical substations, empirical formulas and suitable techniques are developed to calculate their parameters for uniform soil models or layered soil structures. However, underground electrical substations represent a finite heterogeneity inside the ground, and so, a specific approach that allows to model this soil structure is necessary. In this work the authors carried out a numerical approach with a realistic approximation to soil structure based on the Boundary Element Method and on the weighted residual methods of Point Collocation and Bubnov-Galerkin Method to design and analyze the grounding grid of underground electrical substations, and to calculate their main parameters, which are the ground resistance, the ground potential rise, and the step, touch and mesh voltage, as well as the voltage distributions. Finally, grounding systems analysis for real underground transformer substations has been done.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Rollover Stability Analysis of a Double-Deck Bus Under Crosswind Effects by Computational Simulation

Hugo Guillermo Castro*, Rodrigo Rafael Paz**, Facundo Del Pin***, Iñaki Caldichouri****

*Instituto de Modelado e Innovación Tecnológica (IMIT-UNNE) - CONICET - UTN Facultad Regional Resistencia, **Livermore Software Technology Corporation (LSTC) - CONICET, ***Livermore Software Technology Corporation (LSTC), ****Livermore Software Technology Corporation (LSTC)

ABSTRACT

Every road vehicle under motion experiences forces and moments caused by different sources, being the wind one of the most important. Historically, several researches (computational and experimental) have dealt with the effects of the wind over road vehicles [1]. Particularly, high sided road vehicles (e.g., double-deck buses) are highly demanded because their passenger transportation capability, being the most used mean of passenger transportation in some countries of Latin America. This type of vehicle have its centre of mass in a relatively high location so in combination with moderate velocities may give rise to rollover instabilities [2]. This scenario is further dangerous when the vehicle motion is developed along a road bend, adding lateral forces due to the centrifugal acceleration effect. In this work, as a typical application of a coupled analysis, an unsteady aerodynamics simulation of a simplified double-deck bus in windy conditions is demonstrated, and the effects of the unsteady aerodynamics on the bus motion are investigated. The obtained results are compared with the results of a conventional quasi-steady analysis. The effects of the aerodynamics clearly indicate the importance of estimating the unsteady aerodynamic forces in a vehicle motion analysis. [1] Fuller, J.; Best, M.; Garret, N.; Passmore, M.; “The importance of unsteady aerodynamics to road vehicle dynamics”, Journal of Wind Engineering and Industrial Aerodynamics, 117 pp. 1-10, 2013. [2] Dorigatti, F.; Sterling, M.; Rocchi, D.; Belloli, M.; Quinn, A.D.; Baker, C.J.; Ozkan, E.; “Wind tunnel measurements of crosswind loads on high sided vehicles over long span bridges”, Journal of Wind Engineering and Industrial Aerodynamics, 107-108 pp. 214 – 224, 2012.

13th World Congress on Computational Mechanics (WCCM XIII) and 2nd Pan American Congress on Computational Mechanics (PANACM II), July 22-27, 2018, New York City, NY, USA

MODELING AND IDENTIFICATION OF A STOCHASTIC MODEL OF VOCAL FOLDS FOR PRODUCING VOICE SIGNALS WITH PATHOLOGICAL CHARACTERISTICSS

E. Cataldo*, C. Soize+ and E. Barrientos*

* Universidade Federal Fluminense, Telecommunications Engineering Department and Graduate program in Telecommunications Engineering, Rua Passo da pátira, 156, Inga, Niteroi, RJ, CEP:24210-240 , Brazil

+ Université Paris-Est, Laboratoire Modelisation et Simulation Multi Echelle, MSME UMR 8208 CNRS, 5 Bd Descartes, 77454 Marne-La-Vallée, France

Key words: *Voice production, stochastic model, jitter, inverse stochastic problem.*

Abstract. This paper aims to propose a stochastic model, considering three control parameters, to generate jitter based on a deterministic one-mass model for the dynamics of the vocal folds and to identify parameters from the stochastic model taking into account real voice signals experimentally obtained. To solve the corresponding stochastic inverse problem, the cost function used is based on the distance between probability density functions of the random variables associated with the fundamental frequencies obtained by the experimental voices and the simulated ones, and also on the distance between features extracted from the voice signals, simulated and experimental, to calculate jitter. The results obtained show that the model proposed is valid and some samples of voices are synthesized considering the identified parameters for normal and pathological cases.

1 INTRODUCTION

The production of a voiced sound starts when the airflow coming from the lungs is modified into the glottal signal, a quasi-periodic signal after passing through the glottis, where the vocal folds are located. The main examples of voiced sounds are the vowels and this paper is based on their production.

The acoustic pressure signal, after passing by the vocal folds, is filtered and amplified by the vocal tract and then radiated by the mouth originating the voice signal. As the vocal folds displacements are not exactly symmetric the time intervals corresponding to the air pulses of the glottal signal have random fluctuations, called jitter.

The stochastic model proposed here has the origin based on the deterministic model

created by Flanagan and Landgraf [1], known as the first model used to generate voice using a nonlinear one-mass mechanical model. More complete deterministic models were created [2;3;4;5] even considering pathological cases in the vocal folds [6] or stress situation [7] but the idea here is to show that it is possible to generate jitter and voice signal with quality from the primary model considering the stiffness as a stochastic process and, mainly, validate the model proposed identifying parameters solving an statistical inverse problem taking into account experimental normal voices and also with pathological characteristics.

2 PRIMARY DETERMINISTIC MODEL

Figure. 1 illustrates a sketch of the model.

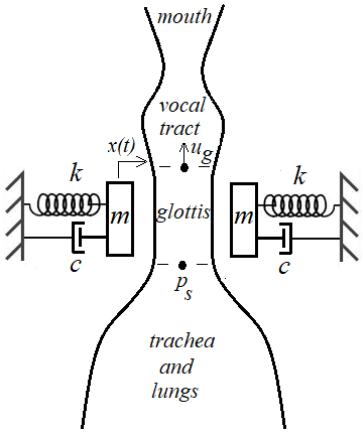


Figure 1: Sketch based on the Flanagan and Landgraf (1968) model.

Each vocal fold is represented by a nonlinear mass-stiffness-damper system and the complete model is composed by the subsystem of the vocal folds (*source*) coupled by the glottal flow to the subsystem of the vocal tract (*filter*). To generate jitter the stiffness will be considered as a stochastic process for which a model is proposed.

3 STOCHASTIC MODELING OF JITTER

The stiffness k is modeled by a stochastic process $\{K(t), t \in \mathbb{R}\}$ with values in $\mathbb{R}^+$. Consequently, the dynamical position of each vocal fold will be given by a stochastic process, named $X(t)$, coupled with the stochastic process associated with the glottal flow (volume flow velocity), noted $U_g(t)$. The stochastic dynamics of the vocal folds is described by Eq. 1:

$$m\,\frac{d^2X(t)}{dt^2} + \{c + c^*(X(t))\}\,\frac{dX(t)}{dt} + K(t)\,X(t) + a_1\,p_B(X(t), U_g(t)) = a_2\,p_s(t)\,, \qquad (1)$$

where $a_1 = 1.87\,\frac{\ell \mathrm{d}}{2}$ and $a_2 = \frac{\ell \mathrm{d}}{2}$, with ℓ the length of each vocal fold and d the vocal fold thickness. The stochastic process $X(t)$ is the displacement of the mass m of one vocal fold, $K(t)$ is its stiffness and c is its damping coefficient when the glottis is opened; when the glottis is closed, there is an additional damping given by $c^*(X(t))$ described in the following, where the Bernoulli pressure $p_B(X(t), U_g(t))$ is also described.

The stochastic process $U_g(t)$ is the acoustic volume velocity through the glottal orifice (the glottal flow). The air pressure that comes from the lungs and forces the vocal folds is called the subglottal pressure and is denoted by $p_s(t)$. The constant parameters have been discussed in the original paper about the corresponding deterministic model[1]. Some information about values can also be found in [8].

A representation of non-Gaussian stochastic process $K(t)$ can be constructed using Information Theory as explained in [9]. Following such a construction, we introduce a Gaussian second-order real-valued stochastic process, $Y = \{Y(t), t \in \mathbb{R}\}$, centered, mean-square continuous, stationary and ergodic, physically realizable. A representation of stochastic process K can then be written as

$$K(t) = k_0 + (\underline{k} - k_0)(\underline{y} + Y(t))^2 \quad , \quad \forall\, t \in \mathbb{R}\,, \tag{2}$$

in which $\underline{y}$ is a parameter (that will be defined later) such that

$$E\{(\underline{y} + Y(t))^2\} = 1 \quad , \quad E\{(\underline{y} + Y(t))^4\} < +\infty\,. \tag{3}$$

The conditions defined by Eq. (3) effectively yields, for all t, $E\{K(t)\} = \underline{k}$ and $E\{K(t)^2\} < +\infty$. Let ω be the angular frequency in rad/s and f be the circular frequency in Hz such that $\omega = 2\pi f$. The Gaussian stochastic process Y is constructed as the linear filtering, $Y = h * N_\infty$, of the centered Gaussian white noise N_∞ (generalized stochastic process) whose power spectral density function is written, for all real ω, as

$$S_N(\omega) = \frac{1}{2\pi}\,, \tag{4}$$

and where $h = \mathcal{F}^{-1}\{H\}$ is the inverse Fourier transform of the complex-valued frequency response function $\omega \mapsto H(\omega)$ that we defined, for all real ω, by

$$H(\omega) = \frac{a}{-\omega^2 + 2i\omega\xi b + b^2}\,, \tag{5}$$

in which, a, b, and ξ are three positive parameters that will be defined later.

Consequently, the power spectral density function $S_Y(\omega)$ of Gaussian stationary stochastic process Y is written, for all real ω, as

$$S_Y(\omega) = \frac{1}{2\pi}\,\frac{a^2}{(b^2 - \omega^2)^2 + 4\xi^2 b^2 \omega^2} \quad , \quad a > 0 \quad , \quad b > 0 \quad , \quad \xi > 0\,. \tag{6}$$

From Eq. (6), it can be deduced that the mean-square derivative $\{\dot{Y}(t), t \in \mathbb{R}\}$ of stochastic process $\{Y(t), t \in \mathbb{R}\}$ is a second-order stochastic process because $\int_{\mathbb{R}} \omega^2\, S_Y(\omega)\, d\omega < +\infty$.

Let $\{\mathbb{Z}(t) = (Y(t), \dot{Y}(t)), t \geq 0\}$ be the stochastic process with values in $\mathbb{R}^2$ solution of the following Itô stochastic differential equation,

$$d\mathbb{Z} = [\alpha]\,\mathbb{Z}\,dt + \beta\,dW(t) \quad , \quad t > 0\,, \tag{7}$$

with the initial condition $\mathbb{Z}(0) = (0, 0)$, in which $\{W(t), t \geq 0\}$ is the real-valued normalized Wiener stochastic process indexed by $[0, +\infty[$, where $[\alpha]$ is the (2×2) real matrix and β is the real vector such that

$$[\alpha] = \begin{bmatrix} 0 & 1 \\ -b^2 & -2\xi b \end{bmatrix} \quad , \quad \beta = \begin{bmatrix} 0 \\ a \end{bmatrix}. \tag{8}$$

It can be proved (see for instance [10]) that Eq. (7) has a unique solution $\{\mathbb{Z}(t), t \geq 0\}$ such that, for $t_0 \to +\infty$, the stochastic process $\{\mathbb{Z}(t), t \geq t_0\}$ is asymptotically stationary and tends to the stationary Gaussian stochastic process $\{(Y(t), \dot{Y}(t)), t \in \mathbb{R}\}$ in which $Y = h * N_\infty$. The first condition defined by Eq. (3) yields,

$$\underline{y}^2 + \int_{-\infty}^{+\infty} S_Y(\omega) d\omega = 1 \quad \Longrightarrow \quad \underline{y}^2 = 1 - \frac{a^2}{4\xi b^3}\,. \tag{9}$$

Consequently, the parameters must satisfied the following conditions,

$$0 < a^2 < 4\xi b^3 \quad , \quad b > 0 \quad , \quad \xi > 0. \tag{10}$$

In order to control the bandwidth of stationary stochastic process Y, we introduce the parameter $\epsilon > 0$ [10] that is defined by

$$\epsilon = \sqrt{1 - \frac{m_2^2}{m_0 m_4}} \quad , \quad m_{2p} = \int_{\mathbb{R}} \omega^{2p}\, S_Y(\omega)\, d\omega \quad , \quad p = 0, 1, 2\,. \tag{11}$$

Parameter ϵ is estimated using the simulated signals and is discussed in the next section. It is important to say that the bandwidth is related to the quality of the synthesized sounds [11] and this is one of the main reasons to introduce it in this paper, discussing the relation between the presence of jitter and the quality of the voice.

4 SIMULATION

The objective of this section is to generate voice signals with jitter using the stochastic model proposed and to analyze the sensitivity of the stochastic model with respect to parameters a, b, and ξ.

As the main idea is to generate jitter, a way to measure it will also be discussed. There are different ways to analyze jitter effects [12]. At first, it is important to define the random variable associated with the duration of the glottal cycle, which is defined as

the duration between two successive times, the first one corresponding to the instant the vocal folds (glottis) opens and the second one the instant when it closes completely. The corresponding random variable will be denoted by T_{fund}. To calculate T_{fund} from $X(t)$, it was used an algorithm based on an implementation of the RAPT pitch tracker [13].

During the simulations, the values of parameters a, b, and ξ, as well as the mean of the fundamental frequency, will vary. All the other parameters will be fixed and their values are $p_s(t) = 800\,Pa$, $m = 0.24 \times 10^{-2}\,kg$, $c = 346.3\,m/s$, $k_0 = 40\,N/m$, $\underline{k} = 115\,N/m$, $a_1 = 1.87\,\ell\,d/2$ and $a_2 = \ell\,d/2$, with $\ell = 1.4 \times 10^{-2} m$ and d $= 0.3 \times 10^{-2}\,m$. The other parameters that are necessary to produce the sounds, including values related to the vocal tract, are given in (Cataldo and Soize, 2017). In particular, the parameter A_{g0} and the air density ρ are chosen such that $A_{g0} = 0.04 \times 10^{-2}\,m^2$ and $\rho = 0.12\,kg/m^3$.

The objective of this section is to perform a sensitivity analysis of the parameters in order to better understand how to proceed to solve the inverse problem to identify parameters of the model corresponding to experimental voice which will be discussed further in the paper.

Another important objective of this section is to show that with these three parameters a, b and ξ, there are different possibilities to generate jitter, but also to control the distribution of the fundamental frequency.

Although jitter is a variation of the glottal cycle and consequently this variation is related to the random variable $F_{\text{fund}} = 1/T_{\text{fund}}$, the shape of the curve corresponding to the probability density function of F_{fund} is not so easily controlled with the variation of jitter. It means that, to identify parameters of the model, it is important to minimize the distance between measures of jitter (from simulated and experimental signals) but also distance between probability density functions of F_{fund} (simulated and experimental). So, this section will give the feeling of how to vary the parameters in order to better minimize those distances.

Thirteen cases were simulated. For each case simulated, the corresponding voice signal will be synthesized and available to be heard following the link:

https://www.dropbox.com/sh/eo49b4usr1n4iz4/AADU8gI-JGWAeWqmxwE5u7nwa?dl=0 .

All the values of the parameters considered and also the value calculated for ε for all the simulations considered are summarized in Tab. 1.

Case	a	c_b	ξ	Relative jitter	ϵ
I	10	1	0.01	0.16%	0.43
II	200	1	0.01	0.32%	0.43
III	600	1	0.01	0.77%	0.43
IV	1200	1	0.01	3.48%	0.43
V	10	1	0.2	0.09%	0.9
VI	600	1	0.2	0.48%	0.9
VII	1800	1	0.2	1.43%	0.9
VIII	3000	1	0.2	2.51%	0.9
IX	10	1	0.5	0.09%	0.96
X	1000	1	0.5	0.80%	0.96
XI	3000	1	0.5	2.23%	0.96
XII	3000	1.5	0.5	0.90%	0.93
XIII	3000	2	0.5	0.64%	0.92

Table 1: Value of bandwidth parameter ε of stationary stochastic process Y for all the simulation cases.

As the idea is to discuss the sensitivity of the parameters with the specific objective of solving the inverse stochastic problem, some of these cases will be selected and the graphs showed and discussed and graphs of the probability density function will be constructed for some cases.

5 STATISTICAL INVERSE PROBLEM

In order to validate the model proposed, parameters a, b, and ξ are identified using experimental voice signals. This identification is carried out by introducing a cost function that is constructed writing that the probability density function associated with the simulated voice is close to the probability density function of the experimental voice and also, the jitter obtained for the simulated voice is close to the jitter of the experimental voice. The four measures of jitter are used. The cost function, denoted by $J_{\text{cost}}(a,b,\xi)$, is then defined by

$$
\begin{aligned}
J_{\text{cost}}(a,b,\xi) = \frac{1}{2}\mathit{Dist}_{\text{dens}}(a,b,\xi) + \frac{1}{4}\mathit{JitterRel}_{\text{dist}}(a,b,\xi) \\
+ \frac{1}{4}\mathit{JitterAbs}_{\text{dist}}(a,b,\xi) + \frac{1}{4}\mathit{JitterRAP}_{\text{dist}}(a,b,\xi) \\
+ \frac{1}{4}\mathit{JitterPPQ5}_{\text{dist}}(a,b,\xi)\,,
\end{aligned}
\tag{12}
$$

in which, each quantity appearing in the right-hand side member is defined hereinafter. (i) Let $f \mapsto f_S(f;a,b,\xi)$ be the probability density function on $[0\,,+\infty[$ of random variable

$F_{\text{fund}}(a,b,\xi)$ associated with the simulated voice and $f \mapsto f_R(f)$ be the probability density function on $[0\,,+\infty[$ of the random variable associated with the experimental voice. The distance between these two probability density functions is written as

$$\mathit{Dist}_{\text{dens}}(a,b,\xi) = \frac{1}{2}\int_0^{+\infty} \mid f_S(f;a,b) - f_R(f) \mid \, df\,. \tag{13}$$

The probability density functions are estimated by using the Gaussian kernel estimation method from the nonparametric statistics[14]. For each value of (a,b,ξ), probability density function $f_S(.;a,b,\xi)$ of $F_{\text{fund}}(a,b,\xi)$ is estimated using the realization of the stochastic process corresponding to the glottal flow computed with the stochastic model and probability density function f_R of F_{fund} is estimated using the realization of the experimental glottal signal obtained through a filtering inverse algorithm (PSIAIF) [15] of the experimental voice.

(ii) For each given value of vector (a,b,ξ), N realizations $\{\theta_k, k = 1,\ldots,N\}$ of the voice signal are computed, which allows for computing the jitter quantities. Let $\mathit{Jitter}_{\text{sim}}$ represent one of these four jitter quantities: $\mathit{JitterRel}_{\text{sim}}$, $\mathit{JitterAbs}_{\text{sim}}$, $\mathit{JitterRAP}_{\text{sim}}$, or $\mathit{JitterPPQ5}_{\text{sim}}$. Let $\mathit{Jitter}_{\text{exp}}$ be the jitter calculated with the experimental signal. Then, a distance between $\mathit{Jitter}_{\text{sim}}$ and $\mathit{Jitter}_{\text{exp}}$ can be defined by

$$\mathit{Jitter}_{\text{dist}} = \frac{\left|\mathit{Jitter}_{\text{sim}} - \mathit{Jitter}_{\text{exp}}\right|}{\mathit{Jitter}_{\text{exp}}}\,. \tag{14}$$

The optimal values a^{opt}, b^{opt} , and ξ^{opt} are then computed by solving the following optimization problem,

$$(a^{\text{opt}}, b^{\text{opt}}, \xi^{\text{opt}}) = \arg \min_{(a,b,\xi)\in\mathcal{C}} J_{\text{cost}}(a,b,\xi)\,, \tag{15}$$

in which the admissible set $\mathcal{C}$ is defined, using Eq. (10), by

$$\mathcal{C} = \{(a,b,\xi) \in \mathbb{R}^3 \quad \text{such that} \quad 0 < a^2 < 4\xi b^3 \quad , \quad b > 0 \quad , \quad \xi > 0\}\,. \tag{16}$$

The values of the fixed parameters considered for the corresponding deterministic model are the same as considered for the simulations.

The first case to be taken into account is a voice signal from a woman producing an /e/ vowel. The parameters corresponding to the mean value $\underline{k}$ of K is considered in a way that the mean of the random variable associated with the fundamental frequency simulated is very near of the one for the real voices. Then, the optimal values a^{opt}, b^{opt} and ξ^{opt} of parameters a, b and ξ are identified by solving the optimization problem defined by Eq. (15).

5.1 Algorithm used

- Step 1: From the experimental voice signal obtained with the vowel produced all the values corresponding to the random variable $F_{\text{fund}} = 1/T_{\text{fund}}$ are obtained using the

algorithm (Talkin, 1995) and the probability density function $f \mapsto F_R(f)$ associated is estimated. The mean value of random variable F_{fund} is calculated and is used in the other steps. From this signal, the four measures of jitter are obtained: $\mathit{JitterRel}_{\text{exp}}$, $\mathit{JitterAbs}_{\text{exp}}$, $\mathit{JitterRAP}_{\text{exp}}$, and $\mathit{JitterPPQ5}_{\text{exp}}$.

- Step 2: Using the model proposed, one signal is simulated in a way that the mean of random variable F_{fund} of this signal was near from the mean value calculated in step 1. It is not difficult to generate this signal because there are parameters in the model directly related to the fundamental frequency as, for example, f_p. However, some essays are necessary in order to obtain a mean value near the one wished. At the same time, values for a, b, and ξ have been calculated so that the estimated probability density function of random variable F_{fund} for the simulated voice signal is near from the probability density function estimated in step 1. This step 2 takes some time because it is a step of essays. Values are obtained and they will serve as start for the grid variation of the values of the fundamental frequency and also of the parameters a, b, and ξ, consequently four loops are constructed.

- Step 3: For each value of the fundamental frequency and of the triplet (a, b, ξ), the Monte Carlo Method is used for the estimation of the probability density functions and the computation of cost function $J_{cost}(a, b, \xi)$.

- Step 4: The minimum value of the cost function estimated in Step 3 is the objective that has to be reached.

5.2 IDENTIFYING PARAMETERS

5.2.1 The first experimental voice signal considered is a female production of a vowel /e/.

After solving the inverse stochastic problem, the optimal values obtained were: $a^{opt} = 200$, $b^{opt} = (1/2)\pi f_p$, $f_p = 200\,Hz$ and $\xi^{opt} = 0.9$. Table 2 shows the values of jitter calculated for the experimental voice and for the simulated voice, after solving the inverse problem. The value obtained for the bandwidth parameter is $\epsilon = 0.98$.

Jitter	Experimental	Simulated
JitterRel	0.48%	0.52%
JitterAbs	$2.37e-05\,s$	$2.54e-05\,s$
JitterRAP	0.26%	0.30%
JitterPPQ5	0.29%	0.32%

Table 2: Jitter values for a female production of a vowel /a/, without pathological characteristics

.

As we have already discussed, not only the measures of jitter have to be taken into account but also the distance between the probability density functions $f_S(.\,; a^{\text{opt}}, b^{\text{opt}}, \xi^{\text{opt}})$ and f_R (simulated and experimental) shown in Fig. 2.

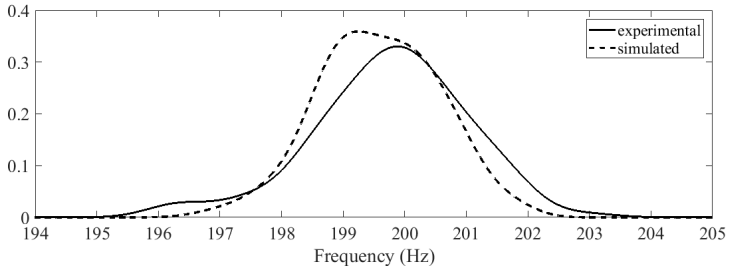


Figure 2: pdf of the random fundamental frequency corresponding to a real voice (solid line) and corresponding to the simulated for the optimal values of the parameters (dotted line) in the case without pathological characteristics.

It is important to say that if the distance between the pdfs was not taken into consideration inside the cost function, the values obtained to the jitter measures would be: *JitterRel* $= 0.50\%$, *JitterAbs* $= 2.4404e-05\,s$, *JitterRAP* $= 0.30\%$ and *JitterPPQ5*$5 = 0.31\%$ and in this case the distance between the pdfs would be a little bit greater.

As a way to verify what happens when a sound is synthesized considering these optimal values of the parameters, a voice signal has been simulated with the optimal values of the parameters. The experimental signal ($exper_1.wav$) and the corresponding optimal simulated one ($simulated_1.wav$), in the same link presented before for all simulations.

5.2.2 The second case considered is a voice signal from a woman with paralysis of the vocal folds.

After solving the inverse stochastic problem, the optimal values obtained were: $a^{opt} = 1050$, $b^{opt} = (1.5\pi f_p$, $f_p = 226\,Hz$ and $\xi^{opt} = 0.4$. Table 3 shows the values of jitter calculated for the real voice and for the simulated voice, after solving the inverse problem. In this case, the value obtained for the bandwidth parameter is $\epsilon = 0.96$.

Jitter	Experimental	Simulated
JitterRel	3.24%	3.40%
JitterAbs	$1.44e-04\,s$	$1.42e-04\,s$
JitterRAP	2.03%	2.00%
JitterPPQ5	2.05%	2.45%

Table 3: Jitter values for a female production of a vowel /a/, with a pathology

.

Figure 3 shows probability density functions $f_S(.\,; a^{\text{opt}}, b^{\text{opt}}, \xi^{\text{opt}})$ and f_R (simulated and experimental). It is important to note the difference between the values obtained for

jitter, but mainly showing that it is possible to solve the inverse stochastic problem even considering a pathological case.

In this case, the pathological one, the results are better for the distance between the values of jitter for the experimental and simulated signals than those obtained for the normal voice.

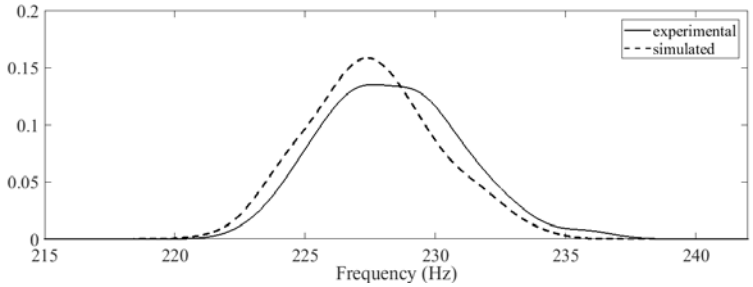


Figure 3: pdf of the random fundamental frequency corresponding to a real voice (solid line) and corresponding to the simulated for the optimal values of the parameters (dotted line) in the case without pathological characteristics.

In the normal case or in the pathological case, the value of ϵ is high. It shows that it is not directly related to the pathology, but to the quality of the synthesized sound.

6 CONCLUSIONS

A stochastic model has been proposed using three control parameters for generating jitter considering a mechanical model for producing voiced sounds. Some pathological cases have been generated and the model has been validated considering an inverse stochastic problem to identify the parameters. With three control parameters more possibilities of different sounds are obtained, including different levels of jitter and, mainly, it is possible to control the quality of the synthesized voice. The inverse stochastic problem solved to identify parameters of the model uses different measures of jitter and also the distance between probability density functions, showing that with more measured features the voices synthesized are more similar of the corresponding experimental voices. The sensitivity analysis performed before was very important to show how to change the jitter and also the distribution of frequencies in order to obtain synthesized voices near experimental voices. A pathological case caused by an unilateral paralysis of the vocal folds has been considered and, even in this case, the parameters of the model has been identified. The bandwidth parameter has been used as a measure of quality of the synthesized voice and it has also been considered when the inverse problem has been solved.

7 ACKNOWLEDGEMENTS

This work was supported by CNPq.

References

[1] Flanagan, J. and Landgraf, L. Self-oscillating source for vocal-tract synthesizers. IEEE Transactions on Audio and Electroacoustics (1968) AU-16, 57–64.

[2] Ishizaka, K. and Flanagan, J. Synthesis of voiced sounds from a two-mass model of the vocal folds. Bell Syst. Tech. J. (1972) 51, 1233–1268.

[3] Avanzini, F., 2008. Simulation of vocal fold oscillation with a pseudo-one-mass physical model. Speech Communication, (2008) 50 (2), 95–108.

[4] Zhang, Y. and Jiang, J. J. Nonlinear dynamic mechanism of vocal tremor from voice analysis and model simulations. Journal of Sound and Vibration (2008) 316 (1–5), 248–262.

[5] Pinheiro, A. P. and Kerschen, G. Vibrational dynamics of vocal folds using nonlinear normal modes. Medical Engineering & Physics, (2013) 35(8), 1079–1088.

[6] Gunter, H. E. Modeling mechanical stresses as a factor in the etiology of benign vocal fold lesions. Journal of Biomechanics (2004) 37 (7), 1119–1124.

[7] Luzan, C. F., Mihaescu, J. C. M., Khosla, S.M. and Gutmark, E. Computational study of false vocal folds effects on unsteady airflows through static models of the human larynx. Journal of Biomechanics (2015) 48 (7), 1248–1257.

[8] Cataldo, E., Soize, C. Voice signals produced with jitter through a stochastic one-mass mechanical model. Journal of Voice, (2017) 31 (1), 111e9–111e18.

[9] Soize, C. Uncertainty Quantification - An accelerated Course with Advanced Applications in Computational Engineering. Interdisciplinary Applied Mathematics Series, Springer, New York, (2017).

[10] Krée P. and Soize C. Mathematics of Random Phenomena. Reidel, Dordrecht, (1986).

[11] Rabiner, L. and Schafer, R. Theory and Application of Digital Signal Processing. Pearson Education, (2011).

[12] Mongia, P. K. and Sharma, R.K. Estimation and statistical analysis of human voice parameters to investigate the influence of psychological stress and to determine the vocal tract transfer function of an individual. Journal of Computer Networks and Communications (2014), 1–17.

[13] A robust algorithm for pitch tracking (rapt). Speech coding and synthesis (1995), 495–518.

[14] Bowman, A. W. and Azzalini, A. Applied smoothing techniques for data analysis: The kernel approach with S-Plus illustrations. Oxford University Press, (1997).

[15] Glottal wave analysis with pitch synchronous iterative adaptive inverse filtering. Speech Communication, (1992) V. 11 (2–3) , 109–118.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Novel OpenSees Element for FPS Bearings with Breakaway Friction

Sara Cattaneo*, Emanuele Gandelli**, Virginio Quaglini***

*Politecnico di Milano, Department of Architecture, Built Environment and Construction Engineering, **Politecnico di Milano, Department of Architecture, Built Environment and Construction Engineering, ***Politecnico di Milano, Department of Architecture, Built Environment and Construction Engineering

ABSTRACT

The increasing use of sliding bearings with curved surfaces, like the Friction Pendulum System (FPS), as seismic isolator, benefits from the improvement of numerical models that can capture their experimental performance and enhance the predictive capability of nonlinear response history analyses. Among the limits of current models, it is noted that effective implementation of the static coefficient of friction of sliding isolators in object-oriented software for structural analysis has not yet been achieved, and the use of the dynamic friction only for design is a common practice. Furthermore, specific guidance in this respect is missing. The formulation proposed in this study aims at filling this gap, by incorporating in an established numerical framework the change in the coefficient of friction occurring in the transition from the sticking, or pre-sliding phase to the dynamic sliding motion. The proposed model has been coded in the object-oriented finite element software OpenSees by modifying the standard "SingleFPSimple3d" element. The hysteretic force – displacement relationship of the FPS isolator in the horizontal direction is mathematically modelled using the theory of plasticity, while two yield conditions are introduced to switch from the static to the dynamic friction coefficient. Other features of the model are the inclusion of the dependency of the dynamic coefficient of friction on the instantaneous values of axial load and slide velocity at the interface, and the accumulated heat generated from energy dissipation. The primary assumptions in the development of the friction model and the verification of the newly developed element are validated by agreement with available data. A case study relevant to a base-isolated concrete, moment resisting frame helps to demonstrate the improved prediction capability of the new bearing element over its standard counterpart when applied to real situations, such as estimating a +50% increase in isolator displacement, superstructure drift and base shear demand under high intensity earthquakes, and possible non-activation of the sliding isolators under weak or medium intensity earthquakes.

13th World Congress on Computational Mechanics (WCCM XIII) and 2nd Pan American Congress on Computational Mechanics (PANACM II), July 22-27, 2018, New York City, NY, USA

CONTROL OF AN ACTIVE CABLE DOME USING MULTI-OBJECTIVE GENETIC ALGORITHMS

STANISLAV KMET*, PETER CAUNER*

*Technical University of Kosice, Faculty of Civil Engineering
Institute of Structural Engineering, Vysokoskolska 4
Kosice, Slovakia
stanislav.kmet@tuke.sk, peter.cauner@tuke.sk

Key words: Cable Dome, Tensegrity, Genetic Algorithm.

Abstract. Control processes of an active Levy cable dome which has the ability to adapt to current loading conditions are presented in the paper. The prototype of Levy cable dome which was developed at the Technical University of Kosice is equipped with sensors and an actuator. Theoretical models in presented numerical studies contain various loading conditions and all vertical compressed members of the studied dome are designed as actuators. The control task is stated as an optimization task where the objective is to reduce excessive displacements and stresses (forces) to acceptable levels with a minimum control effort. Active strut members of the dome can be elongated or contracted modifying internal stress distributions and nodal displacements. Relevant movements of the active struts keep the required reliability (related to serviceability and safety) of the dome subjected to changed loading effects. Multi-objective search is used to select control commands. An appropriate tool for the optimization of the control process is an application of genetic algorithm. Multi-Objective Genetic Algorithm (MOGA) used in Goal Driven Optimization (GDO) as a hybrid variant of the popular Non-dominated Sorted Genetic Algorithm-II (NSGA-II) based on controlled elitism concepts are used in these studies. Initial population, necessary to run the MOGA algorithm, consists of elongations or contractions of the active structural members.

1 INTRODUCTION

Cable domes are lightweight spatial pre-stressed structures that are increasingly investigated as structural solutions for large-span roof systems. The cable dome structures first proposed by Geiger have been developed in recent years due to their innovative forms, lightweight and deployability. They belong to a class of pre-stressed pin-jointed systems that cannot be stable without introducing prestresses to some members [1]. Cable domes are sensitive to asymmetric loads and changes in pre-stress. Active cable systems equipped with sensors and actuators provide shape-control potential that adapts the structure to changing loads and environmental conditions. Structural control is carried out by modifying the prestress state of the cable dome in order to satisfy prescribed reliability criteria due to ultimate and mainly serviceability limit states. Skelton and Sultan (1997) introduced the concept of a controllable tensegrity as a new class of smart structures capable of large displacements [2, 3, 6].

Cable domes have been developed in recent years. The names of Geiger and Levy are associated with these structures (Fig. 1). It is clear that they have been inspired by the tensegrity principle. Two kinds of compressed component can be identified: vertical struts and compressed ring. This last component is on the boundary of the system and not inside it, which excludes these systems from the tensegrity classification (by "extended" definition) [5].

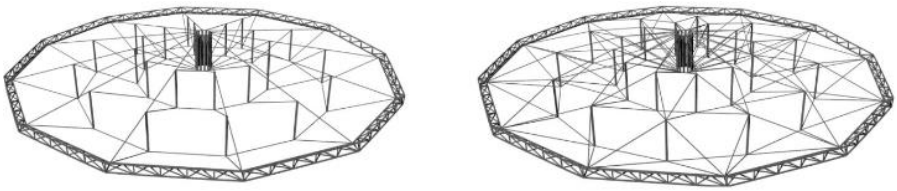


Figure 1. Geiger and Levy cable dome [7]

2 MODEL OF ACTIVE CABLE DOME IN LEVY FORM

The cable domes created of tensioned cables and compressed struts belong to hybrid tensegrity systems. A model of an active cable dome was designed and built in Laboratory of Excellent Research at the Technical University of Kosice. Prototype of cable dome is shown in Fig. 2.

Figure 2. Prototype of Levy cable dome, Laboratory of Excellent Research TU of Kosice

The elementary shape of structure is a cable dome in Levy form with a circular base with diameter 3,0 m. Cable dome consists of 42 tension members and 7 compression members. A central compressed strut is designed as an actuator which is used to modify the geometry and pre-stress of the system. The analyzed cable dome consists of ridge cables, diagonal cables, hoop cables, vertical struts and actuator. Basic geometry of Levy cable dome is shown in Fig. 3.

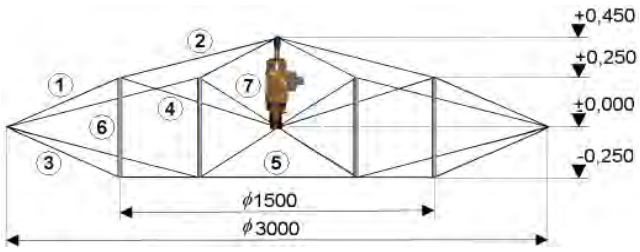


Figure 3. Section view of cable dome in Levy form with geometry and described basic structural members: (1) and (2) ridge cables, (3) and (4) diagonal cables, (5) hoop cables, (6) vertical struts and (7) actuator

Compressed struts of the cable dome are made from steel S235 with Young's modulus of elasticity 210.10^6 Pa and are created from circular hollow sections of 30/5 mm. The length of the struts is 500 mm. For tensile cables 1x19 wires strands with a nominal diameter of 4 mm were used. Cables were made from stainless austenitic steel 1.4401. The cross-sectional area of the cables is 9,55 mm^2 and Young's modulus of elasticity is 130.10^6 Pa. A central compressed strut is actuator which is used to modify the geometry and pre-stress of the system. The theoretical length of the actuator is 450 mm with self-weight of the actuator 16 kg and increased on the bottom point by 55 kg from connecting cylinder.

3 MULTI-OBJECTIVE OPTIMIZATION METHOD

Multi-Objective Genetic Algorithm (MOGA) used in Goal Driven Optimization (GDO) as a hybrid variant of the popular Non-dominated Sorted Genetic Algorithm-II (NSGA-II) based on controlled elitism concepts are used in these studies. Concept of multi-objective optimization is based on optimization process of at least two functions to be minimized respectively maximized. In general, multi-objective criteria are defined by equations:

$$\begin{aligned} & f_m(x) && \mathrm{m} = 1, 2, ..., \mathrm{M} \\ & g_j(x) \geq 0 && \mathrm{j} = 1, 2, ..., \mathrm{J} \\ & h_k(x) = 0 && \mathrm{k} = 1, 2, ..., \mathrm{K} \\ & x_i^{\mathrm{L}} \leq \mathrm{x}_i \leq \mathrm{x}_i^{\mathrm{U}} && \mathrm{i} = 1, 2, ..., \mathrm{n} \end{aligned} \tag{1}$$

where x is vector $x = (x_i, ..., x_n)$, g_j and h_k are boundary functions, last condition represents restriction constraint imposed on the arguments of objective function. Solution which does not satisfy condition (1) is infeasible solution. Set of solutions which satisfy condition (1) are feasible solutions. Set of possible solutions is incoherent and is created by isolated sets of feasible solutions (Pareto front) [8].

3.1 Pareto front

Pareto front is defined like set of points which represents combinations of functions $f_1 ... f_n$, that it is not possible to reduce any value of the objective function f_i, in order to increase the value of some other function f_j. A solution is said to be optimal (Pareto optimal) if it is not dominated by any other solution in the solution space. There are non-dominant solutions on the Pareto front. Dominance of solutions is shown at the Fig. 4 [8, 9].

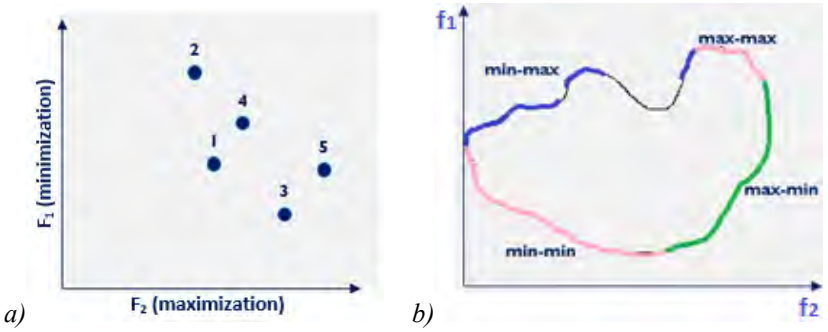


Figure 4. a) Pareto front - example of dominance b) Pareto front

If x_1 and x_2 solving problem, x_1 is dominant to x_2, if x_1 is not worse in all objective functions $f_i(x_1)$ than x_2 and better at least in one case $f_j(x_1)$. Solutions 3 and 5 (Fig. 4) lies on Pareto front (non-dominant solutions) [8, 9].

3.2 Fitness function

The classical approach to solve a multi-objective optimization problem is to assign a weight w_i to each normalized objective function $z_i'(x)$ so that the problem is converted to a single objective problem with a scalar objective function as follows:

$$\min z = w_1 z_1'(x) + w_2 z_2'(x) + ... + w_k z_k'(x) \tag{2}$$

where $z_i'(x)$ is the normalized objective function $z_1(x)$ and $\sum w_i = 1$. This approach is called the priori approach since the user is expected to provide the weights. Solving a problem with the objective function (2) for a given weight vector $w = \{w_1, w_2, ..., w_k\}$ yields a single solution, and if multiple solutions are desired, the problem must be solved multiple times with different weight combinations. Let ∇ be the space of design, each of which has n runs and s factors (design variables), with each factor having q levels (samples per each design variable). Let $h(D)$ be the objective function of $D \in \nabla$. Optimised DOE (Design of experiment) for space-filling design may be generally defined by minimize an objective function $h(D)$, which maximizes the distance between design points in order to find a design $D^* \in \nabla$ and is expressed by a formulation [11]

$$h(D^*) = \min h(D), D \in \nabla. \tag{3}$$

3.3 Multi-objective optimization formulation

The ultimate goal of a multi-objective optimization algorithm is to identify solutions in the Pareto optimal set. However, identifying the entire Pareto optimal set, for many multi-objective problems, is practically impossible due to its size. In addition, for many problems, especially for combinatorial optimization problems, proof of solution optimality is computationally infeasible. Therefore, a practical approach to multi-objective optimization is to investigate a set of solutions (the best-known Pareto set) that represent the Pareto optimal set as well as possible [9].

The concept of Genetic Algorithm (GA) was developed by Holland and his colleagues in the 1960s and 1970s inspired by Darwin's theory of evolution which deduces that after a natural selection and reproduction the best fittest individuals survive over the next generations. GAs implement such notion in order to solve an optimization of various single or multi-objective problems in many fields of engineering [9, 10].

In GA terminology, a solution vector $x \in X$ is called a *chromosome*. Chromosomes are made of discrete units called *genes*. Each gene controls one or more features of the chromosome. GA operate with a collection of chromosomes, called a *population*. The population is normally randomly initialized. As the search evolves, the population includes fitter and fitter solutions, and eventually it converges, meaning that it is dominated by a single solution. The procedure of a generic GA is given as follows [4, 9]:

- *First population MOGA*: Randomly generate N solutions to form the first population, P_1. Evaluate the fitness of solutions in P_1.

- *Crossover*: Generate an offspring population Q_t as follows:
  - Choose two solutions x and y from P_t based on the fitness values.
  - Using a crossover operator, generate offspring and add them to Q_t.
- *Mutation*: Mutate each solution $x \in Q_t$ with a predefined mutation rate.
- *Fitness assignment*: Evaluate and assign a fitness value to each solution $x \in Q_t$ based on its objective function value and infeasibility.
- *Selection*: Select N solutions from Q_t based on their fitness and copy them to P_{t+1}.
- If the *stopping criterion* is satisfied, terminate the search and return to the current population, else, set $t = t+1$ go to Step 2 (Crossover). An operation is repeated until the final Pareto front is obtained [4, 9].

The MOGA is based on controlled elitism concepts. It supports all types of input parameters. The Pareto ranking scheme is done by a fast, non-dominated sorting method that is an order of magnitude faster than traditional Pareto ranking methods. The constraint handling uses the same non-dominance principle as the objectives, thus penalty functions and Lagrange multipliers are not needed. This also ensures that the feasible solutions are always ranked higher than the unfeasible solutions [4, 8].

Control process was carried out in the add-on Workbench module of Ansys Mechanical APDL software. The Workbench is appropriate for finding Pareto optimal (non-dominate) solutions. However, elongations of actuators generating gene of chromosome. Algorithm is shown on the Fig. 5:

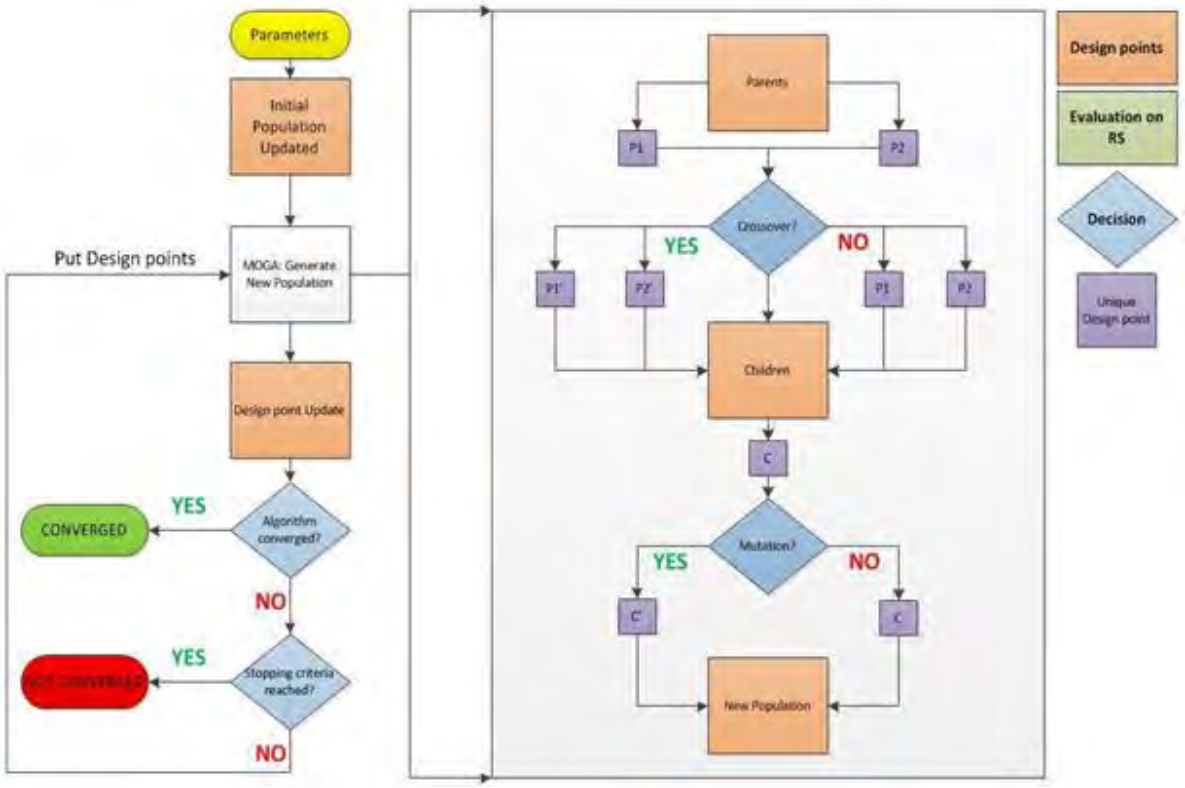


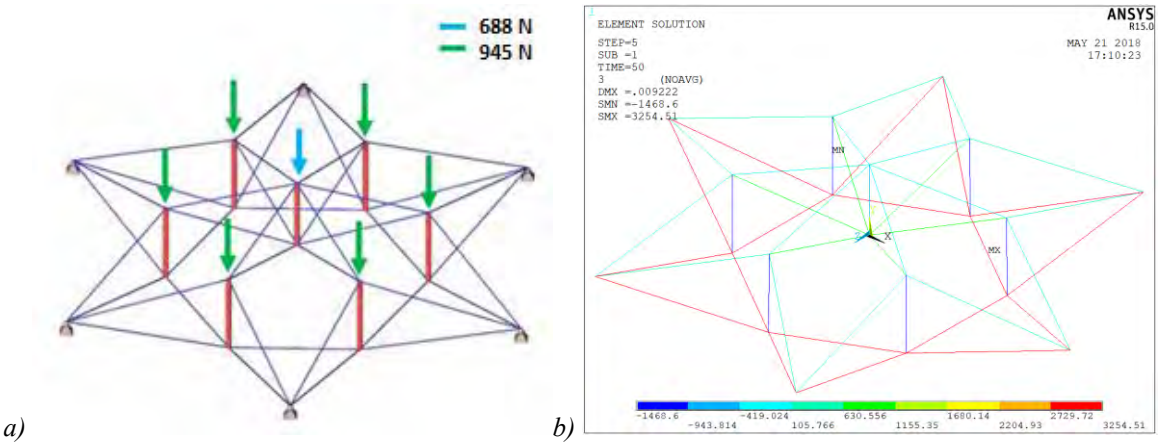
Figure 5. MOGA algorithm [4]

4 ANALYSIS OF CABLE DOME

Numerical analysis was carried out by Ansys Workbench software. All vertical compressed struts were created as actuators in the analysis. Paper consist of two analyses with symmetric and asymmetric load.

4.1 Symmetric load

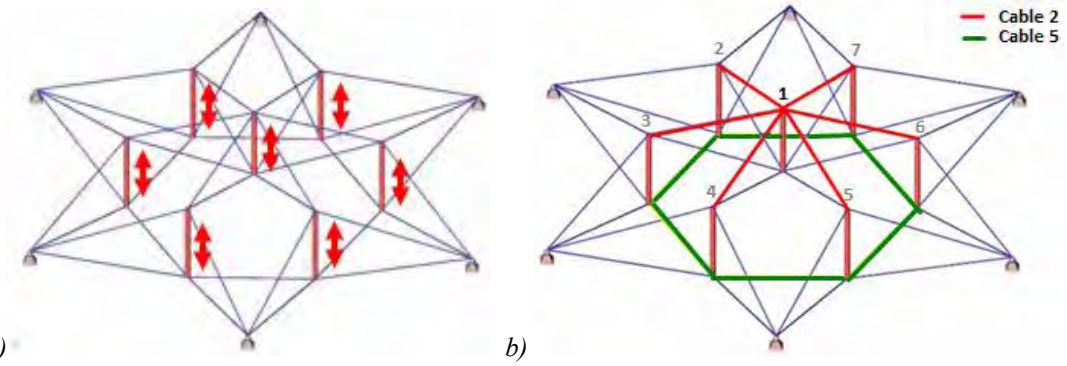
Cable dome was loaded by maximum symmetric load. Nominal value of maximum symmetric load is 1.5 kN.m^{-2}. It leads to reach the minimal forces in cables, however, all cables were still tensioned. Axial forces under maximum symmetric load are shown in Fig. 6. Minimal force in set of ridge cables (Cable 2) is 8.26 N. If load exceeds maximum value of symmetric load, cables are not tensioned yet. It is necessary to elongate actuators to redistribute forces in the cable dome and ensure reliability criteria.



a) *b)*

Figure 6. a) Maximum symmetric load (*1.5* kN.m^{-2}) b) Axial forces under maximum symmetric load

Next optimization consists of finding suitable configurations of elongations of actuators which leads to satisfy prescribed reliability criteria. Obviously, ultimate and serviceability limit states are reached. Location of actuators is shown in Fig. 7.



a) *b)*

Figure 7. a) Actuators b) Investigated set of cables

Optimization by Multi-Objective Genetic Algorithm leads to minimize functions (4) and (5). Optimization process minimizes functions with strict constraint values of maximum forces in cable

set (Cable 5) between 4200 N and 5000 N and minimum forces in the cable set (Cable 2) greater than or equals to 400 N. Investigated sets of cables are shown in the Fig. 7. Input parameters to optimization process are elongations of actuators, which creates gene of chromosome. New population of MOGA is given by genes of these chromosomes. Step of elongations of actuators (AM - active member) is 0.001 m. Lower and upper bound of elongation is shown in Table 1.

$$F_{\min}^{Cable\,2} \geq 400N, (\min) \tag{4}$$

$$4200N \leq F_{\max}^{Cable5} \leq 5000N, (\min) \tag{5}$$

Table 1. Elongations of actuators

[m]	AM-1	AM-2	AM-3	AM-4	AM-5	AM-6	AM-7
Lower Bound	0.001	0.001	0.001	0.001	0.001	0.001	0.001
Upper Bound	0.015	0.01	0.01	0.01	0.01	0.01	0.01

The MOGA configuration generates 200 samples initially, 50 samples per iteration and find 5 candidates in a maximum of 20 iterations. Optimization process converged after 201 evaluations. Maximum Allowable Pareto Percentage is 70 and Convergence Stability Percentage is equal 2. One-point Type of Discrete Crossover was used in optimization. Process of minimization of functions (4) and (5) is shown in Fig. 8.

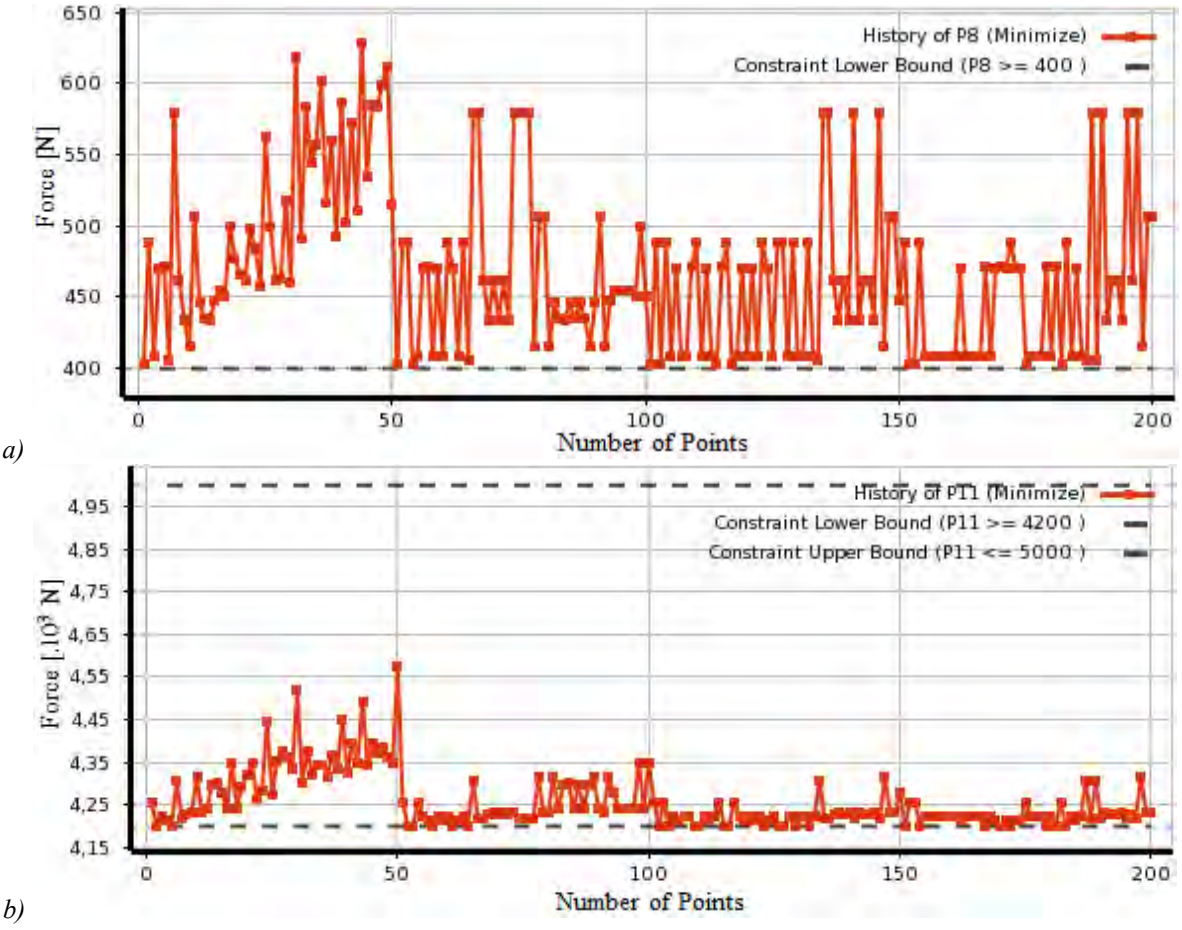


Figure 8. a) Minimization of function $F_{\min}^{Cable\,2}$ b) Minimization of function $F_{\max}^{Cable5}$

Tradeoff chart, as applied to the resulting sample set, shows the Pareto dominant solutions. However, in the MOGA approach, the Pareto fronts are better articulated and most of the feasible solutions lie on the first front, as opposed to the usual results of the Screening approach where the solutions are distributed across all the Pareto fronts. Feasible solutions from Pareto fronts are shown in Fig. 9. Top 5 candidate points from Pareto fronts are in Table 2.

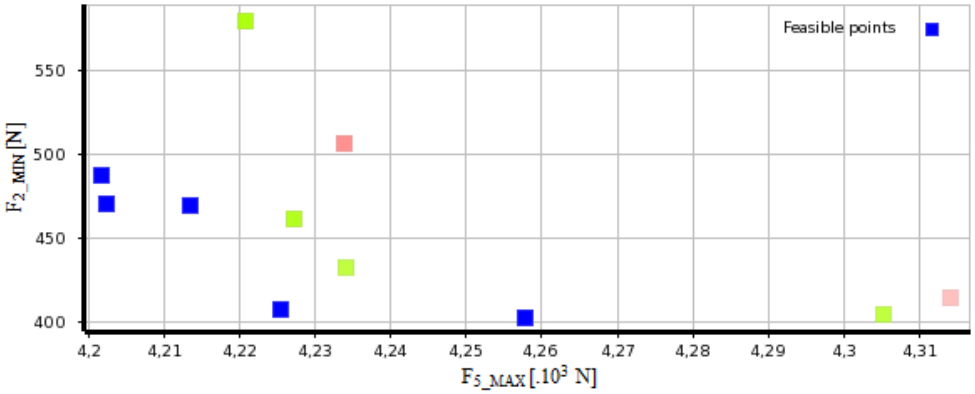
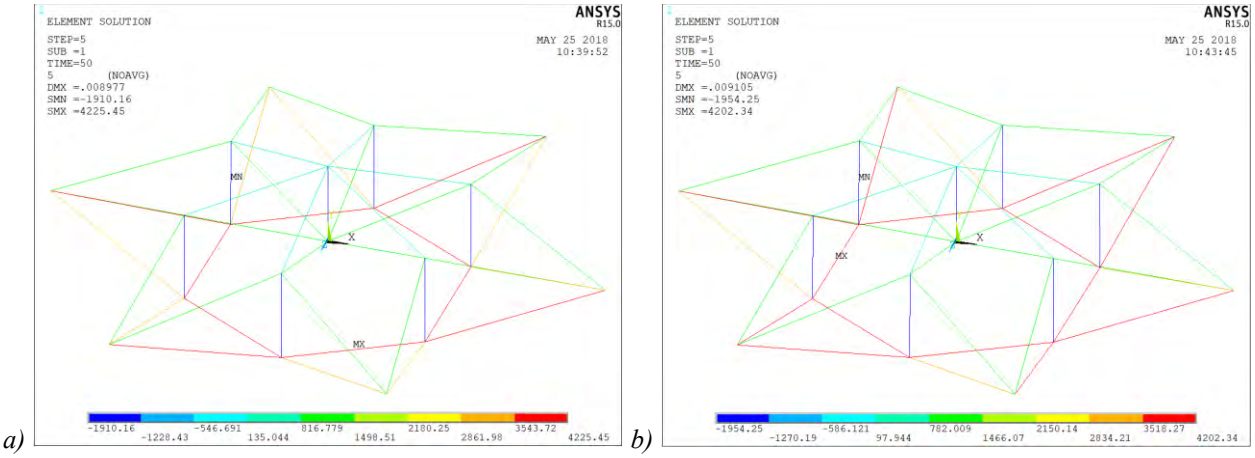


Figure 9. Feasible solutions from Pareto front

Table 2. Top 5 Candidate Points from Pareto Front

[m]	CP-1	CP-2	CP-3	CP-4	CP-5
AM1	0.004	0.006	0.002	0.002	0.003
AM2	0.002	0.004	0.006	0.006	0.006
AM3	0.005	0.007	0.001	0.001	0.007
AM4	0.002	0.003	0.009	0.009	0.001
AM5	0.008	0.002	0.004	0.004	0.007
AM6	0.007	0.005	0.008	0.008	0.004
AM7	0.002	0.005	0.007	0.007	0.009
F_{2_MIN}[N]	408.56	471.32	433.66	433.66	488.08
F_{5_MAX}[N]	4225.5	4202.3	4234.2	4234.2	4201.7

Final axial forces using elongations of actuators from Candidate Points (CP1) and (CP2) after optimization process of Levy cable dome are shown in Fig. 10.



a) *b)*

Figure 10. a) Axial forces - CP1 [N] b) Axial forces – CP2 [N]

4.2 Asymmetric load

Cable dome was loaded by maximum asymmetric load as you can see in Fig.11. Nominal value of maximum asymmetric load is 2.6 kN.m^{-2} and minimal force in set of ridge cables (Cable 2) is 1.32 N.

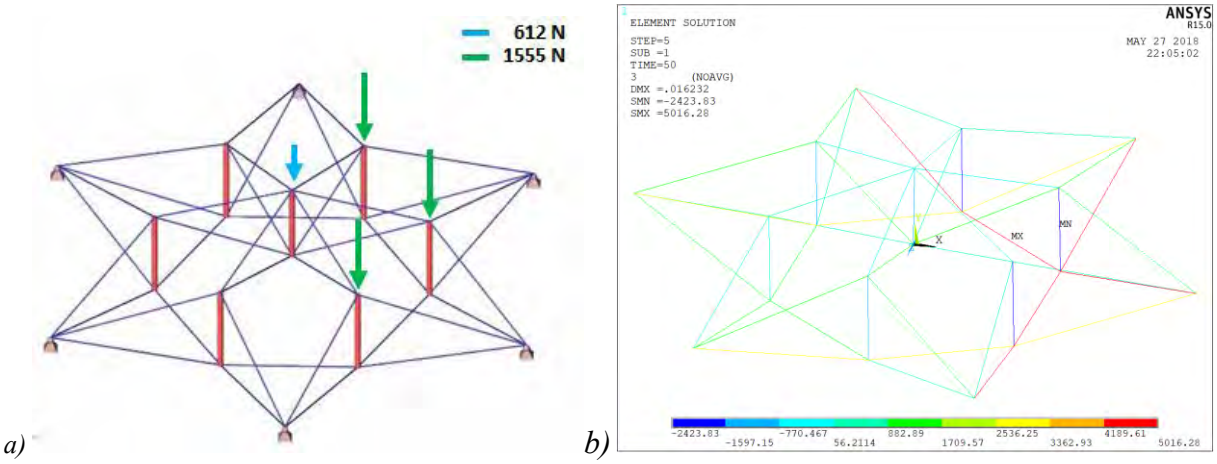


Figure 11. a) Maximum asymmetric load (*2.6* kN.m^{-2}) b) Axial forces under maximum symmetric load

Optimization process leads to minimize functions (6), (7) and (8). Elongations of actuators are in Table 3. MOGA generated 200 samples initially, 50 samples per iteration and found 5 candidates in a maximum of 20 iterations. Optimization converged after 201 evaluations. Top 5 candidate points from Pareto front, as a result of best configuration of elongations of actuators in optimization process, are shown in Table 4. Top 2 CPs are shown in Fig. 12.

$$F_{\min}^{Cable\,2} \geq 400N, (\min) \tag{6}$$

$$F_{\max}^{Cable2} \leq 1000N, (\min) \tag{7}$$

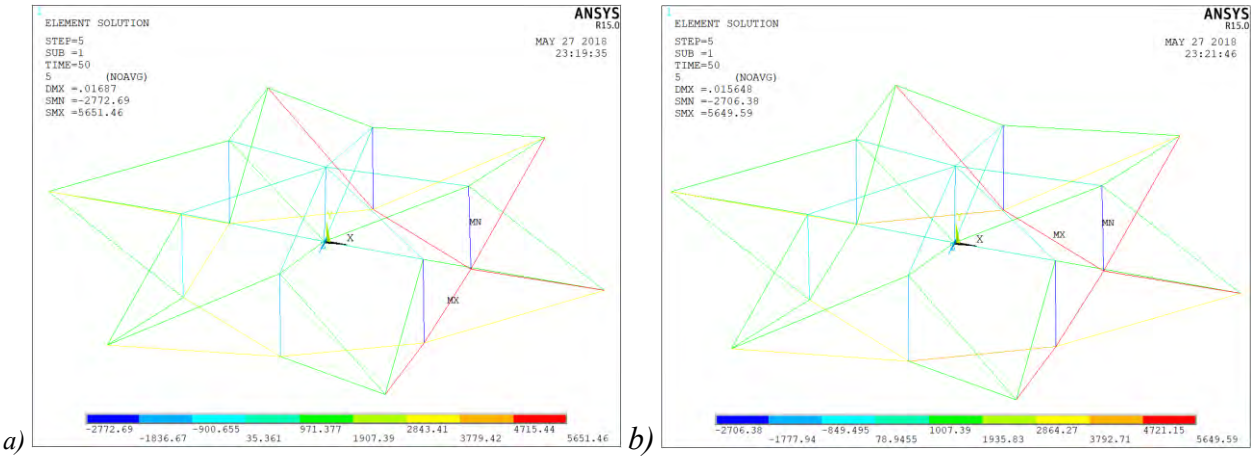
$$5500N \leq F_{\max}^{Cable5} \leq 6500N, (\min) \tag{8}$$

Table 3. Elongations of actuators

[m]	AM-1	AM-2	AM-3	AM-4	AM-5	AM-6	AM-7
Lower Bound	0.001	0.001	0.001	0.001	0.001	0.001	0.001
Upper Bound	0.01	0.01	0.01	0.01	0.01	0.01	0.01

Table 4. Top 5 Candidate Points from Pareto Front

[m]	CP-1	CP-2	CP-3	CP-4	CP-5
AM1	0.001	0.001	0.001	0.001	0.002
AM2	0.002	0.004	0.007	0.007	0.007
AM3	0.005	0.003	0.008	0.008	0.005
AM4	0.008	0.003	0.001	0.001	0.007
AM5	0.006	0.009	0.007	0.007	0.009
AM6	0.004	0.006	0.005	0.005	0.003
AM7	0.004	0.005	0.004	0.004	0.001
F_{2_MIN}[N]	408.11	416.94	414.88	414.88	420.54
F_{2_MAX}[N]	786.44	821.22	895.18	895.18	919.56
F_{5_MAX}[N]	5651.5	5649.6	5579.7	5579.7	5782.4



a) *b)*

Figure 12. a) Axial forces - CP1 [N] b) Axial forces – CP2 [N]

5 CONCLUSIONS

Levy cable dome was analyzed by symmetric and asymmetric load. Top 3 configurations of elongations of actuators during optimization process are shown in Table 5 and Table 6. MOGA generates the best non-dominant solutions from Pareto front. Analysis of cable dome under symmetric load consists of 3 analyses.

Table 5. Top 3 Candidate Points from Pareto Front under symmetric load

Symmetric Load	**Max. Load 1.5 kN.m^{-2}**			**+10% 1.65 kN.m^{-2}**			**+20% 1.8 kN.m^{-2}**		
[m]	**CP-1**	**CP-2**	**CP-3**	**CP-1**	**CP-2**	**CP-3**	**CP-1**	**CP-2**	**CP-3**
AM1	0.004	0.006	0.002	0.004	0.003	0.005	0.005	0.004	0.004
AM2	0.002	0.004	0.006	0.005	0.007	0.004	0.005	0.008	0.007
AM3	0.005	0.007	0.001	0.005	0.003	0.005	0.001	0.006	0.004
AM4	0.002	0.003	0.009	0.004	0.004	0.007	0.008	0.008	0.005
AM5	0.008	0.002	0.004	0.007	0.002	0.004	0.007	0.003	0.005
AM6	0.007	0.005	0.008	0.003	0.009	0.004	0.010	0.009	0.005
AM7	0.002	0.005	0.007	0.006	0.007	0.005	0.003	0.004	0.009
F_{2_MIN} [N]	408.56	471,32	433.66	401.27	402.89	427.3	409.78	403.35	408.06
F_{5_MAX} [N]	4225.5	4202.3	4234.2	4267.3	4276.4	4279.2	4449.9	4523.1	4511.2

Table 6. Top 3 Candidate Points from Pareto Front under asymmetric load

Asymmetric Load	**Max. Load 2.6 kN.m^{-2}**			**+10% 2.86 kN.m^{-2}**			**+20% 3.12 kN.m^{-2}**		
[m]	**CP-1**	**CP-2**	**CP-3**	**CP-1**	**CP-2**	**CP-3**	**CP-1**	**CP-2**	**CP-3**
AM1	0.001	0.001	0.001	0.002	0.003	0.002	0.003	0.009	0.002
AM2	0.002	0.004	0.007	0.007	0.008	0.004	0.008	0.006	0.010
AM3	0.005	0.003	0.008	0.003	0.009	0.002	0.004	0.002	0.005
AM4	0.008	0.003	0.001	0.004	0.002	0.007	0.003	0.001	0.003
AM5	0.006	0.009	0.007	0.002	0.002	0.007	0.004	0.003	0.006
AM6	0.004	0.006	0.005	0.009	0.003	0.007	0.007	0.006	0.009
AM7	0.004	0.005	0.004	0.008	0.007	0.005	0.009	0.004	0.005
F_{2_MIN} [N]	408.11	416.94	414.88	418.63	402.34	422.27	405.84	404.44	413,26
F_{2_MAX} [N]	786.44	821.22	895.18	765.44	825.41	793.69	803.13	833.86	877.99
F_{5_MAX} [N]	5651.5	5649.6	5579.7	6007.9	5965.5	5986.9	6318.8	6241.7	6256.9

Cable dome was loaded by maximum symmetric load (1.5 kN.m^{-2}), maximum load increased by 10% (1.65 kN.m^{-2}) respectively increased by 20% (1.8 kN.m^{-2}). Optimization process of Levy cable dome under asymmetric load consists of analysis under maximum asymmetric load (2.6 kN.m^{-2}), load increased by 10% (2.86 kN.m^{-2}) and 20% (3.12 kN.m^{-2}). Axial forces of optimized Levy cable dome are shown in Fig. 13 and Fig. 14.

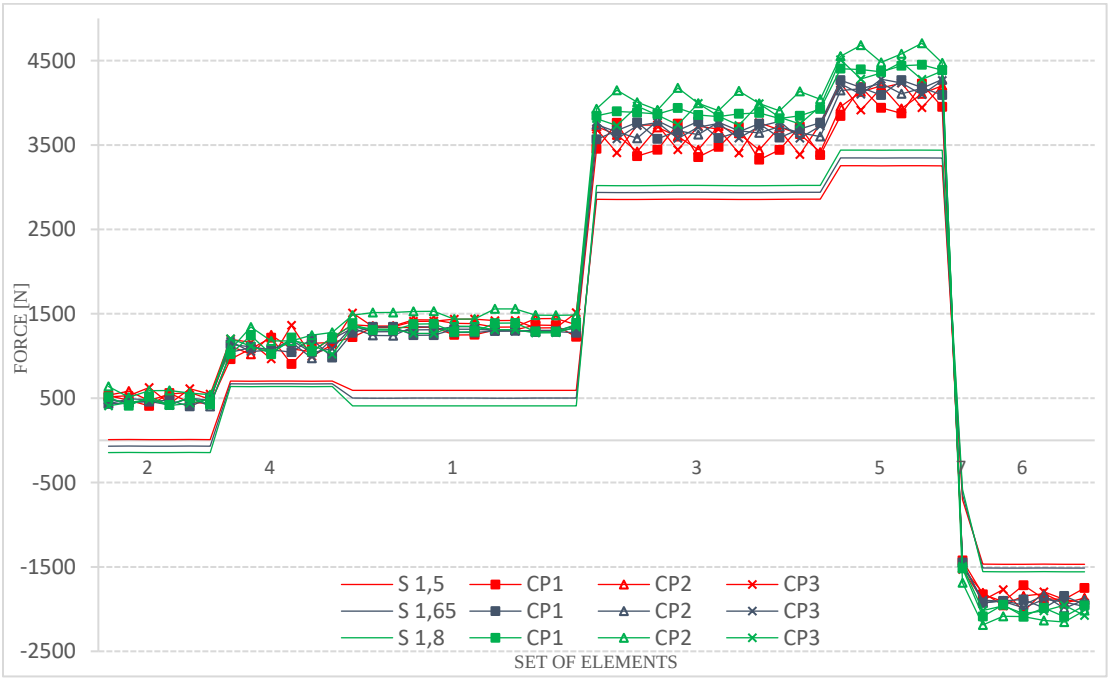


Figure 13. Axial forces – symmetric load [N]

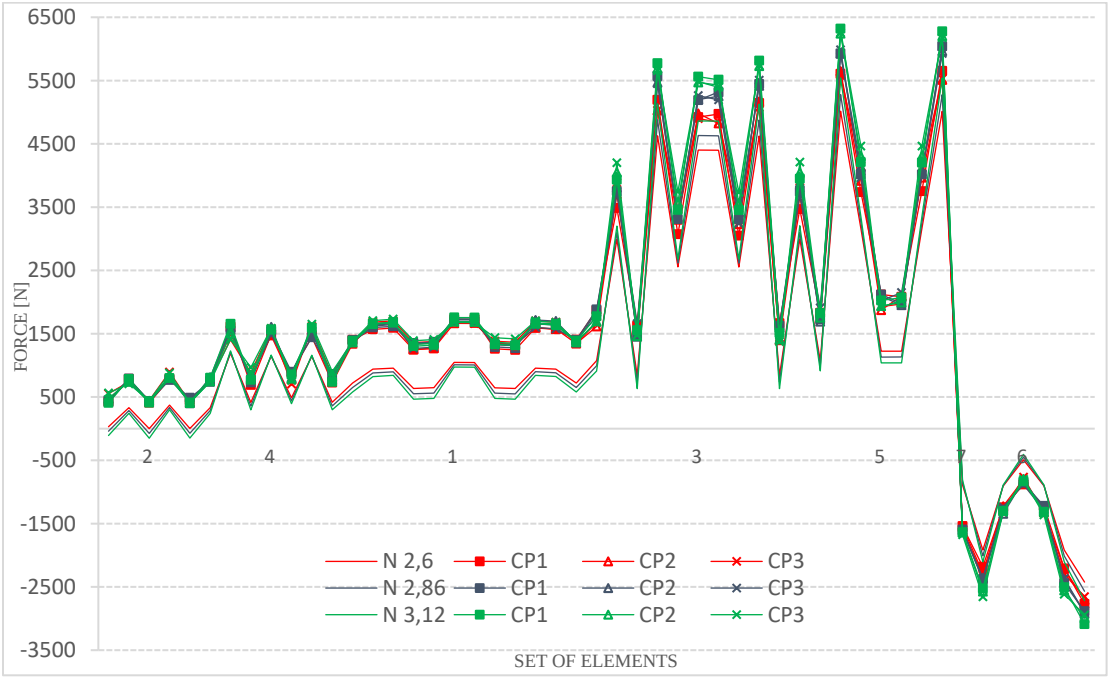


Figure 14. Axial forces – asymmetric load [N]

The objective of the NSGA algorithm (Non-Dominated Sorted Genetic Algorithm–II as a multi-criteria optimization tool MOGA) is to improve finding control commands (necessary movement of the actuators) of the cable dome. MOGA represents an effective way to find optimal solutions at Pareto front.

Acknowledgments

This paper is the result of the Project implementation: University Science Park TECHNICOM for Innovation Applications Supported by Knowledge Technology, ITMS: 26220220182, supported by the Research & Development Operational Programme funded by the ERDF. We support research activities in Slovakia/This project is being co-financed by the European Union.

The paper is carried out within the project No. 1/0302/16, partially founded by the Science Grant Agency of the Ministry of Education of Slovak Republic and the Slovak Academy of Sciences.

REFERENCES

[1] Kmet, S. and Mojdis, M. Time-depended analysis of cable dome using a modified dynamic relaxation method and creep theory, *Computer and Structures*, vol. 125, September 2013, ISSN 0045-7949.

[2] Shea, K., Fest, E. and Smith, I.F.C. Developing Intelligent Tensegrity Structures with Stochastic Search, *Advanced Engineering 129(4)*, 2003, pp.515-526.

[3] Sobek, W., Teuffel, P., Weilandt, A. and Lemaitre, C. Adaptive and lightweight, In *Proc., The Int. Conf. on Adaptable Building Structures, Eindhoven,* pages 234-245, Eindhoven, 2006.

[4] Ansys, Inc. Release documentation of Ansys 15.0, Southpointe, 275 Technology Drive, Canonsburg, November 2013.

[5] Motro, R. Tensegrity: Structural systems of future, *London: Kogan Page Science*, 2003. 238p. ISBN 1-903996-37-6.

[6] Kmet, S. and Mojdis, M. Adaptive Cable Dome, *Journal of Structural Engineering*, vol. 141, Issue 9, 2015, Article number: 04014225.

[7] Telgen, M. V. Parametric design and calculation of circular and elliptical tensegrity domes, *Master Thesis in Structural Design.* Eindhoven: Eindhoven University of Technology, Department of Architecture, Building and Planning. 2012, 211 p.

[8] Zelinka, I. Evolutionary computing techniques – principles and applications. *Brno University of Technology, BEN – technical literature. Prague, CZ.* 2009 (In Czech). 1st edition. ISBN 978-80-7300-218-3.

[9] Konak, A., Coit, D.W. and Smith, A.E. Multi-objective optimization using genetic algorithms: A tutorial, *Reliability Engineering and System Safety,* 2006. 91(9): 992-1007.

[10] Holland, J.H. Adaptation in ntural and artificial systems. Ann Arbor: *University of Michigan Press*; 1975.

[11] Fang, K.T., Li, R. and Sudjianto, A. Design and Modeling for Computer Experiments. *Chapman & Hall/CRC,* Boca Raton; 2006.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Two-scale Uncertainty Model for Transversely Fiber Reinforced Plastics

Ismail Caylak*, Eduard Penner**, Alex Dridger***, Rolf Mahnken****

*Paderborn University, **Paderborn University, ***Paderborn University, ****Paderborn University

ABSTRACT

In recent years, lightweight structures became increasingly important due to their excellent mechanical and lightweight properties. As a special component fiber reinforced plastics (FRP) become prominent. It is well known that material properties of FRP are uncertain due to the manufacturing process. In addition, there are measurement errors and missing or incomplete information on material properties. While several sources of uncertainties exist, these are often distinguished into aleatoric and epistemic uncertainty. Aleatoric uncertainty is presumed to be the intrinsic randomness of a phenomenon and is also called statistical uncertainty that can be modeled with stochastic methods based on the polynomial chaos expansion (PCE). On the other hand, epistemic uncertainty is the vagueness in a system definition due to subjectivity, simplification and incomplete knowledge that can be modeled with fuzzy methods based on the fuzzy set theory. In this presentation, we concentrate on unidirectional FRPs. Due to both constituents, fiber and matrix, composites are essentially heterogeneous, which motivates a two-scale approach. The related transversely isotropic behaviour is investigated with this approach. It takes into account the behavior of fibers and matrix separately, which renders a more realistic material behaviour of FRP. It is based on the idea to substitute the heterogeneous material with an effectively equivalent homogeneous material. As a key idea, the constitutive equations are modeled by a combination of fuzzy-stochastic methods. The stochastic material parameters are expanded with the multivariate PCE, whereas epistemic material parameters are defined as design variables and are modeled as fuzzy sets. An underlying optimization problem for the fuzzy analysis is approximated by discretization techniques, resulting into a separation of minimum and maximum problems. To become more universal, so-called quantities of interest are employed, which allow a general formulation for the target problem of interest. Experimental data of the matrix and the fibers are obtained separately. Then, in the numerical examples we investigate analytical effective properties for fuzzy-stochastic Voigt upper bounds and Reuss lower bounds. Finally, numerical results are compared with existing experimental observations.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Initial Value Problems in Nanotechnology Using Clifford Analysis

Johan Ceballos*, Antonio Di Teodoro**, Alexander López***

*Universidad De Las Américas, **Universidad San Francisco de Quito, ***Universidad Politécnica del Litoral

ABSTRACT

We analyze some initial value problems using Clifford Analysis within the context of nanotechnology focusing on the possible configurations which are compatible with the symmetries of the boundaries of toy-model samples such as, quantum dots and nanoribbons in order to describe the anisotropic electronic transport in two dimensional systems, where the electrons do not obey the Schroedinger equation but the Dirac equation. This, in principle trivial difference, has quite a lot of implications in the physical behavior of new materials such as graphene and related samples. Finally, we present a matrix representation of Clifford Algebras through some algorithms.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Combined Multiscale FEM and DPG Approach for Linear Elasticity

Witold Cecot*, Marta Oleksy**, Marek Klimczak***

*Cracow University of Technology, **Cracow University of Technology, ***Cracow University of Technology

ABSTRACT

The Multiscale Finite Element Method (MsFEM) [1] is one of the promising methods used for modeling of heterogeneous materials. It neither requires the assumption of scale separation nor periodicity of micro-structure. Moreover, it may be easily parallelized, since the essence of the MsFEM is an evaluation of special macro-scale finite element trial (approximating) shape functions that capture the micro-scale details. These functions are computed independently in appropriate patches of elements and the higher order approximation for the MsFEM has already proved to be profitable [2]. Although the method significantly reduces the computational cost, its efficiency and trustworthiness need further improvements. It may be achieved by using the ultra-weak variational formulation of the considered elasticity problem and coupling the MsFEM with the Discontinuous Petrov-Galerkin approach (DPG) [3] that is a new FEM methodology enabling computation of optimal, from the convergence point of view, test functions. Efficiency improvement is expected due to the optimal test functions offered by the DPG methodology since they enable obtaining reasonable results for a relatively small number of degrees of freedom. The ultra-weak formulation additionally simplifies, typically a cumbersome in the MsFEM, determination of boundary conditions for auxiliary, local problems and reduce the domains of the auxiliary problems to only single coarse elements. Reliability of the new version of the MsFEM is enhanced by the DPG guaranteed convergence, a built-in a'posteriori error estimate offered by this methodology and mathematically sound background of this approach. Preliminary numerical results for deformations of heterogeneous elastic bodies confirm expected profits of the proposed coupled MsFEM and DPG methodology. [1] T. Hou and X. Wu. A multiscale finite element method for elliptic problems in composite materials and porous media. Journal of Computational Physics, 134:169-189, 1997. [2] W. Cecot and M. Oleksy. High order FEM for multigrid homogenization. Computers and Mathematics with Applications, 70(7):1370-1390, 2015. [3] L. Demkowicz and J. Gopalakrishnan. A class of discontinuous Petrov-Galerkin methods. Part II. Optimal test functions. Numerical Methods for Partial Differential Equations, 27(1):70-105, 2011.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Triflow : Python Library for Prototyping Coupled Nonlinear PDEs. Application to Heat Transfer in Falling Films

Nicolas Cellier*, Benoît Stutz**, Nadia Caney***, Christian Ruyer-Quil****, Philippe Bandelier*****

*Université de Savoie Mont-Blanc, **Université de Savoie Mont-Blanc, ***Université Grenoble Alpe, ****Université de Savoie Mont-Blanc, *****CEA

ABSTRACT

Triflow is an open source software designed to easily implement systems of coupled non linear partial differential equations. The software appears as a python library. The library fits well with an interactive usage : this allow an effective way to test the models and explore the simulation results. It is based on the method of lines and use a mixed paradigm : the spatial derivatives are discretized and the Jacobian is computed via a symbolic engine in a first time. Then Theano, a modern framework used in deep learning algorithms, is used in order to perform on-the-fly optimisation and compilation of the schemes. High order implicit temporal schemes have been implemented. As an example of the capabilities of the Triflow library, we propose an analysis of the interaction between hydrodynamic wave regimes and heat transfer occurring on heated falling films based on an asymptotic model derived with the WRIBL method. Heat transfer across a wavy film falling on a hot plate depends not only on fluid thermal characteristics, but also on the hydrodynamic state of the flow: experimental works (Gonda, A. et al. Water falling film evaporation on a corrugated plate. Int. J. Therm. Sci. 81, 29–37 (2014).) show a non negligible impact of the hydrodynamic instabilities on transfer intensification compared to flat films. An asymptotic model based on weighted residual integrated boundary layer (WRIBL) method (1. Ruyer-Quil, C. & Manneville, P. Improved modeling of flows down inclined planes. Eur. Phys. J. B 15, 357–369 (2000).) has been written for the fluid dynamic and the heat transfer. Compared to previous attempts (1. Kalliadasis, S., Ruyer-Quil, C., Scheid, B. & Velarde, M. G. Falling Liquid Films. 176, (Springer London, 2012).), this new formulation compares satisfactorily to the solutions to the Fourier equation even at large values of the Prandtl number. Less expensive than direct numerical simulations (DNS), solving this asymptotic model allows for fast exploration of the physical parameters and their impacts on the heat flux and the interaction between hydrodynamics and heat transfer. One of the main goals is to use that tool and the comprehension of these interactions in order to improve the industrial equipments employing heated falling films. One way could be to force beneficial instabilities with the plate shape design. To this aim, we have included the effect of a corrugated plate shape in the models within a soft slope hypothesis.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Unraveling the Structure-property Relationships in Fiber-composite Materials Using Machine Learning and Global Sensitivity Analysis

David Cereceda*, Raman Arora**, Jessica A. Krogstad***, Francisco L. Jiménez****, Michael D. Shields*****, Lori Graham-Brady******

*Villanova University, **Johns Hopkins University, ***University of Illinois at Urbana-Champaign, ****University of Colorado at Boulder, *****Johns Hopkins University, ******Johns Hopkins University

ABSTRACT

The development and deployment of advanced new materials are linked to the understanding of their structure-property relationships. Physically-based approaches have extensively been used for this purpose, but they present some limitations related to their computational cost and the communication of information between the multiple hierarchical length scales involved. For their part, data models are designed to be computationally efficient, but they are not necessarily formulated with an explicit knowledge of the physical behavior of the system under study. In this work, we develop a machine-learning based model that exploits a combination of the physical knowledge of the microstructure with data-driven techniques to predict the local strain field in the material. In particular, we apply this method to extract the structure-property linkages in a two-dimensional metal matrix composite (MMC), by using a fully-connected neural network. As part of the model, global sensitivity analysis is also employed to identify the most prominent microstructural features that drive the mechanical behavior of the material.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Poroelasticity of Sedimentary Basin during Glaciation

Daniele Cerroni*, Paolo Zunino**, Anna Scotti***, Luca Formaggia****

*Politecnico di Milano, **Politecnico di Milano, ***Politecnico di Milano, ****Politecnico di Milano

ABSTRACT

Reconstructing the stress and deformation history of a sedimentary basin is a challenging and important problem in the geosciences and a variety of applications [2]. The mechanical response of a sedimentary basin is the consequence of complex multi-physics processes involving mechanical, geochemical, thermal, geophysical and geological aspects. The strongly coupled nature of the deformation problem may be understood in terms of the feedback underlying crustal dynamics. The pore fluid pressure affects stress, stress changes can lead to fracturing, and fracturing can affect pore fluid pressure. Similarly, stress can affect mineral solubility, causing mineral dissolution which, in turn, can affect rock rheology and, therefore, stress. The basin deformation analysis requires accounting of the coupling among the many interacting reaction, transport and mechanical (RTM) processes. For the mechanical analysis at the macroscopic scale, phenomena that contribute to the compaction of sediments are purely-mechanical compaction which originates mainly from rearrangement of the solid particles during burial and mechano-chemical compaction resulting from dissolution–precipitation mechanisms, generally induced by stress (pressure - dissolution). Purely mechanical phenomena prevail in the upper layers, whereas chemical compaction dominates for deeper burial as stress and temperature increase. Moreover during the glaciation the water inside the porous rock can freeze changing the mechanical and geochemical properties of the medium. The water in the upper layers of the basin can erode and hugely modify the top layer of the basin changing its poromechanical response. In this work we assume that this surface is described by the zero value of a given function of the space. The levelset introduces a discontinuity in the solution and the Extended finite element method is used to take into account this discontinuity.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Flat-top Partition of Unity Method for Electronic Structure Calculations

Ondrej Certik*, Gianmarco Manzini**, Lee Collins***, N. Sukumar****, John Pask*****, Marc Alexander Schweitzer******

*Los Alamos National Laboratory, **Los Alamos National Laboratory, ***Los Alamos National Laboratory, ****UC Davis, *****Lawrence Livermore National Laboratory, ******University of Bonn

ABSTRACT

A flat-top partition of unity method (FT-PUM) will be presented to solve the equations of Kohn-Sham density functional theory. The partition of unity weight functions are multiplied by functions consisting of enrichment functions and polynomials that span the trial space of the standard finite element method. The enrichment functions are derived from solutions of isolated atoms. Convergence studies with the state-of-the-art planewave method will be shown, as well as with non-enriched spectral finite elements. We show that the FT-PUM formulation yields an order of magnitude reduction in the degrees of freedom required to attain chemical accuracy. The method performs similarly to the recently developed partition of unity finite element method (PUFEM), but affords the significant advantage that it produces a well conditioned standard eigenvalue problem, thus facilitating efficient, parallel solution.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Macro-mechanical Modelling of Localized Cracks in Masonry Structures Using a Tracking Algorithm

Miguel Cervera*, Luca Pelà**, Savvas Saloustros***

*UPC-BarcelonaTech/CIMNE, **UPC-BarcelonaTech/CIMNE, ***UPC-BarcelonaTech/CIMNE

ABSTRACT

Masonry refers to a wide diversity of construction techniques and composite materials, varying according to local building traditions and material availability. This variability has impeded the development of a general methodology for the analysis of masonry structures, and has motivated the proposal of different numerical approaches specifically tailored to the simulation of masonry. Despite this extensive inventory of numerical approaches, a common choice for the analysis of large masonry structures is a macro-mechanical material representation through irreducible continuum finite element models. This “macro-modelling” approach allows an easier development of the numerical model and an affordable computational cost for the analysis. Nevertheless, it commonly results in a non-realistic representation of cracking as a smeared quantity over large areas within the structure, which contradicts the localized nature of cracks and hampers the identification of local and global collapse mechanisms. Additionally, cracking tends to propagate along the directions imposed by the sides of the finite elements in a spurious way. To overcome the above limitations, this work presents a numerical model based on the classical smeared crack approach and a novel local tracking algorithm oriented to the analysis of masonry structures under monotonic and cyclic loading [1,2]. The use of the tracking algorithm enhances the crack representation compared with classical smeared crack approaches, facilitating the identification of developing damage patterns on the analyzed structure [3]. In addition to that, the tracking algorithm enhances significantly the mesh-independency of the numerical simulation. At constitutive level, masonry is represented as a homogenized material with average mechanical properties through a local continuum damage mechanics model. A simple and explicit algorithmic formulation is adopted by including the description of irreversible deformations as an additional internal variable into an orthotropic continuum damage model [2]. The proposed methodology is applied to the simulation of experimental results on in-plane loaded masonry walls available in the literature. Keywords: Macro-modelling, tracking algorithm, masonry structures, cracking, cyclic loading References [1] Saloustros S, Pelà L, Cervera M, Roca P (2016) Finite element modelling of internal and multiple localized cracks. Comput Mech 59:299–316. doi: 10.1007/s00466-016-1351-6 [2] Saloustros S, Cervera M, Pelà L (2017) Tracking multi-directional intersecting cracks in numerical modelling of masonry shear walls under cyclic loading. Meccanica (in press) . doi: 10.1007/s11012-017-0712-3 [3] Saloustros S, Pelà L, Cervera M, Roca P (2017) An Enhanced Finite Element Macro-Model for the Realistic Simulation of Localized Cracks in Masonry Structures: A Large-Scale Application. Int J Archit Herit (in press) . doi: 10.1080/15583058.2017.1323245

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Common Implementation of Phase-field and Non-local Implicit Gradient Models for Ductile Failure

Jose Cesar de Sa*, Erfan Azinpour**, Joao Ferreira***, Marco Parente****

*University of Porto, Portugal, **University of Porto, Portugal, ***University of Porto, Portugal, ****University of Porto, Portugal

ABSTRACT

Damage and failure in ductile materials models, with their attractive simplifications of the microstructural complexity associated with these phenomena, comprise the presence of softening at the constitutive level, which is known as a possible source of problems in their numerical implementation. To somehow restore the well-posedness of the set of partial differential equations to be solved, regularized solutions, often resorting to non-local and gradient theories with the recourse of a characteristic length associated with the size of the non-local support region definition, may be utilised. The similar nature of the mathematical coupled temperature-displacement problems and non-local implicit gradient models for material ductile failure is explored using the existing built-in thermo-mechanically coupled finite-element solutions in common commercial software. In particular the nonlocal implicit gradient of the Lemaitre damage model and the phase field model are addressed The diffusive regularization of those material models are associated with the heat conduction equation, therefore circumventing the need of including special user subroutines to implement explicitly the weak form resultant from the coupling between momentum conservation and the evolution of the diffusive field. Using benchmarking examples, the proposed methodology, in what concerns capability to avoid mesh dependency and to predict cracked regions, is assessed.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Application of the Edge-based Gradient Smoothing Technique to Acoustic Radiation and Acoustic Scattering from Rigid and Elastic Structures in Two Dimensions

Yingbin Chai*, Cong Cheng**, Wei Li***, Xiangyu You****

*Huazhong University of Science and Technology, **Huazhong University of Science and Technology, ***Huazhong University of Science and Technology, ****Huazhong University of Science and Technology

ABSTRACT

The acoustic scattering and acoustic radiation from underwater object is a very interesting physical phenomenon in ocean acoustics and is also often encountered in practical ocean engineering applications. Therefore, how to precisely calculate and predict the acoustic scattered field is of great importance to improve the acoustical properties of the ocean engineering structures. In general, the analytical or semi-analytical approaches are only effective for the problems with simple geometries. When it comes to more practical problems with very complicated geometries, the analytical solutions are always impossible to obtain. In these cases, we have to resort to numerical methods. As is well-known to all, the conventional finite element method (FEM) is constrained by the "numerical dispersion error" issue for solving acoustic problems at high frequencies. In this paper, the gradient smoothing technique (GST) which is based on the edges of the elements is combined with the conventional FEM to construct a novel edge-based smoothed FEM (ES-FEM) for two dimensional exterior structural-acoustic problems. In this model, the ends of elements edges are sequentially connected to the centroids of the surrounding elements to form the so-called smoothing domains (SDs). Then the smoothed gradient field can be obtained by performing the GST over these obtained SDs. The present ES-FEM is able to provide a relatively appropriate stiffness of the real system owing to the "softening effects" from the GST. Therefore, the accuracy of the solutions for acoustic radiation and acoustic scattering can be significantly improved. For the purpose of handling the exterior Helmholtz equation, the involved infinite domains are truncated by a predefined artificial boundary B and the Dirichlet-to-Neumann (DtN) map is employed on B to prevent any possible spurious reflecting acoustic waves from the far-field. Several supporting numerical examples demonstrated that the ES-FEM with DtN map was very effective for exterior structural-acoustic problems and could produce more accurate numerical results than the conventional FEM.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Periodic Unsteady Flow Simulation Using Harmonic Balance Method

Zhenxia Chai*, Wei Liu**, Ming Zeng***, Xiaoliang Yang****

*National University of Defense Technology, **National University of Defense Technology, ***National University of Defense Technology, ****National University of Defense Technology

ABSTRACT

In recent years, Fourier-based frequency domain techniques are widely applied to significantly reduce the computational expense for analyzing unsteady periodic problems. Among the frequecy domain algorithms, the harmonic balance method (HBM) proposed is computationally efficient for unsteady flow problems, especially for periodic unsteady flow. The basic principle of this method is to decompose the flow variables into a Fourier serie, which transforms the unsteady flow into several steady problems coupled by a spectral time-derivative operator. The whole time history of a complete unsteady periodic flow can be reconstructed from the steady results. The present research simulates time-periodic unsteady transonic and subsonic flows around pitching airfoils via the solution of unsteady Euler equations, using HBM and compares it with the traditional time domain method (TDM) and experimental data to demonstrate the accuracy, efficiency and memory requirement of HBM. The test cases are NACA 0012 pitching airfoils with transonic and subsonic inflows. The unsteady pitching aerodynamic forces and moments are rebuilt, and the pressure coefficient distributions at different points in a pitching cycle are also reconstructed by HBM. These results are then compared with experimental data and TDM. The results show that for subsonic flow, only one harmonic is enough for HBM computation to achieve the same accuracy with TDM. Meanwhile, for strongly nonlinear unsteady transonic flow, it can be modeled to engineering accuracy with a small number of harmonics. Thus, the HBM is computationally efficient, it can reduce the computing time greatly with only about 1/10 (one-harmonic) and 1/4 (three harmonics) of that needed by the TDM. We also note that, both the computation time and memory requirement of the harmonic balance method increase linearly as the number of harmonics increases. For transonic flow, the reconstructed pressure distributions with three harmonics are agree well with TDM at all points on the aerofoil except where the shock appears and moves. In this region more harmmonics are needed to reconstruct the nonlinear behavior, and then the efficiency of the HBM when compared with the TDM may be lost. Thus, it is necessary to do further studies on adaptive harmonic balance method to solve highly nonlinear time-periodic flows and reduce the computational time and memory requirement.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Fast and Adaptative Boundary Element Methods for 3D Acoustic and Elastodynamic Problems

Stéphanie Chaillat*, Patrick Ciarlet**, Faisal Amlani***, Félix Kpadanou****, Adrien Loseille*****

*CNRS - POEMS, **ENSTA - POEMS, ***ENSTA - POEMS, ****ENSTA - POEMS, *****INRIA

ABSTRACT

The main advantage of the Boundary Element Method (BEM) [1] is that only the domain boundaries (and possibly interfaces) are discretized leading to a drastic reduction of the total number of degrees of freedom. In traditional BE implementation the dimensional advantage with respect to domain discretization methods is offset by the fully-populated nature of the BEM matrix, with set-up and solution times rapidly increasing with the problem size. In the last couple of years, fast BEMs have been proposed to overcome the drawback of the fully populated matrix. The Fast Multipole Method (FMM) is a fast, reliable and approximate method to compute the linear integral operator and is defined together with an iterative solver. The efficiency of the method has been demonstrated for 3D wave problems. However, the iteration count becomes the main limitation to consider realistic problems. Other accelerated BEMs are based on hierarchical matrices. When used in conjunction with an efficient rank revealing algorithm, it leads to a data-sparse and memory efficient approximation of the original matrix. Contrary to the FM-BEM it is a purely algebraic tool which does not require a priori knowledge of the closed-form expression of the fundamental solutions and it is possible to define iterative or direct solvers. Mesh adaptation is an additional technique to reduce the computational cost of the BEM. The principle is to optimize (or at least improve) the positioning of a given number of degrees of freedom on the geometry of the obstacle, in order to yield simulations with superior accuracy compared to those obtained via the use of uniform meshes. If an extensive literature is available for volume methods, much less attention has been devoted to BEMs. In this contribution, we give an overview of recent works to speed-up the solution of 3D acoustic and elastodynamic BEMs. More precisely, we will present - some preconditioning technics for iterative solvers; - iterative and direct solvers based on H-matrices [2]; - an anisotropic metric-based mesh adaptation technic [3]. [1] M. BONNET, Boundary integral equation methods for solids and fluids, John Wiley, 1995. ? [2] S. CHAILLAT, L. DESIDERIO, P. CIARLET, Theory and implementation of H-matrix based iterative and direct solvers for Helmholtz and elastodynamic oscillatory kernels, Journal of Computational Physics 351 (2017), pp 165-186. [3] S. CHAILLAT, S.P. GROTH, A. LOSEILLE, Metric-based anisotropic mesh adaptation for 3D acoustic boundary element methods, submitted.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

PBDW: a non-intrusive Reduced Basis Data Assimilation Method and its application to Outdoor Air Quality Models

Rachida Chakir*, Janell K. Hammond**, Frederic Bourquin***, Yvon Maday****

*Université Paris Est, IFSTTAR, **Université Paris Est, IFSTTAR, ***Université Paris Est, IFSTTAR, ****Sorbonne Université

ABSTRACT

As the population increases, cities must constantly reassess their urban planning. However, this must be done in such a way to preserve the quality of life of its inhabitants. Energy saving, sustainable water and air quality are some of the important challenges associated with growing cities. In this context, the monitoring of the different urban flows (pollution, heat) is very important. For instance data assimilation approach can be used in monitoring. These methods incorporate available measurement data and mathematical model to provide improved approximations of the physical state. The effectiveness of modeling and simulation tools is essential. Advanced physically based models could provide spatially rich small-scale solution, however the use of such models is challenging due to explosive computational times in real-world applications. Beyond computational costs, physical models are often constrained by available knowledge on the physical system. To overcome these difficulties, we resort the Parameterized-Background Data-Weak (PBDW) method introduced in [1]. The PBDW formulation combines a Reduced Basis (RB) [2] from the physically based model and the experimental observations, in order to provide a real-time and state estimate in a non-intrusive manner. The RB is used to diminish the cost of using a high-resolution model by exploiting the parametric structure of the governing equations. In addition, variational data-assimilation techniques are used to correct the model error. In this work we extend the PBDW method to the monitoring of urban air quality as an important use case but also as an example of the very generic approach that proves well suited to online monitoring of urban flows over large scales. We build a RB approximation space from a sample of solutions from air quality models based on CFD with varying meteorological conditions and pollution. The goal is to rapidly estimate online pollutant concentration around an area of interest (up to tens of hectares). In case studies presented here, the method allows to correct for unmodeled physics and treat cases of unknown parameter values, all while significantly reducing online computational time. REFERENCES [1] Y. Maday, A.T Patera, J.D. Penn and M. Yano, “A parameterized-background data-weak approach to variational data assimilation: formulation, analysis, and application to acoustics”, Int. J. Numer. Meth. Engng (2014). [2] Prud’homme, C., Rovas, D. V., Veroy, K., Machiels, L., Maday, Y., Patera, A. T., & Turinici, G. (2002). “Reliable real-time solution of parametrized partial differential equations: Reduced-basis output bound methods”. Journal of Fluids Engineering, 124(1), 70-80

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Use of Modified Johnson-Cook Model in Simulation of Metal-ceramic Composite Cold Spraying

Rohan Chakrabarty*, Jun Song**

*McGill University, **McGill University

ABSTRACT

Owing to the low processing temperatures and subsequent minimal thermal residual stresses, cold spray (CS) process has a significant potential as a fabrication route for freeform components, thus making it a prospective additive manufacturing technology. Over the past decade or so, cold spray experiments have been accompanied with systematic computational modeling to optimize the coating deposition conditions and predict the coating properties and thereby their performance. One of the most widely used plasticity models for prediction of material behavior at high strain rate is Johnson-Cook (JC) model. However, the model's shortcomings at the strain rates experienced during cold spray lead to inaccuracies in the predictions. Still, it is predominantly used owing to its simplicity and rich material parameters database. Though other models such as Preston - Tonks - Wallace (PTW) models have been considered more suitable for the high strain-rate predictions, they require many more material constants and are complex to implement numerically than JC model. Thus, in this study, we have incorporated a modified form of JC model to the cold spray simulations, which accounts for the viscous regimes experienced at high strain rates. The predictions obtained from the modified JC model has been found to be consistent with the cold spray experimental results. This modified JC model is then used to demonstrate the building-up process of the ceramic-metal composite coating. This study contributes important mechanistic knowledge towards understanding and predicting the ceramic retention and composite coating characteristics during cold spraying.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Spatial and Temporal Scale Bridging of Atomistic-Continuum Concurrent Multiscale Models for Inelastic Modelling of Materials

Subhendu Chakraborty*, Somnath Ghosh**

*Student, **Professor

ABSTRACT

Atomistic-continuum concurrent multiscale models are widely used to assess the deformation mechanisms of material. Where only the most critical part of the domain is modelled with atomistic resolution and rest of the domain is considered as continuum. The interface region between these two subdomains works as a medium of information transfer between these two different models. Most of these multiscale models suffer from two critical limitations. First, mismatch of time-scale between atomistic and continuum domain. Second, limited capability to deal with plasticity. In this present study, both of these issues are addressed. To match the time scale between atomistic and continuum domain, a new time marching scheme is proposed. In this scheme, Strain Boost based Hyperdynamics[1] is used to accelerate the time evolution of the atomistic domain. Under each load increment both atomistic and the continuum domain is iteratively evolved until both the convergence in the solution and time match between the domains are obtained. By using this method, the lowest strain rate of 104 is achieved which is impossible to achieve using conventional Molecular Dynamics and within similar computational resource. The proposed method is used to study and parametrize the propagation speed of a preexisting crack in a nickel single crystal. The parameterized crack propagation relation extracted from this concurrent model is used to study the kinetics and energetics of crack evolution for much larger domain using pure continuum scale model[2]. This model is extended further to incorporate the plastic capability for both the atomistic and continuum domain. The continuum domain is modelled using density based CPFE. To transport the plastic state variables from atomistic to continuum, dislocations at the interface region are converted from their discrete representation in the atomistic domain to the density form. This incoming dislocations are considered as incoming flux for the continuum CPFE model. The model is used to study and parametrize the evolution of plastic state variables during inhomogeneous deformation of a nickel single crystal owing to the presence of defects inside the grain. Parametrized relations are used to assess the material behavior for large scale pure continuum simulations. [1] S. Chakraborty, J. Zhang and S. Ghosh. Comp. Mat. Science, 121 (2016) 23-24. [2] J. Zhang, S. Chakraborty and S. Ghosh. J. for Multiscale Comp. Engineering, 15(2): 1-21 (2017).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Control of Discretization and Model Reduction Errors in Shape Optimization Performed Using Isogeometric Analysis (IGA) and Proper Generalized Decomposition (PGD)

Ludovic Chamoin*, Phuong Thai**

*ENS Paris-Saclay, **ENS Paris-Saclay

ABSTRACT

IGA has gained much attention over the last decade, particularly due to the fact that it enables one to solve problems directly on the geometry extracted from a CAD model; it thus simplifies the link between design and analysis [1]. IGA involves, for both the geometry and analysis, smooth and high-order NURBS functions associated with control points and weights. The IGA framework can be effectively coupled with reduced-order modeling (ROM) when dealing with parametrized geometry and shape optimization. To this end, the position of control points and the value of weights become design parameters, and ROM enables to compute efficiently the solutions over the whole parameter space. Here, we focus on ROM performed by means PGD, which is a technique based on a modal decomposition with separation of variables [2]. In the present work, we propose to control error sources inherent to this coupling between IGA and PGD when conducting shape optimization. First, in order to address discretization error, we introduce an a posteriori error estimate based on duality and the Constitutive Relation Error (CRE) concept. It can be used for a large set of mechanics problems, particularly for linear or nonlinear material behaviors described by means of convex potentials (elasticity, visco-plasticity, damage, contact, etc.). To the best knowledge of the authors, it is the first a posteriori error for IGA which is generic and which provides both guaranteed and fully computable bounds. Second, we extend the estimate in order to take into account modal truncation when resorting to PGD solutions. The control of this latter error source uses tools which were primarily introduced in the FEA context [3]. The obtained error estimators and indicators then enable to conduct adaptive processes. The talk will be illustrated with several numerical experiments, for linear or nonlinear (damage) problems, and with a focus on goal-oriented error estimation and adaptivity performance. References: [1] Hughes T.J.R, Cottrell J.A, Bazilevs Y, Isogeometric analysis: CAD, finite elements, NURBS, exact geometry an mesh refinement, Computer Methods in Applied Mechanics and Engineering, 2005, 194:4135-4195 [2] Chinesta F, Keunings R, Leygue A, The Proper Generalized Decompositiion for Advanced Numerical Simulations - A Primer, Springer, 2014 [3] Chamoin L, Pled F, Allier P.E, Ladevèze P, A posteriori error estimation and adaptive strategy for PGD model reduction applied to parametrized linear parabolic problems, Computer Methods in Applied Mechanics and Engineering, 2017, 327:118-146

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Discretely Entropy Stable Discontinuous Galerkin Methods for Nonlinear Conservation Laws

Jesse Chan*

*Rice University

ABSTRACT

High order methods offer several advantages in the approximation of solutions to hyperbolic equations, such as improved accuracy and low numerical dispersion and dissipation. However, high order methods also tend to suffer instabilities when applied to nonlinear hyperbolic equations such as the compressible Euler equations and shallow water equations. Often, these instabilities require filtering, limiting, or artificial dissipation to ensure that the solution does not blow up. At the root of these problems is the fact that the stability of the continuous problem does not imply stability at the discrete level. This talk will show how to construct high order schemes based on summation-by-parts theory which recover a discrete statement of entropy stability, and will discuss the extension of such methods to a more general class of discontinuous Galerkin methods. We will conclude by showing numerical results in one and two dimensions which support the presented theoretical results.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Thermal Simulation of Fused Filament Fabrication with Fiber Filled Composites

Aaditya Chandrasekhar*, Behzad Rankouhi**, Krishnan Suresh***

*University of Wisconsin-Madison, **University of Wisconsin-Madison, ***University of Wisconsin-Madison

ABSTRACT

Due to recent advancements in material technology such as fiber filled matrix, fused filament fabrication (FFF) is being increasingly used to produce functional parts. The preferential orientation of the fibers, combined with the layer-wise printing leads to enhanced anisotropic material behavior. This can be utilized to obtain desired mechanical performance of the fabricated part [1]. However, studies have shown that the temperature history during the printing process can have an adverse effect on the accumulation of residual stress, delamination, and distortion of the part. In this paper, we numerically investigate the evolution of temperature during the printing of a fiber filled composite using an anisotropic model, and an assembly free finite element solver. The anisotropic orientation of each mesh element is obtained from the machine instruction for the printing process (G-code). This is combined with experimentally obtained thermal conductivity tensor [2], to study the effects of raster path and fiber infill percentage on the heat conduction of the part. The numerical results are validated using infrared thermography during fabrication of samples with commercially available carbon fiber-filled polymer. The simulation framework can be used to predict the behavior of the part during and after the fabrication process. References [1] Zhang, P., Liu, J., & To, A. C. (2017). Role of anisotropic properties on topology optimization of additive manufactured load bearing structures. Scripta Materialia, 135, 148–152. https://doi.org/10.1016/j.scriptamat.2016.10.021 [2] Mulholland, T., Goris, S., Boxleitner, J., Osswald, T. A., & Rudolph, N. (2018). Fiber Orientation Effects in Fused Filament Fabrication of Air-Cooled Heat Exchangers. JOM, 1–5. https://doi.org/10.1007/s11837-017-2733-8

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A General Framework for Predicting Friction in Metals

Michael Chandross*, Adam Hinkle**, Andrew Kustas***, Nicolas Argibay****

*Sandia National Laboratories, **Sandia National Laboratories, ***Sandia National Laboratories, ****Sandia National Laboratories

ABSTRACT

While pure metals generally exhibit high friction and wear, nanocrystalline metals often show much lower friction and correspondingly low wear. We have developed and validated a model of friction in FCC metals that links the interfacial grain structure directly with the macroscopically measured friction coefficient. Recent work has shown that similarly low friction is possible in BCC metals, and we present a suite of simulations and experiments that demonstrate a general framework for connecting microstructural evolution and tribological response in both FCC and BCC metals. We show evidence that low friction is linked to grain boundary sliding as the dominant mechanism for stress accommodation. We utilize large-scale molecular dynamics simulations and targeted experiments to explore the various steady-state friction regimes of metals and alloys, with a goal of elucidating the structure-property relationships, allowing for the engineering of tribological materials and contacts based on material properties. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

The Study on Pseudo-elastic Effect of Ni-Ti Shape Memory Alloys

I-Ling Chang*, M.H. Tsai**

*National Cheng Kung University, **National Cheng Kung University

ABSTRACT

The shape memory properties, i.e., phase transformation induced by temperature and stress, of Ni-Ti alloy bulks are investigated using molecular dynamics simulation. First, the phase transformation behaviors of Ni-Ti alloy for various nickel composition ratios are studied under cooling and heating process. W parameter analysis is adopted for phase identification, i.e., martensite and austenite. It is noticed that the transformation temperature decreases as nickel composition ratio increases, which is consistent with experimental observation. Besides, there exists temperature hysteresis in thermal cycle for nickel composition ratio less that 51.5%. Second, the stress-assisted martensitic phase transformation is examined for 51%Ni-Ti alloy under cyclic uniaxial compression loading and unloading. It is noted that the stress needed to induce martensitic phase transformation from austenite at high temperature could become higher or lower with cycles depending on whether the previous loading causes any dislocation inside. The observation could provide an explanation for the contradictive experiment results reported in the literature.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Phase-field Modeling of Grain Growth with CSL Boundaries

Kunok Chang*

*Kyunghee University

ABSTRACT

The phase-field modeling has been actively applied to simulate grain growth phenomena in the solid-state polycrystalline materials. Even though the former works deeply contribute to enhance the fundamental understanding of the grain growth phenomena, they assumed the isotropic grain boundary energy and mobility for the simplicity. In recent years, parallel computing technology, such as GPGPU (General-Purpose computing on Graphics Processing Units) and OpenMP has developed dramatically, and anisotropic grain growth simulation can now be performed on a box-sized workstation rather than a clustered supercomputer. The stress corrosion cracking phenomenon is a long-standing challenge in the field of nuclear engineering because it poses a threat to the integrity of the Ni-based alloy in the secondary system of the nuclear power system. Also, it is well known that CSL (Coincidence Site Lattice) boundary, for example Sigma 3 boundary, play a significant role in determining stress corrosion cracking behavior in Alloy 600. Threrefore, understanding of effect of CSL boundary in grain growth of Alloy 600 is highly significant to predict the integrity of the nuclear system. However, incorporating CSL in grain growth simulation requires extremely high computation resources, it has not been considered in the former computational studies of grain growth. In this study, we incorporated not only anisotropic grain boundary energy but also CSL boundary such as sigma 3 grain boundary. We quantitativley analyzed how CSL affects the microstructure evolution of Alloy 600 and the results has been compared with former experimental observations.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Study of Failure of Reinforced Concrete Material with Concrete Damaged Plastic Model

Weitze Chang*

*National Center for Research on Earthquake Engineering, Taiwan

ABSTRACT

Reinforced Concrete (RC) play an important role in modern construction industry caused of its economical, long-life, and easy-molded advantages. However, the combition of steel reinforcing bars and concrete which mixed by rock (coarse aggregates), sand, water, and various power-sized particles makes its dynamic behavior complex and not easy to be predicted, especially especially after failure occurs. Tranditionally, Finite Element Analysis (FEA) is a good choice to model RC material and works well in both elastic and plastic stage, but cannot describe the post-peak part after concrete failure. In this study, the Concrete Damaged Plastic (CDP) model (Lubliner, et al., 1989; ABAQUS Inc., 2010) is introduced to model the dynamic brhavior of RC column in cylical loading test. The fraction and sliding between the interface of steel reinforcing bars and concrete material is also considered. After systematic study of model simplifying, performance improving, and validation with experimental data, this paper show that the proposed simulation can be expected to applied in concrete industry in the future. Keywords: Reinforced concrete, cylical loading test, fracture, concrete damaged plastic model Reference * Lubliner, J., Oliver, J., Oller, S., and Oñate, E. (1989). “A Plastic-Damage Model for Concrete, International Journal of Solids and Structures, 25: 299-326. * ABAQUS Inc., (2010). “Damaged Plasticity Model for Concrete and Other Quasi-brittle Materials,” in Abaqus Analysis User's Manual v6.10, Section 4.5.2, 14 pages.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Projection-based Model Reduction of Nonlinear Structural Dynamics Models with Contact Surfaces

Todd Chapman*, Charbel Farhat**

*Stanford University, **Stanford University

ABSTRACT

Projection-based model order reduction (PMOR) is a potentially enabling technology for the routine analysis of full configuration structural systems through numerical methods. Relatively speaking however, PMOR is still in its infancy in the context on nonlinear analysis but significant progress has been made in the last decade especially in the area of hyper reduction. However, in many scenarios contact must be modeled in order to analyze realistic engineering configurations. Incorporating contact constraints into a projection-based reduced order model (PROM) poses a distinct difficulty since the reduced coordinates are not associated with a mesh while contact is intimately linked to locality on a mesh. Furthermore, in the case of projection-based hyper-reduced order models (HPROMs) the majority of the mesh is discarded after a sampling procedure so that determining the appropriate constraints becomes non-trivial. Enforcement of contact constraints has been addressed in the context of PMOR through the use of Lagrange multipliers for node-to-node contact. The approach requires the collection of dual snapshots which, like the compression of displacement snapshots through a truncated SVD, must be compressed under the additional constraint of nonnegativity. This leads to the construction of a dual reduced order basis (ROB) through nonnegative matrix factorization. The dual ROB associated with the fixed node-to-node contact can then be precomputed offline. However, scenarios involving kinematic nonlinearities and sliding contact in which constraints cannot be reasonably precomputed offline have not been addressed. In addition to these difficulties, the contact PROM with Lagrange Multipliers must satisfy Inf-Sup conditions for solvability which requires that the dual ROB be of a lesser dimension than the primal ROB. The dual subspace must be large enough to accurately reconstruct the contact forces but not so large that it violates solvability of the reduced system of equations. Since contact is often associated with highly concentrated forces, snapshot data will typically be sparse which poses challenges for compression due to the uncertainty principle. This talk presents a one-sided projection method (akin to the mortar method) for the reduction of contact forces arising from large deformation contact. The principle of nonnegative matrix completion is also presented in the context of efficiently compressing dual snapshot data for the construction of an appropriate nonnegative dual basis. These two components are demonstrated in constructing effective PROMs for several challenging contact problems including the underbody blast of an ARES tank.

13th World Congress on Computational Mechanics (WCCM XIII) and 2nd Pan American Congress on Computational Mechanics (PANACM II), July 22-27, 2018, New York City, NY, USA

AN ISOGEOMETRIC FORMULATION FOR LARGE DEFORMATION ANALYSIS OF SOLIDS IN BOUNDARY REPRESENTATION

MARGARITA CHASAPI* AND SVEN KLINKEL*

*Chair of Structural Analysis and Dynamics
RWTH Aachen University
Mies-van-der-Rohe Str. 1, 52074, Aachen, Germany
Email address: chasapi@lbb.rwth-aachen.de, website: http://www.lbb.rwth-aachen.de/

Key words: Isogeometric Analysis, NURBS Basis Functions, Nonlinear Solid Surface, Scaled Boundary Finite Element Method, Large Deformations.

Abstract. This contribution deals with geometrical nonlinear problems within the framework of the so-called scaled boundary isogeometric formulation (SB-IGA). We propose this approach for the isogeometric analysis of surfaces especially, if only a boundary description of the geometry is available. This is for example the case with solids, which are typically modeled only by their boundary surfaces in CAD. To provide a numerical approach for surfaces with arbitrary number of boundaries, we combine the merits of the isogeometric analysis and the scaled boundary finite element method. The main idea lies in the parameterization of the solid in analogy with the scaled boundary finite element method (SB-FEM). Hence, the boundary of the surface is scaled in respect to a specified scaling center inside the domain. To solve the boundary value problem, we apply the weak form of equilibrium in the circumferential direction of the boundary and the radial scaling direction in the interior of the domain. As in standard IGA, the NURBS functions that describe the geometry of the boundary also interpolate the unknown displacement field. We employ NURBS also for the approximation of the solution in radial scaling direction. This approach has shown promising results in the scope of linear elasticity and plasticity problems. Here, a formulation for geometrical nonlinear 2D problems is presented. The derived linearized operator is used within a Newton-Raphson iterative scheme. We study numerical examples in the scope of nonlinear elasticity and plasticity and assess the performance of SB-IGA by comparison to other numerical methods.

1 INTRODUCTION

In the finite element analysis (FEA) framework, Lagrange basis functions form the basis for the approximation of the geometry and the displacement response of the structure. Due to this approximation, the geometry of the analysis model differs from the original geometry of the Computer Aided Design (CAD) software. Hughes introduced the idea of Isogeometric Analysis [1, 2], which circumvents the geometrical approximation error and provides a seamless integration of CAD and FEA software. In IGA, NURBS interpolate the geometry and the solution field.

Thus, the geometry remains *exact* throughout the entire analysis process. Currently, commercial CAD software employ the boundary representation modeling technique for the modeling of solids [3]. Thus, only the boundary surfaces of the solid are available in CAD. This observation motivates the development of a boundary-oriented formulation within the isogeometric analysis framework.

A well-known boundary-oriented method that combines the advantages of the boundary element method (BEM) and the finite element method (FEM) is the scaled boundary finite element method (SB-FEM). It is as a semi-analytical fundamental-solution-less boundary element method [4, 5]. For the parametrization of the structure interior, a radial scaling parameter and a parameter in the circumferential direction along the boundary is defined. The scaling parameter runs from a central point, the scaling center, to the boundary. The position of the scaling center is chosen so, that the total boundary of the domain is visible, which means that the domain occupied by the solid must be star-shaped. Sub-structuring of the domain is, in general, possible. In this way, the domain is covered by scaling the boundary in respect to the scaling center. In the circumferential direction, a standard finite element approach with Lagrange basis functions is employed [4]. NURBS basis functions can be used as given in [6, 7, 8, 9] for the description of the geometry and the approximation of the solution. The weak form of equilibrium is only enforced in the circumferential direction. In the scaling direction, the equilibrium is strongly applied. This results in a second order ordinary differential equation (ODE) in terms of the scaling parameter, which is the so-called scaled boundary finite element equation. For linear elasticity, a unique analytical solution exists, which can be computed with the eigenvalue method. For nonlinear problems, a linearization based on the homotopy analysis method is proposed in [10] and special shape functions based on the solution of linear problems are derived in [11, 12]. Alternatively, the Galerkin projection of the weak form in radial scaling direction allows the treatment of nonlinear problems. This approach has been investigated in [13, 14] for the solution of elasticity and plasticity problems. The performance of B-splines and NURBS for nonlinear problems has been studied e.g. in [15, 16].

This paper deals with an isogeometric formulation for large deformation analysis of surfaces, which are designed by the boundary representation modeling technique in CAD. The geometry and displacement of the boundary is interpolated by NURBS basis functions. Hence, we keep the *exact* geometry of the boundary for the analysis. We employ NURBS for the approximation in scaling direction, which allows for nonlinear behavior. The Galerkin method is applied in both the radial scaling and the circumferential direction. Due to the nonlinear deformation behavior, the iterative Newton-Raphson scheme is employed for the linearization of the solution. Finally, nonlinear problems are assessed by comparison to the isogeometric analysis

2 PARAMETRIZATION

The parametrization of the computational domains follows the idea of the scaled boundary finite element method [4, 5]. The two-dimensional domain Ω is decomposed into sectional subdomains $\partial\Omega_s$, which are parameterized in the same fashion and assembled to cover the whole domain. For the transformation of the geometry, a radial scaling parameter ξ is introduced to describe the interior of each section, as shown in Figure 1. The boundary of the solid is scaled in respect to a scaling center *C*, which is defined such as the total boundary of the solid is visible. This approach requires a star-shaped domain. For domains that do not fulfill this requirement, sub-structuring is

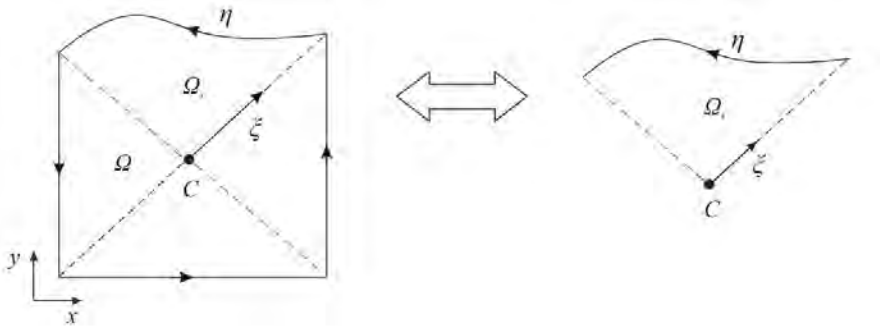


Figure 1: The scaled boundary parametrization of the domain Ω.

possible [4, 7, 12, 14]. The radial scaling parameter ξ runs from the scaling center towards the boundary, where ξ = 0 denotes the scaling center C and ξ = 1 the boundary. The circumferential direction of each section corresponds to the boundary of the domain, which is parameterized with a circumferential parameter η running from η = 0 to η = 1. The coordinates of the scaling center are denoted as $\boldsymbol{x}_0$. Employing this parametrization, the position of a point on the boundary $\boldsymbol{x}_s$ and inside the domain $\boldsymbol{x}$ can be expressed as

$$\boldsymbol{x}_s = \boldsymbol{N}_b(\eta)\mathbf{X}_s \quad \text{on} \quad \partial\Omega, \qquad \boldsymbol{x} = \boldsymbol{x}_0 + \xi(\boldsymbol{x}_s(\eta) - \boldsymbol{x}_0) \quad \text{in} \quad \Omega. \tag{1}$$

The NURBS basis functions $\boldsymbol{N}_b(\eta)$ are employed to describe the boundary of the surface. This fits perfectly to the boundary representation modeling technique employed in CAD. The vector $\mathbf{X}_s$ denotes the coordinates of the control points on the boundary. The Jacobian matrix can be derived by employing the scaled boundary transformation as

$$\boldsymbol{J} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & \xi \end{bmatrix} \underbrace{\begin{bmatrix} x_s - x_0 & y_s - y_0 \\ \frac{\partial x_s}{\partial \eta} & \frac{\partial y_s}{\partial \eta} \end{bmatrix}}_{\bar{\boldsymbol{J}}(\eta)} \tag{2}$$

which results in a multiplicative decomposition with the determinant $\det \boldsymbol{J} = \xi \det \bar{\boldsymbol{J}} = \xi \bar{J}$. An area element can be transformed from the physical to the parameter space by $dA = \xi \bar{J}\, d\xi\, d\eta$. Furthermore, we define the differential operator $\mathbf{D}$ as a function of the submatrices $\mathbf{b}_1(\eta)$, $\mathbf{b}_2(\eta)$

$$\mathbf{D} = \begin{bmatrix} \frac{\partial}{\partial x} & 0 & \frac{\partial}{\partial y} & 0 \\ 0 & \frac{\partial}{\partial y} & 0 & \frac{\partial}{\partial x} \end{bmatrix} = \frac{1}{\bar{J}} \left(\boldsymbol{b}_1^T(\eta) \frac{\partial}{\partial \xi} + \frac{1}{\xi} \boldsymbol{b}_2^T(\eta) \frac{\partial}{\partial \eta} \right), \tag{3}$$

$$\boldsymbol{b}_1^T(\eta) = \begin{bmatrix} y_{s,\eta} & 0 & -x_{s,\eta} & 0 \\ 0 & -x_{s,\eta} & 0 & y_{s,\eta} \end{bmatrix}, \boldsymbol{b}_2^T(\eta) = \begin{bmatrix} y_0 - y_s & 0 & x_s - x_0 & 0 \\ 0 & x_s - x_0 & 0 & y_0 - y_s \end{bmatrix}.$$

3 GOVERNING EQUATIONS

In this section, the two-dimensional boundary value problem for nonlinear elasticity will be formulated. The domain Ω is bounded by $\partial\Omega = \partial_u\Omega \cup \partial_t\Omega$, where $\partial_u\Omega$ is the boundary with a prescribed displacement $\bar{\boldsymbol{u}}$ and $\partial_t\Omega$ is the boundary with a prescribed traction $\bar{\boldsymbol{t}}$. The derivation is restricted to bounded domains without loss of generality. The governing equation reads

$$\text{Div}\,\boldsymbol{P} + \boldsymbol{b} = \boldsymbol{0}. \tag{4}$$

Here the vector $\boldsymbol{P}$ denotes the stress vector in the reference configuration and $\boldsymbol{b}$ the body force. The Dirichlet and Neumann boundary condition is defined as

$$\boldsymbol{u} = \bar{\boldsymbol{u}} \quad \text{on} \quad \partial_u\Omega, \qquad\qquad \boldsymbol{NP} = \bar{\boldsymbol{t}} \quad \text{on} \quad \partial_t\Omega. \tag{5}$$

$\boldsymbol{N}$ is the normal outward vector on the reference configuration and reads

$$\boldsymbol{N} = \begin{bmatrix} N_x & 0 & N_y \\ 0 & N_y & N_x \end{bmatrix}. \tag{6}$$

Considering large deformation theory, the deformation gradient and right Cauchy-Green tensor are given as

$$\boldsymbol{F} = \text{Grad}\boldsymbol{x} = \boldsymbol{I} + \text{Grad}\boldsymbol{u}, \qquad\qquad \boldsymbol{C} = \boldsymbol{F}^T\boldsymbol{F}. \tag{7}$$

We consider a hyperelastic Neo-Hooke material with the strain energy function

$$W(\boldsymbol{C}) = \frac{\mu}{2}(tr\boldsymbol{C} - 3) - \mu\ln(J) + \frac{\Lambda}{4}(J^2 - 1 - 2\ln(J)), \tag{8}$$

where μ is the shear modulus, Λ the Lamé parameter and J = det $\boldsymbol{F}$. The first and second Piola-Kichhoff stress can be expressed as

$$\boldsymbol{S} = 2\frac{\partial W}{\partial \boldsymbol{C}}, \qquad\qquad \boldsymbol{P} = \boldsymbol{FS}. \tag{9}$$

4 DISCRETIZATION WITH NURBS

In this study, we follow the idea of isogeometric analysis, thus NURBS basis functions are employed to describe the geometry of the boundary and to approximate the displacements $\boldsymbol{u}_b(\xi = 1)$ at the boundary of each section Ω_s. The expression for the geometry and displacement of the boundary reads

$$\boldsymbol{x}_s = \sum_{i=1}^{n_{bc}} R_{i,p}(\eta)\, \mathbf{X}_{s,i} = \boldsymbol{N}_b(\eta)\mathbf{X}_s, \qquad \boldsymbol{u}_b = \sum_{i=1}^{n_{bc}} R_{i,p}(\eta)\, \boldsymbol{U}_{s,i} = \boldsymbol{N}_b(\eta)\boldsymbol{U}_s(\xi) \tag{10}$$

where i is the index of the control point along the boundary and n_{bc} the number of control points of section Ω_s. The coordinates of the boundary control points are denoted by $\mathbf{X}_s$ and boundary NURBS by $\boldsymbol{N}_b(\eta)$. In order to construct NURBS, an open knot vector is introduced with $\mathbf{H} = [\eta_1, \eta_2, \ldots, \eta_{n_{bc}+p+1}]$, where $\eta_i \in \mathbb{R}$ is the ith knot and i is the knot index. The B-spline basis functions are employed, which are derived by the Cox de Boor formula [17]. Considering the weighting factor w_i for the ith B-spline function $N_{i,p}$, the NURBS basis function $R_{i,p}$ with polynomial degree p reads

$$R_{i,p} = \frac{N_{i,p} w_i}{\sum_{k=1}^{n_{bc}} N_{k,p} w_k} \tag{11}$$

In the scaling direction, we employ NURBS basis functions to approximate the displacement response. Note, that straight lines represent the scaling direction. The weighting factors are set equal along a radial scaling line, i.e. we have B-splines in the scaling direction. In order to construct the basis functions in scaling direction, the knot vector $\boldsymbol{\Xi} = [\xi_1, \xi_2, \ldots, \xi_{n_{cp}+q+1}]$ is introduced. Here, the number of control points per radial scaling line is n_{cp} and the polynomial degree q. Note, that $\xi_1 = 0$ stands for the scaling center C and $\xi_{n_{cp}+q+1} = 1$ for the boundary. After rearranging all control point vectors $\mathbf{U}_{s,i}$ of Equation (10) in the vector $\mathbf{U}_s$ and approximating with the basis function $R_{j,p}$ in scaling direction, the displacement for one section reads

$$\begin{aligned} \boldsymbol{u}_b &= \underbrace{\begin{bmatrix} R_{1,p} & 0 & R_{2,p} & 0 & \cdots & R_{n_{bc},p} & 0 \\ 0 & R_{1,p} & 0 & R_{2,p} & \cdots & 0 & R_{n_{bc},p} \end{bmatrix}}_{\boldsymbol{N_b}(\eta)} \boldsymbol{U}_s(\xi) \\ &= \boldsymbol{N_b}(\eta) \sum_{j=1}^{n_{cp}} R_{j,q}(\xi)\ \boldsymbol{U}_j = \boldsymbol{N}_b(\eta)\boldsymbol{N}_s(\xi)\boldsymbol{U}. \end{aligned} \tag{12}$$

Note, that for each control point two nodal degrees are assumed, so that the dimension of the displacement vector $\mathbf{U}_{s,i}$ is 2 and of the vector $\mathbf{U}$ is $2 \cdot n_{cp}$ respectively. Figure 2 illustrates an example of the interpolation in the radial scaling and circumferential direction for a section. It is worth noting, that the stiffness matrix of a section can be alternatively derived by employing triangular patches in the framework of isogeometric analysis. In the following, we express the discretized form of the operator $\mathbf{D}^h$ as a function of the submatrices $\boldsymbol{b}_1(\eta)$ and $\boldsymbol{b}_2(\eta)$

$$\mathbf{D}^h = \frac{1}{\bar{J}}\left(\boldsymbol{b}_1 \boldsymbol{N}_b \boldsymbol{N}_{s,\xi} + \frac{1}{\xi}\boldsymbol{b}_2 \boldsymbol{N}_{b,\eta} \boldsymbol{N}_s\right). \tag{13}$$

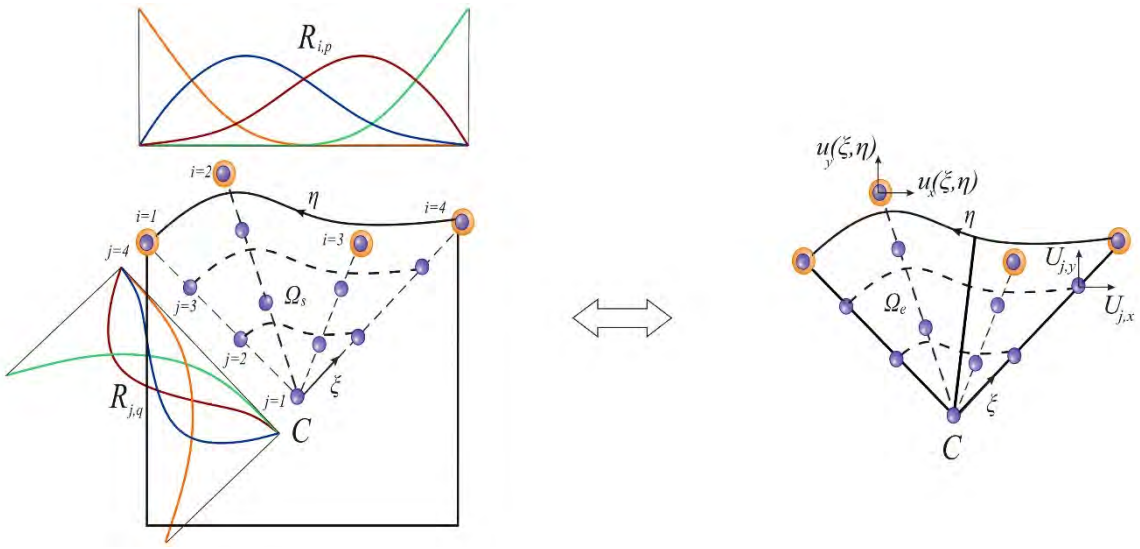


Figure 2: NURBS basis functions in parameter space of section Ω_s.

For the solution, we employ the Galerkin method. Considering Equation (4) and the boundary conditions in Equation (5) it holds

$$\sum_{s=1}^{nsec} \delta \boldsymbol{U}_j^T \left[\int_{\Omega_s} \xi \boldsymbol{D}^{h^T} \widehat{\boldsymbol{F}}^T \boldsymbol{S} \, \bar{J} \mathrm{d}\xi \mathrm{d}\eta \boldsymbol{U}_j - \int_{\Omega_s} \xi \boldsymbol{N}^T \boldsymbol{b} \, \bar{J} \mathrm{d}\xi \mathrm{d}\eta - \int_{\partial\Omega_s} \boldsymbol{N}^T \boldsymbol{b}_2^T \widehat{\boldsymbol{F}} \boldsymbol{S} \, l \, \mathrm{d}\xi \boldsymbol{U}_j \right] = \boldsymbol{0}. \tag{14}$$

Here, the vector $\boldsymbol{N} = \boldsymbol{N}_b(\eta)\boldsymbol{N}_s(\xi)$ denotes the shape functions per radial scaling line and l is the integration length per radial scaling line. The vector $\widehat{\boldsymbol{F}}$ contains the components of the deformation gradient. For the sake of simplicity, the body forces are neglected. By applying a linearization to the weak form with a displacement increment of $\Delta\boldsymbol{u} = \boldsymbol{u}^{k+1} - \boldsymbol{u}^k$ we derive

$$\mathrm{D}\boldsymbol{G}^k(\boldsymbol{u}^k, \delta\boldsymbol{u})\Delta\boldsymbol{u} = \sum_{s=1}^{nsec} \delta \boldsymbol{U}_j^T \int_{\Omega_s} \underbrace{\xi \boldsymbol{D}^{h^T} \left(\widehat{\boldsymbol{F}}^T \mathbb{C}_T \widehat{\boldsymbol{F}} + \widehat{\boldsymbol{S}} \right) \boldsymbol{D}^h \bar{J} \, \mathrm{d}\xi \mathrm{d}\eta}_{\boldsymbol{K}} \Delta \boldsymbol{U}_j \tag{15}$$

where $\boldsymbol{K}$ denotes the stiffness matrix and $\mathbb{C}_T$ the consistent tangent modulus. Moreover, $\widehat{\boldsymbol{S}}$ contains the components of the second Piola-Kirchhoff stress. Having derived all necessary equations, we can now apply this formulation for geometrical nonlinear analysis of boundary represented surfaces.

5 NUMERICAL EXAMPLES

This section illustrates the performance of the proposed formulation by means of two numerical examples. The accuracy and efficiency of the proposed approach is evaluated by comparison to the isogeometric analysis.

5.1 Cook's membrane

The proposed formulation is employed for the nonlinear analysis of Cook's membrane. The geometry and boundary conditions are presented in Figure 3. The scaling center *C* is defined here as the geometric center of the domain. The computational domain is partitioned into 4 sections. The boundary and scaling direction of each section is initially defined with the polynomial degree p = 2 and extends to p = 4 and p = 6. Additionally, *h*-refinement is performed for each polynomial degree. Plain strain state is assumed. The trapezoidal plate of Figure 3 is subjected to combined bending and shear. Reference results are available in the literature for large deformation analysis [18, 19].

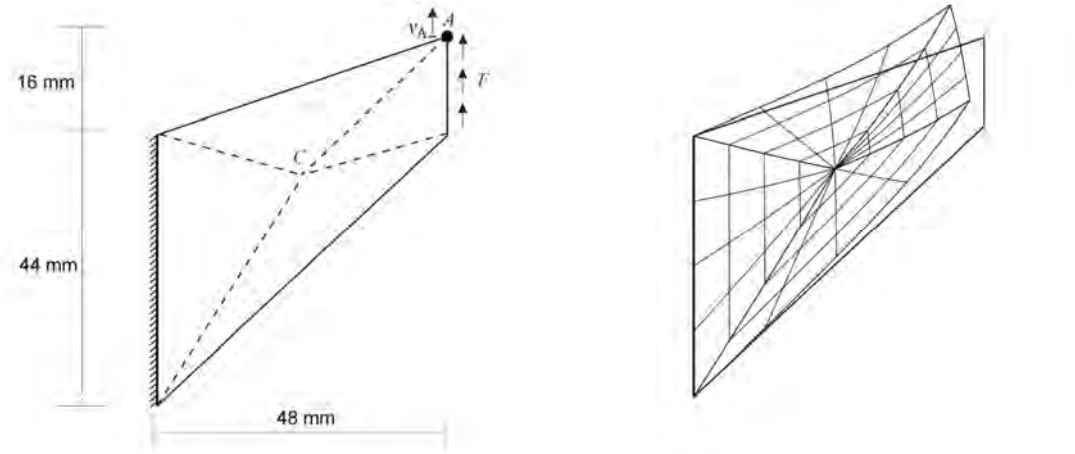


Figure 3: Problem definition and final deformed configuration.

For better illustration, we first refer to the small strain range and study the performance for nonlinear material behavior. A J_2-plasticity model is employed for the analysis in analogy to [14]. The material properties are the elasticity modulus E = 207 MPa, the Poisson's ratio ν = 0.3, the yield stress σ_y = 0.45 MPa and the linear isotropic hardening modulus H = 0.12924. The unit vertical force F = 1.0 N is applied per load step. In Figure 4 we observe the load deformation curve for the vertical displacement v_A. For comparison, an isogeometric computation is performed. Both solutions are computed with a mesh of sixth order shape functions and almost the same degrees of freedom. The results imply that there is a good agreement between the proposed formulation and isogeometric analysis in the small strain range. Furthermore, we consider nonlinear deformation behavior. The material properties are set according to reference studies in the literature for better comparison [19]. Here, the bulk modulus is κ = 40.0942 10^4 MPa and the shear modulus μ = 80.1938 MPa. This leads to a nearly incompressible state. The unit force F = 1.0 N is applied per load step in 100 load steps. The final deformed mesh can be seen in Figure 3. For comparison, we perform the computation on isogeometric *k*-refined meshes. The results can be observed in Figure 5. The results with quadratic polynomial degree seem to suffer from locking for both the proposed approach and IGA. The proposed formulation performs better than IGA for coarse discretizations, whereas IGA performs better for finer discretizations.

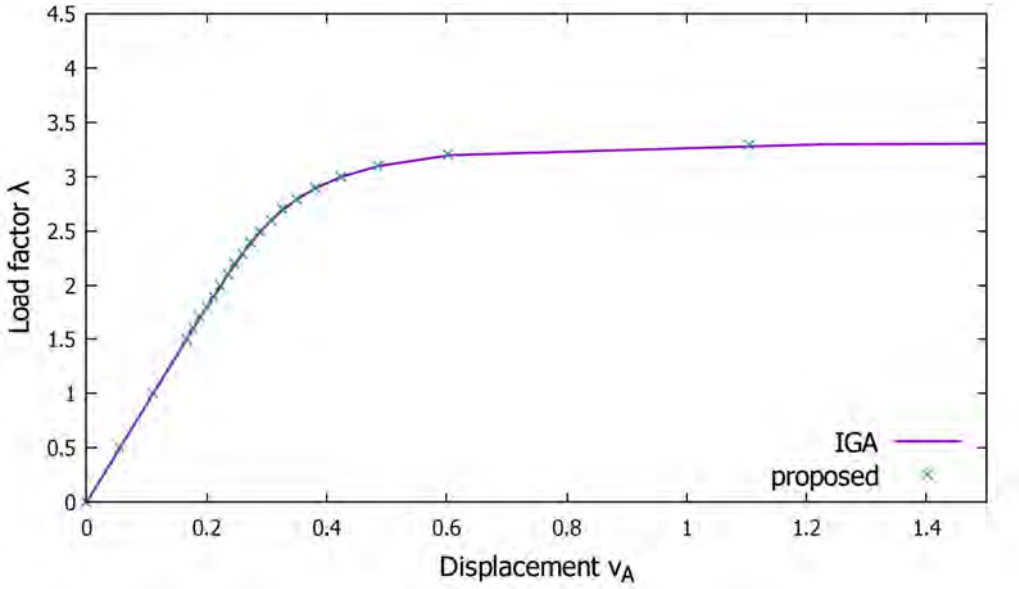


Figure 4: Load deformation curve and comparison with IGA.

Both solutions converge to the same value, which agrees very well with the reference results in the literature [19]. For higher polynomial degrees, locking is alleviated without any treatment of the incompressibility. The results indicate a very good agreement for higher polynomial degrees. The It can be concluded that the proposed formulation converges for all polynomial degrees and is in general comparable to isogeometric analysis.

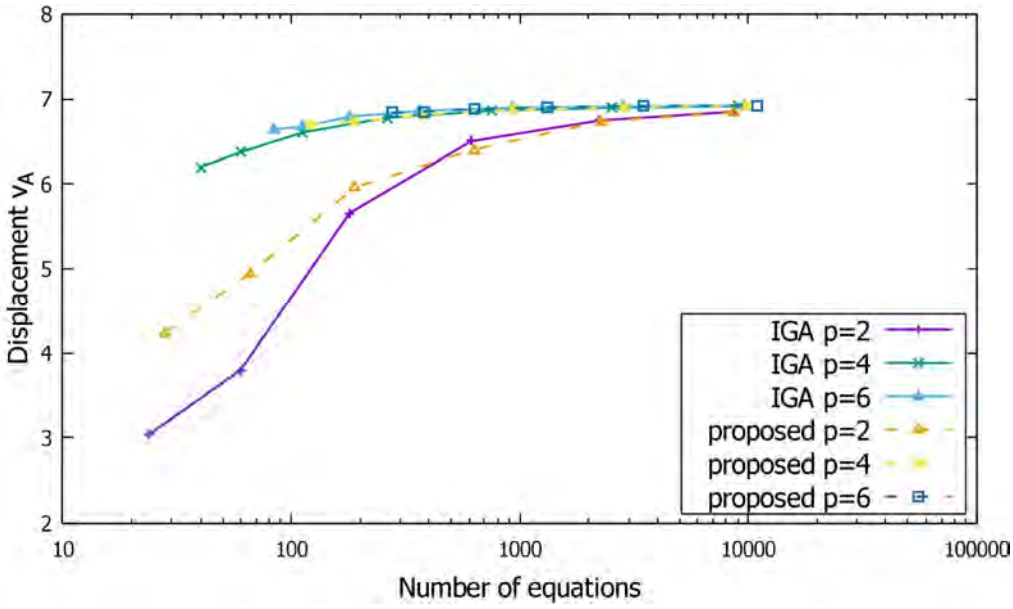


Figure 5: Convergence study and comparison with IGA.

5.2 Notched plate

The second numerical example concerns a notched plate with the geometry and boundary conditions shown in Figure 6. The objective of this test is to demonstrate the applicability of the formulation for non-convex polygonal domains with arbitrary number of boundaries. In the present study, we restrict ourselves to bounded domains. Therefore, the domain is sub-structured here in two subdomains with scaling center C_1 and C_2 respectively. Note, that an application of the formulation to unbounded domains is in principle possible. Plain strain state is assumed. The material properties are the shear modulus $\mu = 0.3422$ N/mm^2 and the Lamé constant $\Lambda = 99.771867$ N/mm^2. Displacement control is applied in 50 steps, with a total prescribed displacement u = 100 mm on the right edge of the plate.

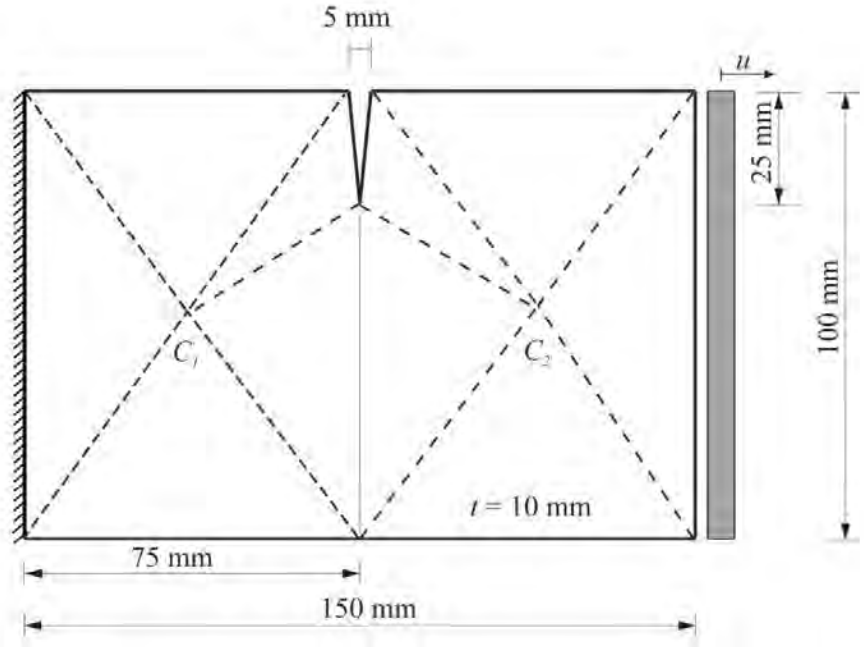


Figure 6: Problem definition and loading. [11]

For the computation, the polynomial degree is chosen as p = 4 for the boundary and the scaling direction. The horizontal reaction force of the plate is monitored. For comparison, an isogeometric mesh with polynomial degree p = 4 and nearly the same degrees of freedom is computed. Due to the geometry, 4 rectangular patches are employed to model the area around the notch with IGA. Figure 7 depicts the force displacement curve for both solutions. The results indicate a very good agreement. It can be concluded, that the proposed formulation seems to be a promising approach for the modeling of domains with arbitrary number of edges that does not induce any significant modeling effort.

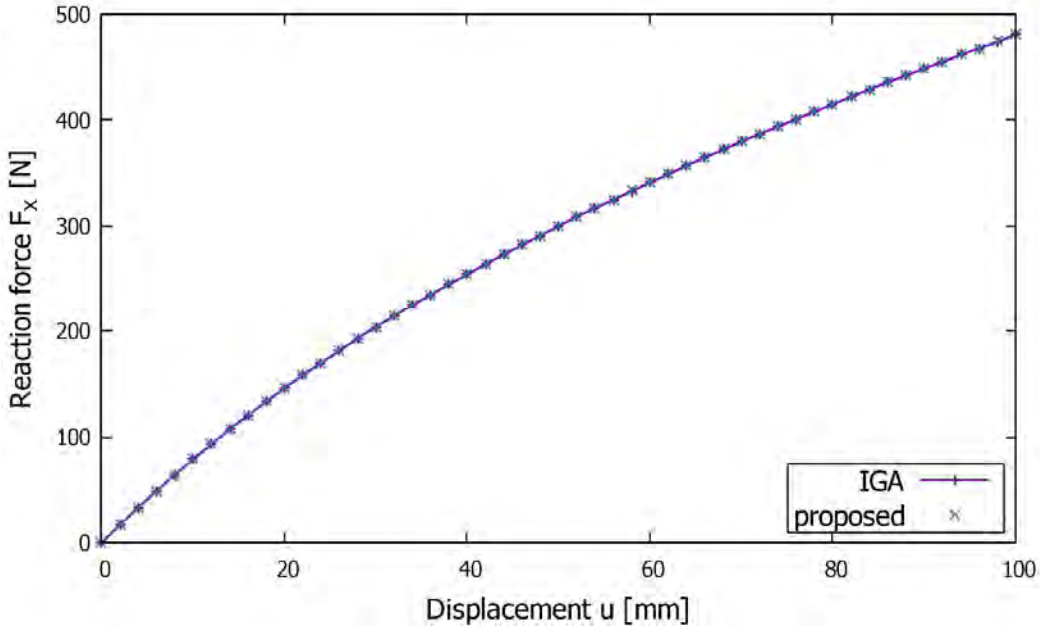


Figure 7: Reaction force displacement curve and comparison with IGA.

6 CONCLUSIONS

This paper deals with an isogeometric formulation for geometrical nonlinear analysis of boundary represented solids. The proposed approach fits perfectly the boundary representation modeling technique employed in CAD to model solids. To parameterize the boundary surfaces of the solid, the idea of the scaled boundary finite element method is employed. NURBS basis functions describe the geometry and approximate the solution. Hence, the *exact* geometry of the boundary is exploited for the analysis. For the solution, we employ the Galerkin method. The linearized operator is derived and used within an iterative Newton-Raphson scheme. We assess the formulation based on numerical examples of nonlinear elasticity and plasticity. For comparison, we employ the isogeometric analysis. The results indicate a good agreement with the isogeometric analysis. The proposed formulation is applicable to domains with arbitrary number of edges and sub-structuring is in general possible. An algorithmic framework for the optimal decomposition of arbitrary domains is a subject of future research. Finally, it can be concluded that the proposed formulation seems to be a promising alternative to isogeometric analysis, if only the geometry of the boundary is available.

ACKNOWLEDGMENTS

The first author wishes to acknowledge the support of the International Association for Computational Mechanics (IACM) for the participation at the 13th World Congress on Computational Mechanics. The financial support of the German Research Foundation (DFG) for the research is also acknowledged.

REFERENCES

[1] Hughes, T.J.R, Cottrell, J.A. and Bazilevs, Y. Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement. Comput. Methods Appl. Mech. Engrg. (2005) 194:4135-4195.

[2] Cottrell, J.A., Hughes, T.J.R. and Bazilevs, Y. Isogeometric Analysis: Toward Integration of CAD and FEA. John Wiley & Sons, (2009).

[3] Stroud, I. Boundary Representation Modelling Techniques. Springer, (2006).

[4] Song, C. and Wolf, J.P. The scaled boundary finite-element method – alias consistent infinitesimal finite-element cell method – for elastodynamics. Comput. Methods Appl. Mech. Engrg. (1997) 147:329-355.

[5] Song, C. A matrix function solution for the scaled boundary finite-element equation in statics. Comput. Methods Appl. Mech. Engrg. (2004) 193:2325-2356.

[6] Lin, G., Zhang, Y., Hu, Z. and Zhong, H. Scaled boundary isogeometric analysis for 2D elastostatics. Science China Physics, Mechanics and Astronomy (2014) 57:286-300.

[7] Natarajan, S., Wang, J.C., Song, C. and Birk, C. Isogeometric analysis enhanced by the scaled boundary finite element method. Comput. Methods Appl. Mech. Engrg. (2015) 283:733-762.

[8] Klinkel, S., Chen, L. and Dornisch, W. A NURBS based hybrid collocation-Galerkin method for the analysis of boundary represented solids. Comput. Methods Appl. Mech. Engrg. (2015) 284:689-711.

[9] Chen, L., Dornisch, W. and Klinkel, S. Hybrid collocation-Galerkin approach for the analysis of surface represented 3D-solids employing SB-FEM. Comput. Methods Appl. Mech. Engrg. (2008) 295: 268–289.

[10] Lin, Z. and Liao, S. The scaled boundary FEM for nonlinear problems. Commun. Nonlinear Sci. Numer. Simulat. (2011) 16:63-75.

[11] Behnke, R., Mundil, M., Birk, C. and Kaliske, M. A physically and geometrically nonlinear scaled-boundary-based finite element formulation for fracture in elastomers. Internat. J. Numer. Methods Engrg. (2014) 99:966-999.

[12] Ooi, E., Song, C. and Tin-Loi, F. A scaled boundary polygon formulation for elasto-plastic analyses. Comput. Methods Appl. Mech. Engrg. (2014) 268:905-937.

[13] Chen, L., Simeon, B. and Klinkel,S. A NURBS based Galerkin approach for the analysis of solids in boundary representation. Comput. Methods Appl. Mech. Engrg. (2016) 305:777-805.

[14] Chasapi, M. and Klinkel, S. A scaled boundary isogeometric formulation for the elasto-plastic analysis of solids in boundary representation. Comput. Methods Appl. Mech. Engrg. (2018) 333:475-496.

[15] Breitenberger, M., Apostolatos, A., Philipp, B., Wüchner, R. and Bletzinger, K.-U. Analysis in computer aided design: Nonlinear isogeometric B-Rep analysis of shell structures. Comput. Methods Appl. Mech. Engrg. (2015) 284:401-457.

[16] Schillinger, D., Ruess, M., Zander, N., Bazilevs, Y., Düster, A. and Rank, E. Small and large deformation analysis with the *p*- and B-spline versions of the Finite Cell Method. Comput. Mech. (2012) 50:445-478.

[17] Piegl, L. and Tiller,W. The NURBS Book, in: Monographs in Visual Communications. Springer, (1997).

[18] Mathisen, K., Okstad, K.M., Kvamsdal, T. and Raknes, S. Isogeometric analysis of finite deformation nearly incompressible solids. J. Struct. Mech. (2011) 44:260-278.

[19] Elguedj, T., Bazilevs, Y., Calo, V. and Hughes, T. $\bar{B}$ and $\bar{F}$ projection methods for nearly incompressible linear and non-linear elasticity and plasticity using higher-order NURBS elements. Comput. Methods Appl. Mech. Engrg. (2008) 197:2732-2762.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Error Estimation for Stress Distributions in Polycrystalline Alloys

Kamalika Chatterjee*, Robert Carson**, Paul Dawson***

*Cornell University, **Cornell University, ***Cornell University

ABSTRACT

Crystal based finite element modeling is an invaluable tool for predicting stress distributions in polycrystalline structural alloys such as Ti-6Al-4V. The accuracy of the prediction depends on estimation and control of the errors associated with discretization. In the current work, the errors in the stress distribution are estimated in virtual polycrystalline samples of alpha-Titanium (hcp phase of Ti-6Al-4V). To estimate the error, the discontinuous stress field (element-by-element stresses) over a grain is smoothed by projecting the stress components to the nodes [1]. The differences between the continuous (smooth) and discontinuous stress fields, calculated at individual gauss points are utilized to estimate the L2 norm of errors for corresponding elements and grains. Error estimations are performed for different cases of microstructures and sample instantiations (using Neper [2]). Magnitudes of the errors are found to depend on microstructural features. For example, the locations of sharp orientation gradients developed through heterogeneous deformation in the polycrystal are associated with significant errors. Mesh refinement is performed at those locations based on the numerical solution obtained using a trial mesh. Simulations then are repeated using the refined mesh to reduce the errors in the problematic regions. The mesh refinement technique introduced in this work helps improve the prediction of stress distributions in polycrystalline aggregates.
[1] Zienkiewicz, O. C., & Zhu, J. Z. (1987). International journal for numerical methods in engineering, 24(2), 337-357. [2] Quey, R., Dawson, P. R., & Barbe, F. (2011). Computer Methods in Applied Mechanics and Engineering, 200(17), 1729-1745.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Computing Singularly Perturbed Differential Equations and Plasticity Without Constitutive Assumptions

Sabyasachi Chatterjee*, Amit Acharya**

*Carnegie Mellon University, **Carnegie Mellon University

ABSTRACT

Obtaining coarse response of systems of ordinary differential equations (ODE) containing rapidly oscillatory response as well as fast monotonic decay without detailed information on the evolution of the original (fine) variables is an interesting, but challenging task. For a given autonomous system of ODE, we consider developing practical models for determining the slow/coarse behavior of the ODE system which reflect a measurement of the underlying dynamics. We study equations with and without apriori split into slow and fast components. When there is a vast separation of the time-scales of the coarse and the fine dynamics, computing the ordinary differential equation takes a lot of computing time and is not practical. The goal of our study is to suggest efficient computational tools that help revealing the limit behavior of such systems. We define coarse variables using modern mathematical tools like Young Measure and Practical Time Averaging (PTA) which incorporates many rigorous ideas. The computational algorithm reveals an approximation of the limit dynamics which is an approximation of the full solution. We also discuss how to determine the fine initial conditions which ensures a correct coarse response. Finally, we apply this method to develop a macroscopic model to compute the plastic strength and study the microstructure of crystalline materials at the meso-macro scale from the underlying motion of crystal defects. We couple an exact, non-closed partial differential equation based theory (Mesoscale Field Dislocation Mechanics, MFDM) representing the evolution of space-time averaged dislocation dynamics, that contains well-defined place-holders for microscopic dislocation dynamics based input. These inputs are prescribed by a carefully designed coupling, on the slow time-scale of meso-macro response, with time-averaged response of fast, local discrete Dislocation dynamics (DD) simulations. The rationale behind adopting such a coupled PDE-ODE approach instead of a completely DD based approach is primarily the vast separation in time-scales between plasticity applications that operate at quasi-static loading rates and the fundamental time scale of dislocation motion as embodied in DD which makes it impractical to reach appreciable applied strain using DD alone. The constitutive equations are replaced by inputs from Discrete Dislocation Dynamics while the associated elastic boundary value problem is solved using finite element method with a limited set of assumptions.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Posteriori Analysis and Efficient Refinement Strategies for the Poisson-Boltzmann Equation

Jehanzeb Chaudhry*

*University of New Mexico

ABSTRACT

The Poisson-Boltzmann equation (PBE) is a second order nonlinear partial differential equation that models the electrostatic interactions of charged bodies such as molecules and proteins in an electrolyte solvent. The PBE is a challenging equation to solve numerically due to the presence of singularities, discontinuous coefficients and boundary conditions. Hence, there is often large error in the numerical solution of the PBE that needs to be quantified. The focus of this presentation is robust error estimation and refinement strategies for computing a quantity of interest (QoI), such as the solvation free energy, from the solution of the PBE. We employ adjoint based a posteriori analysis to accurately quantify the error in a QoI computed from the finite element solution of the PBE. We identify various sources of error and propose novel refinement strategies based on a posteriori error estimates.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Multifidelity Robust Optimization with Information Reuse

Anirban Chaudhuri*, Karen Willcox**

*Massachusetts Institute of Technology, **Massachusetts Institute of Technology

ABSTRACT

This work presents a multifidelity method for optimization under uncertainty. Accounting for uncertainties during optimization ensures a robust design that is more likely to meet performance requirements. Designing robust systems can be computationally prohibitive due to the numerous evaluations of expensive high-fidelity numerical models required to estimate system level statistics at each optimization iteration. In this work, we focus on the robust optimization problem formulated as a linear combination of the mean and the standard deviation of the quantity of interest. We propose a multifidelity Monte Carlo approach combined with information reuse to estimate the mean and the variance of the system outputs using the same set of samples. The method leverages multiple low-fidelity models and the existing information from the designs visited during the prior optimization iterations. The information reuse from previously visited designs takes advantage of model autocorrelation between similar designs during the optimization. Nested control variates are used to combine the multiple fidelities and reuse the information from previous optimization iterations. We optimally allocate resources between the different fidelities that minimizes the variance in the nested control variate estimators for both the mean and the variance for a given budget. The multifidelity robust optimization method with information reuse maintains the same level of accuracy as a regular Monte Carlo estimate using only high-fidelity solves. However, the use of cheaper low-fidelity models and existing information leads to significant computational savings for the multifidelity robust optimization method as compared to a regular Monte-Carlo-sampling-based approach.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Computation of Incompressible Navier-Stokes Equations by Local Radial Basis Function Collocation Method

Bang-Fuh Chen*, Bing-Han Lin**, Chia-Cheng Tsai***

*National Sun Yat-sen University, **National Sun Yat-sen University, ***National Kaohsiung Marine University

ABSTRACT

A meshless local radial-basis-function collocation method (LRBFCM) based on the multiquadric type radial basis function is used to solve incompressible Navier-Stokes equations. The projection method, sometimes called fractional-step methods, is implemented in the present study. The usage of non-uniformly distributed nodes makes the nodes generation in the computational domain become quite simple in LRBFCM. Two numerical cases are provided to verify the accuracy and the stability of the proposed numerical scheme, which include Taylor's decaying vortices and lid-driven square cavity flow. Convergence rates of pressure and velocity confirm the second-order accuracy of the algorithms. The numerical solutions of lid-driven square cavity flow were obtained for Reynolds numbers up to 1000, and very good agreements with the existing results are obtained. The success of these numerical simulations indicates the potential of the proposed numerical model in simulating incompressible flow geometrical and dynamic complexity.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

On Study of Hybrid TMD and TLD System on Structure Motion Control

Bangfuh Chen*, Chih-hua Wu**

*professor, **PhD

ABSTRACT

In this paper, the hybrid tuned mass damper (TMD) and tuned liquid damper (TLD) are used to suppress the dynamic motion of a structure. The time-independent finite difference method is used to evaluate the sloshing liquids in the TLD and the Runge-Kutta method to calculate the dynamic response of TMD. The effects of TMD on base structure (BS) motion suppression are significant when the external forcing frequency is close to the resonant frequencies of the coupled system. Extensive researchers had reported suggested mass ratio, liquid ratio, tuned mass and tuned liquid frequencies. However, the precise physics explanation of the phenomenon are incomplete and rarely discussed, whereas they are clearly explained in this study. In this study, we will clarify the optimal value of the TLD frequency on structure motion reduction control is exactly equal to the exciting frequency. The addition of TLD to the system would further reduce the dynamic response of the structure when the natural frequency of the liquid tank is equal to the external forcing frequency and the out-of-phase occurs between sloshing-induced and external forces and both forces cancel each other and the resultant force acting on the structure nearly vanishes so does the structure motion. According to the numerical simulations of this study and experimental measurements of the associated study, we may suggest a practical design approach of the hybrid TMD+TLD system for a structure motion control. 1. Determine the fundamental frequency of the structure. 2. Determine the response spectrum of the possible of expected ground motion. 3. Determine the most thread exciting frequencies to the structure. 4. Select the tuning frequency of TLD according to step 3. And use to determine the tank width and water depth. 5. One also need to be noted, the smaller liquid depth ratio provides better motion response reduction. In order to avoid slamming and breaking wave occurred in the TLD, the suggested liquid depth ratio is as small as 0.1 and the tank width and liquid depth can be determined according to this number. (Chen and Yang 2017). Chen, Bangfuh and Yang Binhan, (2017) , Experimental study of a hybrid TMD and TLD on structure motion reduction, Ocean Engineering, submitted.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Higher Order, Adaptively Integrated Cohesive Element

Boyang Chen*, Raffaele Russo**

*TU Delft, Faculty of Aerospace Engineering, **TU Delft, Faculty of Aerospace Engineering

ABSTRACT

Cohesive Elements (CE) are known to suffer from the limitation that its size must be several times smaller than the cohesive zone length. The willingness of the authors is to present, with this paper, an adaptively integrated cohesive element which employs a higher-order interpolation of the separations. The validation of the CE has been made by simulating delamination problems chosen from already verified cases in literature (Turon, et al., 2007). For the case of a DCB problem, the cohesive zone length was estimated to be 0.8 mm. Using linear CEs would require a maximum element size of 0.25 mm in order to accurately capture the experimental curve. With 2 mm and larger linear CEs, the results would be far off from the experimental ones. The authors present here a 2D, two-node cohesive element. In addition to the usual two displacement degrees of freedom, each node contains an additional rotational degree of freedom, thereby achieving a higher-order interpolation of the separation field. While the interpolation remains unchanged during analysis (i.e., no additional partitioning or enrichment involved), the integration scheme changes with respect to the damage/failure status of the element. Comparisons with the results of the linear CE demonstrate that the proposed element is able to substantially improve the prediction accuracy of large cohesive elements (2 mm to 5 mm elements). The predicted delamination initiation load of 2.5-mm CE was 171% of the experimental value with linear CEs, and this is now improved to 104% with the proposed element. In the case of even larger CEs, 4-mm linear CE predicts 321% of the experimental initiation strength while the proposed 5-mm element's prediction is at 108%. In terms of propagation, linear 2.5-mm and 4-mm CEs' predictions are far off the experimental curve, while the proposed 2.5-mm and 5-mm elements' predictions stay relatively close to the experimental curve, with largest discrepancies of around 10% of the peak load.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Phase-Field Modeling of Dendrite Formation in Lithium Metal Batteries

Chih-Hung Chen*, Chun-Wei Pao**

*Research Center for Applied Sciences, Academia Sinica, Taiwan, **Research Center for Applied Sciences, Academia Sinica, Taiwan

ABSTRACT

Lithium metal is widely considered to be an ideal anode material for next-generation rechargeable batteries for its high theoretical capacity (3,860 mAh/g) and low electrochemical potential (–3.04 V). However, lithium-metal-based batteries are still not commercially available due to the fact that uncontrollable lithium dendrites can easily form during battery charging and then lead to short-circuit risk and poor cycling performance. It has be known that various lithium dendritic patterns, such as needle-like, mossy, and fractal, can develop under different charging conditions. Although recent studies have found a link between the dendritic patterns and applied current density, the growth mechanism of lithium dendrites in three-dimensions remains poorly understood. In order to investigate the evolution of the electrode/electrolyte interface and its stability, we propose a multi-scale phase-field model for lithium dendrite formation. By introducing a phase order parameter to distinguish the electrode and electrolyte, this method is applicable to describe the electrolyte/electrode interface migration and microstructure evolution. The governing equations of motion for ionic concentration, electric potential and phase order parameter are variationally derived. The classical Butler-Volmer reaction kinetics is used to describe the nonlinear relationship between current density and overpotential at the electrode/electrolyte interface. By imposing relevant boundary conditions for electric potential and current density, we first demonstrate that this model is able to reproduce the sharp interface Butler-Volmer reaction kinetics in one dimension. Different dendritic patterns are observed in our preliminary thin three dimensional simulations. We perform fully three dimensional simulations to investigate the effects of applied electric potential on the dendritic patterns. In addition, recent experimental studies have shown that the lithium dendrite growth can be greatly stabilized by applying a pulse charging scheme. We apply this model to study the effect of pulse frequency on the dendritic patterns and the simulation results are compared with experimental observations.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Multiscale Non-Equilibrium Molecular Dynamics Simulation and Applications

Chuin-Shan David Chen*, Chi-Hua Yu**, Yu-Chuan Hsu***

*National Taiwan University, **National Taiwan University, ***National Taiwan University

ABSTRACT

Atomistic-based multiscale modeling theory and computational method for static problems have been successfully developed in the past decade. The advance has transformed the way we design micro and nanoscale materials for static problems. In contrast, the development of dynamic multiscale method for non-equilibrium simulations is limited, mainly due to spurious wave-reflection problems on the interface between atoms and continuum. In this talk, I will present our recent work on developing a novel multiscale non-equilibrium molecular dynamics (NEMD) simulation method based on the concept of time history kernels in real space [1]. The concept of finite-size virtual domain allows us to construct a novel multiscale NEMD. Dynamic responses of atoms in the virtual domain can be effectively constructed through a careful choice of time history kernels. The proposed method allows us to overcome the length scale limitation posed on NEMD simulations. Applications of the multiscale NEMD method for wave propagation and thermal transport will be addressed. [1] C-S Lee, Y-Y Chen, C-H Yu, Y-C Hsu, C-S Chen (2017), "Semi-analytical solution for the generalized absorbing boundary condition in molecular dynamics simulations," Computational Mechanics, 60, 23-37.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Residual Crushing Performance of Square Carbon Fiber Reinforced Plastic (CFRP) Composite Tubes after Transverse Low-Velocity Impact

Dongdong Chen*, Xintao Huo**, Shaowei Tong***, Guangyong Sun****, Xinglong Liu*****

*State Key Laboratory of Advanced Design and Manufacture for Vehicle Body, Hunan University, Changsha, 410082, China, **State Key Laboratory of Advanced Design and Manufacture for Vehicle Body, Hunan University, Changsha, 410082, China, ***State Key Laboratory of Advanced Design and Manufacture for Vehicle Body, Hunan University, Changsha, 410082, China, ****School of Aerospace, Mechanical and Mechatronic Engineering, The University of Sydney, Sydney, NSW 2006, Australia, *****State Key Laboratory of Advanced Design and Manufacture for Vehicle Body, Hunan University, Changsha, 410082, China

ABSTRACT

With the increasing demand of light-weight for vehicles, carbon fiber reinforced plastic (CFRP) composite, which has a better strength to weight ratio, has been widely used as energy absorption structures, such as crash boxes for progressive folding energy absorption under axial compressive loads. During its whole life time, various impact cases may happen, such as drop out of tools or collision of stones. While CFRP are usually rather sensitive to dynamic impact loadings and even minor, invisible damage could cause the performance reduction. However, studies existed on residual properties of CFRP tubes mainly considered the impact in axial direction, limited studies were available to evaluate the effect of transverse impact on residual axial compression characteristic. This work aims to study the residual crushing performance of square CFRP tubes after transverse low-velocity impact with experimental and numerical methods. Firstly, serials of low-velocity impact tests were conducted to examine the damage modes with the increase of impact energy. Then the quasi-static axial compression tests were carried out to characterize the degradation of residual crushing performance induced by the impact. The main damage modes are matrix cracking for lower impact energies, delamination and fiber breakage for high impact energies. Peak forces of impact force-displacement curves increase with the increase of impact energy. It is also found that the degradation of residual compression properties could be divided into different regions. Different with the progressive crushing mode seen in the un-impacted tubes, collapse and unstable local buckling were observed in the axial crushing tests. The peak load and specific energy absorption of the performed tubes were also analyzed with un-impacted tubes finally. Together with cross-section views in impact position, the performance reduction during axial compression caused by impact were explored, which showed a shear failure mode. Finally, a finite element model was established for describe the dynamic behavior of CFRP tubes and validated with experimental results with a user-defined material subroutine VUMAT.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

An Efficient Computational Fluid Dynamics-based Aeroelastic Reduced Order Model for Aeroelastic Global Optimization

Gang Chen*, Dongfeng Li**, Yixing Wang***, Andrea Da Ronch****, Yueming Li*****

*State Key Laboratory for Strength and Vibration of Mechanical Structures, School of Aerospace, Xi'an Jiaotong University, **State Key Laboratory for Strength and Vibration of Mechanical Structures, School of Aerospace, Xi'an Jiaotong University, ***State Key Laboratory for Strength and Vibration of Mechanical Structures, School of Aerospace, Xi'an Jiaotong University, ****Faculty of Engineering and the Environment, University of Southampton, Southampton, *****State Key Laboratory for Strength and Vibration of Mechanical Structures, School of Aerospace, Xi'an Jiaotong University

ABSTRACT

This paper presents an aeroelastic optimization study for three dimensional wing at global level. The study employs Genetic Algorithms (GAs) as an optimization tool in combination with an efficient Computational Fluid Dynamics-based aeroelastic Reduced-Order Model (ROM). The Proper Orthogonal Decomposition (POD) method has been shown its accuracy and efficiency for aeroelastic analysis at fixed flight condition for a frozen model configuration. POD vectors generated from unsteady flow solution snapshots based on one set of structural modeshapes. In the aeroelastic optimization process, in order to keep the ROM's accuracy, a new CFD-based POD/ROM could be reconstructed when modeshapes changed, these reconstruction procedures take a considerable time, and greatly increasing the time cost of the aircraft design. In this study, the aeroelastic modeling counts for both stiffness and mass matrix variation of wing structure at global level to maximize flutter speed. Finally, the most feasible and optimal solutions were effectively obtained by the presented aeroelastic optimization.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Feature-Based Recombination Deep Neural Network for Reduce Order of Aero-elastic System

Gang Chen*, Dongfeng Li**, Yixing Wang***

*Xi'an Jiaotong University, **Xi'an Jiaotong University, ***Xi'an Jiaotong University

ABSTRACT

A recombination DNN (Deep Neural Networks) model based features of flow field to reduce order of aero-elastic system is carried out in this paper. NN (Neural Networks) is an efficient model for reducing order of flow and aero-elastic system. However, traditional NN models are actually system identification methods. Different from these, the proposed DNN model improve the accuracy and generalization capability through using convolutional neural network to extract the information of flow field in each time step. In order to synthesize different kinds of input variables, a novel serial network is also introduced. Of particular interest about NN is to determine the weights of neuron. The synthesized network with an improved Back-Propagation (BP) algorithm is employed to ascertain parameters of NN model through deep learning process. Using NACA0012 2D aero-elastic model, the DNN is fed by the basic variables at every coarse grid of flow field as the input and the aerodynamic forces as the target data, which is computed by the full order Euler computations. The DNN is iteratively trained using the proposed improved BP algorithm to predict the aerodynamic forces in different time steps and the results are compared with the full-order computations which show good consistence. At last, combining the proposed DNN with the structural motion equations, a Reduced Order Model (ROM) for aero-elastic system is obtained. Using the ROM, we do a flutter analysis for NACA0012. And a sensitivity study is performed to identify the hyper-parameters of DNN for predicting flow field such as the number of neurons, the number of layers and the kernel size of convolutional neural network, and so on. Within the error threshold, the proposed DNN model has reduced nearly four orders of magnitude about the degree of freedom compared the full order computation and significantly cuts down the consumed computational resources. We also try to transfer the form of Euler equation to explore why DNN can predict so good results. Some useful theoretical conclusions about predicting flow with DNN are found. The proposed feature-based recombination DNN has an important and wide significance to the design and control of aircraft, especially when unsteady or aero-elastic effect is prominent.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Fully Implicit, Conservative, Multidimensional Electromagnetic Particle-In-Cell Algorithms for Multiscale Kinetic Plasma Simulation on Curvilinear Meshes

Guangye Chen*, Luis Chacon**

*LANL, **LANL

ABSTRACT

Particle-in-cell (PIC) simulation techniques are widely used for first-principles simulations of plasma dynamics. Classical PIC employs an explicit approach (e.g. leap-frog) to advance the Vlasov-Maxwell/Poisson system using particles coupled to a grid. Explicit PIC is subject to both temporal (CFL) and spatial (aliasing) stability constraints, challenging system-scale kinetic simulations, even with modern super-computers. Implicit algorithms can potentially eliminate these stability constraints, thus holding promise for significant speedups. Implicit PIC algorithms have been explored since the late 1970's, but have suffered from various ailments originating in the lack of non-linear consistency and of strict conservation properties. In this presentation, we discuss a multi-dimensional, nonlinearly implicit, conservative electromagnetic PIC algorithm [1,2]. The approach delivers both accuracy and efficiency for multi-scale plasma kinetic simulations, and extends previous proof-of-principle 1D studies [3]. To avoid noise issues associated with numerical Cherenkov radiation for large implicit timesteps, we consider the Darwin approximation to Maxwell's equations, which projects out the light wave analytically. The formulation conserves exactly total energy, local charge, canonical momentum in the ignorable directions, and preserves the Coulomb gauge. Linear momentum is not exactly conserved, but errors are controlled by an adaptive particle sub-stepping orbit integrator. Key to the performance of the algorithm is a moment-based preconditioner, featuring the correct asymptotic limits. The formulation has been extended to curvilinear meshes [2], which opens the possibility of accurate body-fitted and/or spatially adaptive PIC simulations. The superior accuracy and efficiency properties of the scheme will be demonstrated with various numerical examples. [1] G. Chen, L. Chacón, Comput. Phys. Commun. 197, 73-87 (2015). [2] L. Chacón and G. Chen, J. Comput. Phys., 316, 578–597 (2016) [3] G. Chen, L. Chacón, and D.C. Barnes, J. Comput. Phys., 230 (18), 7018-7036 (2011).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Self-stabilized Peridynamic Correspondence Material Model

Hailong Chen*, Benjamin Spencer**

*Idaho National Laboratory, **Idaho National Laboratory

ABSTRACT

Non-Ordinary State-based Peridynamic (NOSPD) correspondence models are very useful in applying classical continuum material constitutive models to peridynamics but suffer from some practical difficulties, such as non-invertibility. This non-invertibility can be understood as existence of many possible deformations of a family that result in the same force state. As a consequence there would be many possible deformation states of the entire body for a given loading history. This has the practical effect in computations of resulting in zero-energy modes of deformation in the numerical mesh that need to be suppressed. Various remedies for zero-energy modes control are available in the literature, and these methods can be categorized into two groups: fictitious spring-force based methods and stabilized field state based methods. Although can be used to alleviate the instability due to existence of zero-energy modes, these methods do not provide resolution to the fundamental problem in correspondence formulation. Issues such as adjustment of control parameters based on material model and discretization scheme and strain/stress oscillations still exist in these stabilization schemes. In this presentation, we will present a Self-stabilized Non-Ordinary State-based Peridynamic (SNOSPD) correspondence material model based on the concept of bond-oriented reduced deformation gradient to better solve material instability issues. The proposed bond-oriented reduced deformation gradient is formulated for the purpose of accurate calculation of force state within each individual bond. The content of this presentation will be organized as follows: we will first briefly review some details on continuous deformation gradient in Continuum Theory and how the conventional peridynamic nodal deformation gradient is deduced from deformation states of a family. Following this, review of the conventional correspondence material model will be presented. Existence of zero-energy modes in NOSPD will be analytical examined. After that, details on formulation of the proposed bond-oriented reduced deformation gradient and derivation of force state will be discussed. Numerical results on various problems will be presented to establish the validity and accuracy of the proposed formulation. Discussions and conclusions are made based on comparison with other control schemes.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Numerical Investigation of Air-gun Bubble Dynamics Based on FEM

Hailong Chen*, Xiugang Lu**, Shuai Zhang***, Shiping Wang****

*Harbin Engineering University, **Harbin Engineering University, ***Harbin Engineering University, ****Harbin Engineering University

ABSTRACT

In this paper, a high pressure bubble model is built with ABAQUS software based on finite element method (FEM) to simplify the excitation process of seismic air-gun. This model is validated by comparing its predictions with the air-gun experiments in an open top tank. Numerical simulation of the air-gun bubble subjected to various boundary conditions and at different depths is carried out and discussed. The relationships between initial gas pressure and the first maximum bubble radius as well as the first period of oscillation are studied. Meanwhile, the jet dynamics and the migrating behaviors of the bubble under the effect of buoyancy are carefully investigated. This paper provides a basic understanding of the pressure field and shockwave of seismic air-gun bubble which is wildly applied to ocean seabed geophysical exploration and the shock testing of naval vessels. Keywords: Seismic air-gun, Bubble dynamics, Pressure field, Finite element method, ABAQUS

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Identification of Transient Boundary Conditions with Improved Cuckoo Search Algorithm and Polynomial Approximation

Haolong Chen*, Bo Yu**, Huanlin Zhou***, Zeng Meng****

*School of Civil Engineering, Hefei University of Technology, Hefei, P.R.China, **School of Civil Engineering, Hefei University of Technology, Hefei, P.R.China, ***School of Civil Engineering, Hefei University of Technology, Hefei, P.R.China, ****School of Civil Engineering, Hefei University of Technology, Hefei, P.R.China

ABSTRACT

The cuckoo search (CS) algorithm combined with Broyden-Fletcher-Goldfarb-Shanno (BFGS) algorithm (CS-BFGS) is proposed to identify time-dependent boundary conditions for 2-D transient heat conduction problems in functionally gradient materials. Firstly the nonlinear partial differential equation is linearized by the analog equation method. The dual reciprocity boundary element method (DRBEM) is used to solve the direct problem. Then taking the unknown boundary conditions as a polynomial function of coordinates with time-dependent coefficients, the CS-BFGS is applied to obtain the unknown coefficients of the polynomial function. As a result, the time-dependent boundary conditions are evaluated. The convergence speed of the improved CS algorithm is faster than the CS algorithm. What's more, the effect of the polynomial degree is discussed. As the polynomial degree increases, the inverse results are more accurate but the iterative number and computation time also increase. Finally, the influences of the position and number of measurement points, and random errors on the inverse results are investigated. With the measurement points closer to the boundary, with the increase of measurement point number and with the decrease of measurement errors, the results are more accurate.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Artificial Neural Network Potential for Methylammonium Lead Iodide and Lead Iodide

Hsin-An Chen*, Chun-Wei Pao**

*Research Center for Applied Sciences, Academia Sinica, Taipei, Taiwan, **Research Center for Applied Sciences, Academia Sinica, Taipei, Taiwan

ABSTRACT

Recently, organic-inorganic metal halide perovskite solar cell has attracted great attentions because of its high absorption coefficient, high power conversion efficiency (>20%, increasing rapidly), easy processing and low cost in fabrications. The most notable light-harvesting material used in the perovkite solar cell is methylammonium lead iodide (MAPbI3), which is typically synthesized from lead iodide (PbI2) and methylammonium iodide (MAI). Among all factors influencing performance of the perovskite solar cell, the surface morphology and the grain size of perovskite MAPbI3 in the cell are the most important ones, which govern the power conversion efficiency. However, the reaction mechanism for the synthesis of perovskite MAPbI3 from PbI2 is still not concluded. To elucidate the detail of the reaction mechanism, atomistic molecular simulations of the formation of MAPbI3 within PbI2 is required. However, ab initio molecular simulations are extremely time and resource-consuming and therefore not suitable for studying the MAPbI3 reaction pathways or microstructures. In the present study, we demonstrate that by utilizing tens of thousand MAPbI3 and PbI2 structures and energies from ab initio calculations as training sets, we are able to train an artificial neural network (ANN) model potential for classical molecular simulations of PbI2 and MAPbI3 perovskite systems. This ANN model potential provides good predictions in system energetics and can be used for large-scale simulations well beyond the reach of conventional ab initio calculations for studying the microstructure evolution of MAPbI3 perovskite crystals.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Performance Comparison of Nodally Integrated Galerkin Meshfree Methods and Nodally Collocated Strong Form Meshfree Methods

J. S. Chen*, Mike Hillman**

*University of California, San Diego, **The Pennsylvania State University

ABSTRACT

For a truly meshfree technique, Galerkin meshfree methods rely chiefly on nodal integration of the weak form [1]. In the case of Strong Form Collocation meshfree methods, direct collocation at the nodes can be employed [2]. In this paper, performance of these node-based Galerkin and collocation meshfree methods is compared in terms of accuracy, efficiency, and stability [3]. Considering both accuracy and efficiency, the overall effectiveness in terms of CPU time versus error is also assessed. Based on the numerical experiments, the Galerkin meshfree methods with smoothed gradients and variationally consistent integration yield the most effective solution technique, while direct collocation of the strong form at nodal locations has comparable effectiveness. References 1. Chen, J. S., Hillman, M., Rüter, M., “An Arbitrary Order Variationally Consistent Integration Method for Galerkin Meshfree Methods,” International Journal for Numerical Methods in Engineering, Vol. 95, pp. 387–418, 2013. 2. Hu, H. Y., Chen, J. S., and Hu, W., “Weighted Radial Basis Collocation Method for Boundary Value Problems,” International Journal for Numerical Methods in Engineering, Vol. 69, pp. 2736-2757, 2007. 3. Hillman, M. and Chen, J. S., Performance Comparison of Nodally Integrated Galerkin Meshfree Methods and Nodally Collocated Strong Form Meshfree Methods. Advances in Computational Plasticity, [Ed. Onate, E.], Springer, pp. 145-164, 2018.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Implicit Gradient for Numerical Solution of PDEs

J. S. Chen*, Mike Hillman**

*University of California, San Diego, **The Pennsylvania State University

ABSTRACT

Implicit gradient (IG) is expressed in an integral equation with embedded gradient consistency without explicit derivatives. It offers a paradigm for constructing approximation of function derivatives for the numerical solution of PDEs, either by using strong forms or weak forms. A straightforward application of IG is for the gradient typed regularization of ill-posed problems, such as the strain localization problems. GI can also be used to construct stabilization of convection dominated problems and as the stabilization of nodally integrated Galerkin equation. Without the need of taking directives of approximation functions, GI also offers computational efficiency for Meshfree based numerical solution of PDEs. This talk will introduce continuous and discrete GI for approximation of derivatives, discuss the gradient consistency of GI and its convergence properties in solving PDEs, and demonstrate its applications to strain localization, convection dominated problems, and modeling of damage and fracture processes in solids subjected to extreme loadings.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Wave Amplification in an Array of Open Caissons

Jiahn-Horng Chen*, Yan-Xiang Lin**, Da-Wei Chen***

*National Taiwan Ocean University, **National Taiwan Ocean University, ***National Taiwan Ocean University

ABSTRACT

Harbour resonance provides a possible way to amplify wave energy for wave energy converters (WEC) operating in regions of medium wave energy density. In the present paper, we conducted a computational study on the amplification effect for an array of cylindrical caissons with an opening of angle ?. The parameters include the distance between two adjacent caissons, the angle of caisson opening, and the amplitude and period of the incident waves. The open source code OpenFOAM was employed for all computations. The volume of fluid (VOF) method was used to capture the free surface. Both linear and nonlinear incident waves were used for upstream boundary conditions. The results show that proper combitions of these parameters can result in significant wave amplifications in the caisson. Meanwhile, the wave outside the caisson can be significantly reduced after it passes the array.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Strong-Form Formulated Generalized Displacement Control Method for Nonlinear Analysis

Jian-Yu Chen*, Judy Yang**

*National Chiao Tung University, **National Chiao Tung University

ABSTRACT

In the traditional analysis of geometric nonlinearity, the most popular method is formulated on the basis of weak-form such as the finite element method. Due to the element nature, its application is limited by the numerical integration in the governing equation and the quality control of deformed mesh. The meshfree methods have been developed and become one leading research topic in the field of computational mechanics since 1990s. In particular, the strong form collocation methods require no additional efforts to deal with numerical integration and impose Dirichlet boundary conditions, thereby making the collocation methods computationally efficient. Concerning geometric nonlinearity, how to accurately reflect the change in the slope of the load-deflection curve of the structure and remain numerically stable are of major concerns in the incremental-iterative process. As a result, we propose a strong-form formulated generalized displacement control method to analyze geometrically nonlinear problems, where the radial basis collocation method is adopted. The numerical examples demonstrate the ability of the proposed method for large deformation analysis.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Biomechanical Assessment of Femoral Neck Convex Deformity Using Patient-Specific FE Analysis

Junning Chen*, Matthew Wilson**, Tengteng Tang***, Christopher Smith****, Peter Fratzl*****, Richard Weinkamer******, Rizhi Wang*******

*Department of Engineering, University of Exeter, Exeter, United Kingdom, **Exeter Hip Unit, Royal Devon & Exeter NHS Foundation Trust, Exeter, United Kingdom, ***Department of Materials Engineering, University of British Columbia, Vancouver, BC, Canada, ****Department of Engineering, University of Exeter, Exeter, United Kingdom, *****Department of Biomaterials, Max Planck Institute of Colloids and Interfaces, 14476 Potsdam, Germany, ******Department of Biomaterials, Max Planck Institute of Colloids and Interfaces, 14476 Potsdam, Germany, *******Department of Materials Engineering, University of British Columbia, Vancouver, BC, Canada

ABSTRACT

Femoral neck convex deformity has been known as the cam type impingement in the hip joint, and has a very high prevalence in elder population. Recent research on cam-impingement has shown increasing evidence in active young adults [1]. The morphological changes near the femoral head and neck junction lead to severe pain during movement and a reduced range of motion; in the long term, it will result in osteoarthritis [1]. There has also been rising concern for its association with the increasing risk of hip fracture [2]. Hip arthroplasty was one of the most common and successful surgical procedures to provide sufficient clearance in the joint by shaving down the bony bump at the deformity, therefore improving the range of motion and reducing pain. Despite a growing interest in diagnosing and treating hip impingement, little has yet been revealed on the biomechanical effects of either deformity or surgical intervention to proximal femur integrity and fracture risk. This study aims 1) to establish a numerical framework to quantitatively assess its biomechanical changes, by combining ex vivo high resolution peripheral quantitative computed tomography (HR-pQCT) and in silico finite element analysis (FEA); and 2) to evaluate the potential surgical effects after hip arthroplasty by using patient-specific modelling technique to virtually simulate surgery outcomes. Two proximal femora were used in this study, one freshly frozen human cadaveric femur diagnosed with impingement and one control with no observed abnormality. Both samples were scanned with HR-pQCT with a voxel size of 41 μm3. The obtained images were segmented in ScanIP Ver. 7. Two patient-specific geometric models were created by an inverse engineering approach with non-uniform rational basis splines (NURBS). On the pathological model, three different extents of tissue removal were virtually performed to simulate the surgical procedure, providing three post-surgical models on the same patient profile. All five models were imported to ABAQUS Ver. 6.14 for voxel-based heterogeneous micro-FEA. Our results suggested that the convex deformity led to severe stress concentration in the local region compared to the control, indicating raised risk of fracture under impact, and a balanced surgical plan is preferred to provide the minimal joint clearance without significantly increasing the fracture risk. References [1] E. Dickenson, et al. (2015) Prevalence of Cam Hip Shape Morphology: a Systematic Review. Osteoarthritis and Cartilage. 24(6): pp. 949-961. [2] K.L. Bell, et al. (1999) Structure of the Femoral Neck in Hip Fracture: Cortical Bone Loss in the Inferoanterior to Superoposterior Axis. Journal of Bone Mineral Research. 14: pp. 111-9.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Seismic Study of a Transition Tunnel by Using Numerical Simulations

Juntao Chen*, Haitao Yu**, Yong Yuan***

*Tongji University, **Tongji University, ***Tongji University

ABSTRACT

Tunnels can be constructed by immersed, TBM, drill-and-blast, cut-and-cover, or combination of aforementioned methods. Thus, the cross-section of tunnel constructed by means of different tunneling methods is generally different. When this is the case of TBM connected with drill-and-blast directly, a transition portion is needed to accommodate the shapes of cross-section formed by the two types of tunneling methods. This paper is focused to study the seismic response of the transition tunnel connecting TBM segmental lined tunnel and drill-and-blast tunnel by conducting numerical simulations. The transition tunnel is composed of four portions including segmental lined tunnel section, segmental lined tunnel with inner, multi-lined tunnel section and drill-and-blast tunnel section. In addition, during the numerical simulation, strong earthquake motions are considered to study the damage mechanism of the tunnel structure. Based on results, the ovaling deformation and stress distribution for each tunnel section is first compared and studied; then, the influence of the change of tunnel cross-section and stiffness on the seismic response of tunnel is full analyzed; at last, the damage model of the transition tunnel under strong earthquake is discussed.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Powell–Sabin B-splines for Cohesive Fracture Analysis

Lin Chen*, René de Borst**

*University of Sheffield, **University of Sheffield

ABSTRACT

The numerical simulation of fracture is a technically relevant and scientifically challenging issue, and has been a focal point of attention since the early simulations in the 1960s. From the very beginning, two different approaches have been pursued, discrete methods in which cracks are treated as geometric discontinuities, leading to topological changes, and the distributed, or smeared approach, in which discontinuity is modelled by distributing it over a small, but finite band. For the discrete method, the cohesive zone model is often used to model fracture processes in many quasi-brittle and ductile materials, in particular when the size of the fracture process zone is non-negligible compared to the structural dimensions. It can easily be incorporated in finite element formulations (FEM), especially when the crack path is pre-defined. Over the past decades, various FEM technologies have been proposed which can achieve this, such as interface elements and embedded discontinuities. Recently, isogeometric analysis (IGA) has also been used for crack propagation [1, 2]. The crack segment is represented by the NURBS or T-spline basis functions. IGA can accurately predict the local stress field. However, NURBS and T-splines have some limitations when modelling (cohesive) fracture, and a discrete representation of a crack fails in some situations. This restriction is due to the crack segment insertion in the parameter domain and the reparameterization in the physical domain [2]. In this contribution, we employ the Powell–Sabin B-splines, which are based on triangles, to model cohesive crack propagation. The crack is introduced directly in the physical domain. Due to the use of triangles, re-meshing is more straightforward. To implement the proposed method in existing finite element programs, Bézier extraction is employed. It is ideal for adopting an element-wise point of view for crack propagation and extension. The accuracy of the approach to model free crack propagation is demonstrated by several numerical examples, including an L-shaped beam, a SEN beam, and the Nooru-Mohamed concrete panel. References [1] Verhoosel, C.V., Scott, M.A., de Borst, R.., and Hughes, T.J.R. An isogeometric approach to cohesive zone modeling. International Journal for Numerical Methods in Engineering 87: 1?5 (2011): 336-360. [2] Chen. L, Verhoosel, C.V., de Borst. R.. An isogeometric method for cohesive fracture analysis. International Journal for Numerical Methods in Engineering, submitted.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Life-time Based Design of Transmission Mechanism of Micro-positioning Stage

Min Chen*, Shunqi Zhang**, Xiang Wang***, Derrick Tate****

*Xi'an Jiaotong-Liverpool University, **Shanghai University, ***Xi'an Jiaotong-Liverpool University, ****Xi'an Jiaotong-Liverpool University

ABSTRACT

The micro-positioning driven by piezoelectric actuator is a key technology used in a broad variety of applications, like the precision manufacture, optical measurement and microsurgery. The output accuracy is mainly determined by two factors, the actuator and the transmission flexure hinges. The flexure hinges perform their function through local deformation, which tends to lead to stress concentration and fatigue failure. This paper presents a general numerical approach, namely limit and shakedown analysis, to predict the safety state of smart structures made of heterogeneous materials under unknown cyclic loadings. With the homogenization theory and finite element approach, the shakedown problem is converted to a large-scale nonlinear optimization programming. Furthermore, a general platform in with the combination of FEM and interior-point-algorithm based optimization tool is developed, which make the practical application possible.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Scan Pattern Integrated Structural Topology Optimization for Laser Powder Bed Fusion Process Based on Inherent Strain Theory

Qian Chen*, Jikai Liu**, Xuan Liang***, Albert To****

*Department of Mechanical Engineering and Material Science, University of Pittsburgh, **Department of Mechanical Engineering and Material Science, University of Pittsburgh, ***Department of Mechanical Engineering and Material Science, University of Pittsburgh, ****Department of Mechanical Engineering and Material Science, University of Pittsburgh

ABSTRACT

Inherent strain theory based fast method has recently been proposed for additive manufacturing(AM) process simulation. Inherent strain theory based topology optimization, which can significantly reduce simulation time, is now possible and has been actively explored to reduce the thermal process induced defects, such as residual distortion and stress. On the other hand, the laser sintering path dependency issue has not been considered in these optimization issues. More specifically, the extracted inherent strain for laser powder bed fusion process is sintering path dependent, which is generally larger in the raster direction than transverse direction. In fact, Optimizing the laser sintering path is an alternative solution to further reduce these thermal process induced defects. Hence, to fill the gap, a laser scan pattern integrated structural topology optimization method is proposed to address two critical problems.: 1) Scan pattern optimization for fixed geometry to minimize residual stress, and 2) Concurrent structural topology and scan pattern optimization for the same optimization purpose. The scan pattern is optimized instead of the sintering path since the EOS M290 is a closed system which has the embedded scan pattern that can only be parametrically altered. To fit the cyclic characteristic of topology optimization, full-body inherent strain method will be utilized to replace the more accurate layer-by-layer approach, and a less time-consuming one-step static analysis will be performed in each optimization loop. Anisotropic thermal expansion coefficients will be applied to the activate the inherent strain. Effectiveness of the proposed method will be proved by several numerical cases and experimental validation.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Resolving Large-scale Geophysical Flows over Unstructured Meshes: a Class of New Vorticity-Divergence Based Numerical Schemes

Qingshan Chen*, Lili Ju**, Roger Temam***

*Clemson University, **University of South Carolina, ***Indiana University Bloomington

ABSTRACT

Unstructured meshes have been gaining popularity in recent years, because they are almost free of polar singularities, and remain highly scalable even at eddy resolving resolutions. However, to unleash the full potential of these meshes, new schemes are needed. The classical C-grid scheme, which is widely popular on structured meshes, has serious issues concerning the reconstruction of the tangential velocity component. This talk presents new numerical schemes based on an old idea, namely the collocated vorticity-divergence formulation (so-called Z-grid), for large-scale geophysical flows on unstructured centroidal Voronoi meshes. Using the finite-volume discretization technique, the schemes conserve the mass and the absolute vorticity locally, and the potential enstrophy globally. It is also shown that, in an area-averaged sense, the schemes reproduce the Lagrangian transport property for potential vorticity, which is fundamental to the understanding of the dynamics of large-scale geophysical flows. A major challenge of vorticity-divergence based numerical schemes is the specification of the boundary conditions for the PDEs. The current project adopts a hybrid approach that combines explicit and implicit implementations of the boundary conditions on the streamfunction and the velocity potential. This talk will go over the analytical and practical aspects of the schemes, and finish with some high-resolution numerical results.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Dynamic Analysis for Parallel Stabilized Platform

Qunkai Chen*, Chenliang Li**, Yuefa Zhou***

*College of Aerospace Engineering and Civil Engineering, Harbin Engineering University, Room 2035, Building 11, No.145, Nantong Street, Nan gang District, 150001 Harbin, Heilongjiang Province, P.R. China, **College of Aerospace Engineering and Civil Engineering, Harbin Engineering University, Room 2035, Building 11, No.145, Nantong Street, Nan gang District, 150001 Harbin, Heilongjiang Province, P.R. China, ***College of Aerospace Engineering and Civil Engineering, Harbin Engineering University, Room 2035, Building 11, No.145, Nantong Street, Nan gang District, 150001 Harbin, Heilongjiang Province, P.R. China

ABSTRACT

This paper studies on the multi-degree of freedom electro –hydraulic hybrid stabilized platform, which is consisting of up platform and lower platform. Both of them are the six-DOF parallel platform supported by six extensible links (Stewart platform). The function of lower platform is to simulate yawing, rolling and pitching motions, and the function of up platform can be utilized as stabilized platform to isolate the disturbance, to keep parallel to the horizontal plane or track certain target. Kinematics and dynamics of this structure are analyzed. The inverse kinematics of multi-degree of freedom electro –hydraulic hybrid stabilized platform are analyzed in this paper, and the inverse dynamics equation of multi-degree of freedom electro –hydraulic hybrid stabilized platform are studied by Kane formulation. ; using the software program of MATLAB to the motion model for motion simulation and dynamic simulation and draw simulation graphs, and through analyzing and summarizing, draw conclusions. Meanwhile the driving forces-time results from MATLAB are compared with the results form ADAMS software, which verify the correctness of this approach. The results obtained would be useful for the design and analysis of practical manufacture.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Implementation of Anisotropic Cam Clay Model into Abaqus and Its Application to Cavity Expansion Problem

Shengli Chen*, Kai Liu**

*LOUISIANA STATE UNIVERSITY, **LOUISIANA STATE UNIVERSITY

ABSTRACT

Dafalias' (1987) anisotropic Cam Clay model, based strictly on the critical state concept, is one of the most widely used anisotropic elastoplastic constitutive models for clays, attributed mainly to its relative simplicity, yet still capable of capturing the essential features of the anisotropic soil behaviour. This paper develops an implicit integration algorithm for the anisotropic Cam Clay soil model, using the standard return mapping approach (elastic predictor-plastic corrector), to obtain the updated stresses for the given strain increments. It is found that the formulation of the constitutive integration involves essentially 19 simultaneous equations, which contains 6 stresses ?_ij, 6 plastic strain increments ?d??_ij^p, and 7 state variables ?_ij and p_c^ ' as the unknowns to be solved for. The integration algorithm for the anisotropic Cam Clay model is implemented into the finite element analysis commercial program, ABAQUS, through the material interface of UMAT (user defined material subroutine), and then used for the analysis of the fundamental cavity expansion problem. The predictions from the ABAQUS simulations are generally in excellent agreement with the available analytical solutions, thus demonstrating the accuracy and robustness of the proposed integration scheme.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Discontinuous Galerkin/Cohesive Zone Approach for Impact Failure Analyses of Automotive Laminated Glass

Shunhua Chen*, Naoto Mitsume**, Wei Gao***, Tomonori Yamada****, Mengyan Zang*****, Shinobu Yoshimura******

*The University of Tokyo, **The University of Tokyo, ***Guangdong University of Technology, ****The University of Tokyo, *****South China University of Technology, ******The University of Tokyo

ABSTRACT

Automotive laminated glass is a simple sandwiched composite structure, which is comprised of two soda-lime glass sheets bonded by one plastic interlayer, polyvinyl butyral (PVB). It is considered to be a safety component of a vehicle because of its excellent performance in absorbing impact energy and bonding glass fragments. Meanwhile, the impact failure patterns of an automotive windshield glazing contribute to traffic accident reconstruction. The purpose of this work is to develop a discontinuous Galerkin(DG)/cohesive zone approach for the impact failure, including glass cracking and possible debonding, of laminated glass. This approach models inter-element failure by switching the interface constraints from a DG formulation to an extrinsic cohesive expression, which is able to get rid of the so-called artificial compliance and time discontinuity problems existing in cohesive zone models, while being quite scalable for parallel computing. A laminated glass finite element model is proposed, which allows for the use of non-matching finite element meshes for adhesion modeling between glass and PVB, and gradual coarsening glass meshes for the areas away from the impact zone, and thus to reduce computational cost. In order to better capture the impact force history, the cohesive strengths in the impact zone are determined by a glass strength distribution considering initial flaws[1]. However, for the other areas where the crack behaviors have relatively small influences on the impact force history, the cohesive strengths are artificially adjusted so as to satisfy the minimum mesh size requirements in the context of cohesive zone modeling. Finally, the impact fracture behavior of a laminated glass plate is simulated. The effectiveness of the developed computational approach is validated by comparing the numerical results with the experimental ones[2] in terms of crack velocity history and cracking sequence. The impact cracking mechanism of a laminated glass plate is thoroughly discussed as well. Reference: [1] Alter, Christian, Stefan Kolling, and Jens Schneider. "An enhanced non-local failure criterion for laminated glass under low velocity impact. " International Journal of Impact Engineering 109 (2017): 342-353. [2] Xiaoqing Xu, Jun Xu, Jingjing Chen et al. "Investigation of dynamic multi-cracking behavior in PVB laminated glass plates. " International Journal of Impact Engineering 100 (2017): 62-74.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Efficient Meshfree Method for Additive Manufacturing Process

Songtao Chen*, Qinglin Duan**, Yining Wang***, Shuhui Li****

*Department of Engineering Mechanics, Dalian University of Technology, **Department of Engineering Mechanics, Dalian University of Technology, ***Department of Engineering Mechanics, Dalian University of Technology, ****Department of Engineering Mechanics, Dalian University of Technology

ABSTRACT

Additive manufacturing (AM) is an advanced model-free manufacturing technology by means of the layered deposition of materials and in recent years it attracts intensive attentions. The metal additive manufacturing process induced high temperature gradient due to the non-uniform heat input which would detrimentally affect the microstructure, material properties, residual stress, and distortion. Therefore, the thermal history of metal additive manufacturing is significant in predicting the quality of component. Recently, many FEM models have been established to investigate thermal behavior during AM. For example, Denlinger et al. [1] developed a three-dimensional finite element model for the prediction of temperature, residual stress, and distortion in multi-layer Laser Powder-Bed Fusion builds. However, the temperature gradient around the molten pool is very high and fluctuates violently and FEM (usually only linear approximation is employed) is difficult to describe such high gradients accurately. Furthermore, the size of heat affected zone (only several tens of microns) is very small compared to the entire component. However, FEM is inconvenient to implement local refinement whereas uniform grids lead to high computational cost. Meshfree methods, such as the element-free Galerkin (EFG) method [2], possess apparent advantages in constructing high order approximation and adaptive refinement (or coarsening) since construction of meshfree approximation is only dependent on a set of scattered nodes, instead of a mesh. Especially, Duan et al. [3] developed an improved EFG method by correcting nodal derivatives at quadrature points based on the Hu-Washizu three-field variational principle. This method remarkably reduces the number of quadrature points for high order approximation and significantly improves computational efficiency. It is named as consistent element-free Galerkin (CEFG) method since it is able to exactly pass patch tests in a consistent manner. In this work, application of the CEFG method to simulate additive manufacturing process is presented. By making full use of the merit of meshfree approximation, “mesh” coarsening is conveniently and adaptively employed in regions far from current manufacturing layer. This reduces the scale of the computation and accelerates the simulation tremendously. Numerical results also demonstrate that the proposed method is able to simulate the evolution of the thermal fields in additive manufacturing process.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Topology Optimization for Twist Chirality of Materials Induced by Axial Strain

Wei Chen*, Xiaodong Huang**

*Swinburne University of Technology, **Swinburne University of Technology

ABSTRACT

An object or system is chiral if it is distinguishable from its mirror image. The chirality is widely observed in biological materials and structures. Artificial chiral structures inspired by natural materials have also demonstrated significant applications in industry. With growing interest in chiral material design, most of the research work follows the traditional trail-and-error approach. To achieve the chirality of materials, a systematic design method, e.g., utilizing topology optimization technique, has never been reported. In this paper we propose a systematic topology optimization method on designing materials of tubes or beams exhibiting the twist chirality under the axial strain. Such a twist chirality of the structure has many potential applications. The optimization objective is to maximize the twist angle of a structure constructed by optimally designing microstructures of cellular or composite materials. The proposed two-scale topology optimization problem is solved by the extended bi-directional evolutionary structural optimization (BESO) method. The results show that various topological patterns of microstructures are achieved and the resulting structures exhibit the desirable twist chirality. However, the twist chirality of the structure somewhat depend on the size of the material unit cell. Numerical analysis indicates that, with the decrease of the unit cell size, the twist angle of structures gradually increases or decreases and finally approaches its bound, which corresponds to the one obtained by the proposed topology optimization.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Design Optimization of Underwater Acoustic Anechoic Layers Under Set Frequency Bands

Wenjiong Chen*, Chenjing Ren**, Shutian Liu***

*Dalian University of Technology, **Dalian University of Technology, ***Dalian University of Technology

ABSTRACT

Thin rubber layers with air-filled cavities can be used as anechoic submarine coatings. The size and shape of the air-filled cavity (i.e the hole structure) are have greatly influence upon the acoustic performance of the underwater sound absorption coatings. In this paper, a methodology is proposed for designing the hole structure for maximizing the acoustic absorption of the underwater acoustic anechoic layers under set frequency bands. The acoustic cavity structure is separated into several cylindrical channel structures with gradient inner diameters. Therefore, based on the one-dimensional physical model of uniform cylindrical channel, the equivalent parameters (equivalent density and equivalent modulus) each sound absorption layer can be obtained. Then, the sound absorption performance of composite-gradient absorptive coating is calculated by the transfer matrix method. Moreover, the influence of structural parameters and material parameters on the sound absorption performance of the coating is discussed. Finally, the genetic algorithm is employed to optimize the hole structure for maximizing the sound absorption coefficient in specific frequency bands. Utilizing the constructed optimization model, the parameters of hole structure are derived with optimal sound absorption under the set frequency bands, which is a helpful guidance on the design of anechoic coatings.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Numerical Simulation of Water Entry of Three-dimensional Oblique Cylinder by MPSGPU-SJTU

Xiang Chen*, Decheng Wan**

*Shanghai Jiao Tong University, **Shanghai Jiao Tong University

ABSTRACT

Water entry is a very complex flow problem in the naval architecture and ocean engineering, which always accompanies with the slamming, the large deformation of free surface and moving boundary. Thus, numerically simulating water entry is a challenging task of researchers. In the present work, the moving particle semi-implicit method (MPS), a fully Lagrangian particle method for incompressible fluid, is used to simulate this problem. However, most previous researches of our group focus on two-dimensional water entry problems because of huge computation time on CPU. GPU parallel acceleration technique widely used in scientific calculations is applied to improve computational efficiency of MPS. In addition, the motion function of multi-degree of freedom (multi-DOF) is developed for real three-dimensional water entry problem. In this paper, the cylinder model with an oblique angle of 35° is the same as experimental model by Sun et al. in 2015. The cylinder vertically enters the still water with an initial velocity of 1.92 m/s. The motions of surge, heave and pitch are free. The simulation of whole process is carried out by our in-house slover MPSGPU-SJTU, which is developed on improved MPS and GPU acceleration technique. In the previous work by Tang et al. in 2016, only half of computational domain is simulated due to the symmetry of this problem. Because of the improvement of computational efficiency, the whole computational domain is built to capture more details of fluid flied in this work. By GPU calculation, the motions of cylinder are accurately predicted. And details of pressure field and free surface deformation can be observed by GPU simulation. The numerical results show a good agreement with the corresponding experimental data and SPH results. In addition, the computation times of one hundred steps between GPU and CPU is compared. These comparisons show that MPS method coupling with GPU acceleration technique is feasible and faster for the direct numerical study of multi-DOF three-dimensional water entry problem.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Fully Implicit NS Solver for Thermo-Chemical Non-equilibrium Flow Using GMRES Algorithm

Xianliang Chen*, Song Fu**

*School of Aerospace Engineering, Tsinghua University, Beijing, 100084, China, **School of Aerospace Engineering, Tsinghua University, Beijing, 100084, China

ABSTRACT

A significant characteristic of hypersonic flow is the steeply rising temperature within field as Mach number increases. Extremely high temperature of air will excite vibrational energy internally within molecules and cause dissociation and even ionization within the gas[1], leading to considerable deviations from conventional calorically-perfect gas assumption. Meanwhile, thermal and chemical equilibrium of air cannot be reached everywhere, especially behind shocks, due to the finite rate of energy relaxation and reaction, thus a wide variety of non-equilibrium models are developed in the pursuit of more appropriate simulations of hypersonic flow. The increase of complexity in models and difficulty in numerical treatment results in greatly increased computing time and memory, therefore efficient non-equilibrium solver is expected. In this paper, iterative method GMRES(Generalized Minimum RESidual) is introduced as time-stepping method in thermo-chemical non-equilibrium flow, leading to a fast, robust Navier-Stokes solver. LUSGS(Lower-Upper Symmetric Gauss-Seidel) method is used as preconditioner to utilize the advantage of its robustness and low-memory requirement[2]. The numerical results obtained indicate that the efficiency of implicit stepping outperforms explicit counterparts in orders because of the great numerical stiffness of vibrational and chemical source terms. Within implicit methods, the combination of GMRES and LUSGS still results in acceleration of convergence compared to LUSGS alone. Key words: Non-equilibrium Flow, GMRES REFERENCE [1] Anderson J D. Hypersonic and High-Temperature Gas Dynamics, Second Edition[M]. McGraw-Hill, 2006. [2] Hong L, Baum J D, Löhner R. A Fast, Matrix-free Implicit Method for Compressible Flows on Unstructured Grids[J]. Journal of Computational Physics, 1998, 146(2):73-78.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Numerical Analysis on the Buckling, Postbuckling and Delamination Growth of Variable Angle Tow Composite Plates with Delamination Using Cohesive Zone Model

Xiaodong Chen*, Zhangming Wu**, Guojun Nie***, Wuxiang Liu****

*Tongji University, **Cardiff University, ***Tongji University, ****Tongji University

ABSTRACT

Variable angle tow (VAT) composite plates have been made possible by using advanced automated fibre placement (AFP) technology. Such designs have shown considerable freedom in stiffness tailoring to exploit the enhanced performance for lightweight composite plates or structures. Unfortunately, VAT composite plates are not immune to the occurrence of delamination, which may lead to the undesirable loss of both stiffness and strength. In the present study, the compressive behavior of VAT composite plates with delamination damage was numerically evaluated to explore the complex mechanisms of interaction between postbuckling and delamination growth. Both through-the-width and embedded delaminations involved in composite laminates are constructed in the numerical simulation. A three-dimensional solid element is employed to discretize the VAT composite plate, and the bonded interface where delamination is expected to propagate is modelled by using an in-house cohesive element available in Abaqus software. The cohesive element has a bilinear constitutive relationship in terms of traction and separation, which allows modelling of progressive damage and failure in cohesive layers. Within the framework based on the continuum damage mechanics, both delamination initiation and growth occurred in VAT composite plates are predicted. Numerical results obtained using FEA incorporated with the progressive damage model are compared with those in existing literatures and a good agreement between them is found. Effects of the pre-existing delamination and varying fibre orientation angles on the buckling, postbuckling and delamination growth of VAT composite plates are thoroughly investigated in numerical examples. It is shown that the compressive strength of delaminated composite plates is significantly affected by the delamination growth during the postbuckling process. The numerical study also shows that the residual buckling resistance of delaminated composite plates can be significantly improved through using the VAT design concept. In addition, the mechanism of taking advantages of VAT laminates to improve both buckling and postbuckling properties of delaminated composite plates is studied in details. This research provides preliminary fundamentals for the designers to perform the damage tolerance design of VAT composite structures.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Development of an Integrated 1D-0D Simulation System with Functions of 3D Modeling & Visualization

Yan Chen*, Masaharu Kobayashi**, Changyoung Yuhn***, Hao Zhang****, Marie Oshima*****

*Graduate School of Interdisciplinary Information Studies, The University of Tokyo, **Graduate School of Interdisciplinary Information Studies, The University of Tokyo, ***Department of Mechanical Engineering, The University of Tokyo, ****Department of Mechanical Engineering, The University of Tokyo, *****Institute of Industrial Science / Graduate School of Interdisciplinary Information Studies, The University of Tokyo

ABSTRACT

To evaluate the effects of surgery and predict changes in the flow distribution afterwards, we have been developing a patient-specific 1D-0D blood flow simulation system. When the postoperative effects are examined, the global circulatory system must be considered in order to emulate alteration of blood flow after surgery [1]. Although a 3D simulation can provide information about local blood flow, the 1D-0D simulation reflects the changes in the global cardiovascular system with much more reasonable costs than the 3D simulation. On the contrary, since there is no 3D geometry information presented in 1D-0D simulation, it is difficult to grasp the 3 dimensional behavior of blood flow. Therefore, we developed modules for geometric modeling and visualization based on V-modeler [2], which is in-house 3D-modeling and visualization system in order to visualize the blood flow by dynamically mapping the simulation results onto a 3D surface model of large arteries in the cardiovascular system. To construct the visualization module, we used both patient-specific geometry data, which are acquired from patient-specific medical images, and statistic geometry data. We applied a method of deformable model so as to connect 1D simulation results of patient-specific parts with 0D ones of statistic parts in order to represent the physiological characteristics of global blood flow. In addition, we have also developed a method to change geometry interactively to mimic a surgery such as CAS (Carotid artery stenting). For instance, it enables users to create new geometry by changing the radii of vessel geometry, and send the information on the new geometry as input data to the simulation. As the result, the present methods on 3D modeling and visualization enables the 1D-0D simulation to be displayed with dynamic 3D information. Reference [1] Zhang, H., N. Fujiwara, M. Kobayashi, S. Yamada, F. Liang, S. Takagi, and M. Oshima. Development of a Numerical Method for Patient-Specific Cerebral Circulation Using 1D-0D Simulation of the Entire Cardiovascular System with SPECT Data. 44:2363, 2016. [2] Kobayashi, M., K. Hoshina, S. Yamamoto, Y. Nemoto, T. Akai, K. Shigematsu, T. Watanabe, M. Oshima. Development of an Image-Based Modeling System to Investigate Evolutional Geometric Changes of a Stent Graft in an Abdominal Aortic Aneurysm. Circulation advpub, 2015.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Mechanics of Cancer Cell Cluster Passage Through Micro-constrictions

Yeng-Long Chen*

*Academia Sinica

ABSTRACT

Cancer cells and clusters may be able to enter and exit through micro-constrictions in the blood vessels during the metastatic stage. The constrictions could be more than an order of magnitude smaller than the clusters, which begs the question of how the passage occurs. The extravasation process involves severe cell deformation and sufficiently strong inter-cell adhesion during the contraction flow. Using advanced modeling that couples fluid flow, cell mechanics, and inter-cell adhesion, we investigated the mechanics of how cell clusters are able to traverse a much smaller capillary. We found that depending on the inter-cellular adhesion, the cluster could become stuck, pass through intact, or break up during passage [1]. The model predictions capture the qualitative behavior of cancer cell cluster passage through microfluidic constrictions, suggesting possible pathway for future treatments.
[1] S.H. Au, B.D. Storey, J.C. Moore, Q. Tang,Y.L. Chen, S. Javaid, A.F. Sarioglu, R. J. Sullivan, M.W. Madden, R. O'Keefe, D.M. Langenau, D.A. Haber, S. Maheswaran, S.L. Stott and M. Toner* (2016) Clusters of circulating tumor cells traverse capillary-sized vessels, Proc. Natl. Acad. Sci. U.S.A. 113, 4947

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Full Atomic Modeling of the Parathyroid Hormone/parathyroid Hormone-related Protein Type 1 Receptor and Its Ligand Binding

Yi-Hsiang Chen*, Shu-Wei Chang**, Chuin-Shan Chen***

*National Taiwan University, **National Taiwan University, ***National Taiwan University

ABSTRACT

Parathyroid hormone/parathyroid hormone-related protein type 1 receptor, known as PTHR1, is a class B G protein-coupled receptor. It has been considered as a drug target for bone-related diseases, such as Eiken syndrome, Hypoparathyroidism and Osteoporosis. Binding of the PTHR1 and its ligands, parathyroid hormone (PTH) and parathyroid hormone-related protein (PTHrP), leads to the conformational change of PTHR1 transferring the signal for crucial biochemical reactions such as blood calcium ion balance, bone turnover regulation and skeletal development. The abnormal PTHR1, mutated in certain critical sequences, results in many diseases, such as Blomstrand's lethal chondroplasia, Ollier's disease, Jansen's metaphyseal chondroplasia and Brachydactyl type E. However, the structure of the transmembrane domain of PTHR1 and how the ligand alters the structure of PTHR1 are still unclear. Understanding these molecular mechanisms will help enable possible treatments for the receptor/hormone related diseases. In this study, we combine homology modeling and molecular dynamics simulations to investigate the structure of full length PTHR1. We use the crystal structures of glucagon receptor and corticotropin-releasing factor receptor 1 as templates to create the homology model of PTHR1. The full atomistic model of the PTHR1 is compared with the class A receptors and two available class B receptors. The intramolecular interactions and structural features of the PTHR1 are analyzed to provide fundamental insights into the structure of the PTHR1. Furthermore, we use molecular dynamics simulations to investigate the interactions between the PTHR1 and the native ligands including PTH and PTHrP. The intermolecular hydrogen bonds, binding sites, binding affinity, and conformational changes of PTHR1 are analyzed. In the last part, we investigate the effects of three types of mutations which have been found on PTHR1/PTHrP, including (a) extracellular domain mutations: P132L (Blomstrand's lethal Chondroplasia and Familial primary failure of tooth eruption), R150C (Ollier's disease) and R174C (Familial primary failure of tooth eruption); (b) transmembrane domain mutations: H223R, T410P and I458R (all related to Jansen's metaphyseal chondroplasia); (c) PTHrP mutations, L8P and L24P (both related to Brachydactyl type E). This study provides an effective framework to understand the structure of class B G-Protein coupled receptors. The model is in a good agreement with previous experimental studies. The results of the structure of PTHR1, the binding mechanism of its ligands and the molecular origin of receptor related mutations provide molecular insights into receptor-related diseases and could enable the design of novel drugs.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Stiffness Thresholds of Carbon Nanotube Networks

Yuli Chen*, Fei Pan**

*Institute of Solid Mechanics, Beihang University, **Institute of Solid Mechanics, Beihang University

ABSTRACT

For carbon nanotube (CNT) networks (CNTNs), with increasing network density, there may be sudden changes in the properties, such as the sudden change in electrical conductivity at the electrical percolation threshold. In this work, the stiffness of CNTNs is studied and especially the existence of stiffness thresholds are revealed. Two critical network densities divide the stiffness behavior into three stages: zero stiffness, bending dominated and stretching dominated stages. The first critical network density is a criterion to judge whether or not the network is capable of carrying load, defined as the stiffness threshold. The second critical network density is a criterion to measure whether or not most of the CNTs in network are utilized effectively to carry load, defined as bending-stretching transitional threshold. Both thresholds are found to be intrinsic features of CNTNs, independent of loading conditions. Based on the geometric probability analysis, a theoretical methodology is developed to predict the two thresholds and explain their underlying mechanisms, and a simple piecewise expression is summarized to describe the stiffness of CNT networks, in which the relative stiffness of networks depends only on the relative network density and the CNT aspect ratio. Based on the two stiffness thresholds, the out-of-plane bending of film-like CNTNs is studied. The pure bending of CNTNs consists of two types of deformation, the out-of-plane deformation and the in-plane deformation, which both contribute to the bending stiffness. The bending stiffness presents a four-stage regime with the network density, which is divided by the electrical percolation threshold and two stiffness thresholds. Using the energy theorems and superposition method, a simple piecewise analytical expression for bending stiffness is proposed. This work provides a solid theoretical foundation for the design and property prediction of CNTNs, and the method and results can also be extended to other networks constructed by nanotubes and nanowires. Reference [1] Chen Y, Pan F, Guo Z, et al. Stiffness threshold of randomly distributed carbon nanotube networks [J]. J Mech Phys Solids, 2015, 84.395-423. [2] Pan F, Chen Y, Qin Q. Stiffness thresholds of buckypapers under arbitrary loads [J]. Mech Mater, 2016, 96. 151-68. [3] Pan F, Chen Y, Liu Y, et al. Out-of-plane bending of carbon nanotube films [J]. Int J Solids Struct, 2017, 106–107: 183-199.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Adaptive Time-stepping Algorithm for Simulating Snap-through Instability in Bistable Structures

Zi Chen*, Yin Liu**, Guangchao Wan***

*Thayer School of Engineering, Dartmouth College, Hanover, NH 03755, USA, **Thayer School of Engineering, Dartmouth College, Hanover, NH 03755, USA, ***Thayer School of Engineering, Dartmouth College, Hanover, NH 03755, USA

ABSTRACT

Snap-through instability, typically featuring a rapid shape transition, has been found useful in a wide range of natural and engineered structures, such as the Venus flytrap and bistable composites. The snap-through behaviors have a common feature in that the time scale of the deformation is much smaller than that in other deformation stages, which brings challenges for numerical simulations, such as intensive computation induced by the usage of extremely small size of time step and numerical divergence arising from large shape change in a very short time. In this talk, we will introduce nonlinear dynamical finite element (FE) computational framework for efficiently capturing the shape evolution of structures with snap-through instability. The nonlinear dynamical FE equations are first discretized in the time domain based on the Newmark scheme. Next, unlike the traditional time-stepping scheme where a fixed value (or the range) of time step is required before simulation, both the displacement and time increments are introduced as unknowns in the incremental FE formulations, and an arc-length equation, related to the total displacement increment is introduced to complete the equation system. In the algorithm, the time-step size can be automatically adjusted based on the prescribed arc-length and the displacement increment, which permits the usage of large time-step sizes for slow deformation and small time-step sizes for fast deformation. Furthermore, we will introduce several numerical examples involving snap-through instability, including a 2D simply-supported pre-buckled beam and a 3D bistable trilayer composite shell, which demonstrate that the algorithm can efficiently simulate dynamical snap-through behaviors with automatic adjustment of the time-step size.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

3D Numerical Simulation of the Chip Geometry during Machining

Kévin Chenegrin*, Eric Feulvarch**, Habib Karaouni***, Mathieu Girinon****, Frédéric Valiorgue*****

*Univ. Lyon, ENISE, LTDS, UMR 5513 CNRS - SAFRAN Tech, **Univ. Lyon, ENISE, LTDS, UMR 5513 CNRS, ***SAFRAN Tech, ****CETIM, *****Univ. Lyon, ENISE, LTDS, UMR 5513 CNRS

ABSTRACT

This work focuses on the development of a 3D finite element model simulating a turning operation in the thermal and mechanical steady state. It is based on the work of Girinon et al. [1] which proposed an approach based on a Eulerian formulation which allows representing the material flow without the need for simulating the transient step (chip formation and element damaging). This modelling makes it possible to know temperature distribution in the chip, the machined part, the tool and tool-holder. This numerical simulation has been successfully applied for the computation of residual stresses during a drilling operation [2]. Unfortunately, such an approach needs to know the geometry of the chip that can be obtained from experimental Quick Stop Tests (QST). The objective of this communication is to propose a numerical technique avoiding experiments by computing the quasi-stationary geometry of the chip in 3D in a Eulerian Framework with the software SYSWELD. The chip geometry is compared to experimental observations for a turning operation. [1] M. Girinon, F. Valiorgue, V. Robin, and E. Feulvarch, 3D stationary simulation of a turning operation with an Eulerian approach, Appl. Therm. Eng., vol. 76, pp. 134-146, (2015). [2] M. Girinon, F. Valiorgue, H. Karaouni, and E. Feulvarch, 3D numerical simulation of drilling residual stresses, Comptes Rendus Mecanique, in press, (2018).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

FEM-Cluster Based Reduction Method for Efficient Numerical Prediction of Effective Properties of Heterogeneous Materials

Gengdong Cheng*, Xikui Li**, Yinghao Nie***, Hengyang Li****

*Dalian University of Technology, **Dalian University of Technology, ***Dalian University of Technology, ****Dalian University of Technology

ABSTRACT

A novel FEM-Cluster reduced order method which enables efficient numerical prediction of effective properties of heterogeneous material in nonlinear range is proposed. The cluster concept initially presented in the work by WK Liu et al [1] is introduced and extended to derive a full FEM multi-scale formulation of the Representative Unit Cell (RUC) to circumvent the heavy computational burden required for a direct numerical simulation (DNS) of the high-fidelity RUC. The proposed method is formulated in a consistent framework of finite element method. It provides a two-phases, comprising the offline and the online phases, numerical algorithm for predicting effective nonlinear mechanical properties of heterogeneous materials. The basic theory of RUC is introduced and the finite element implementation of the RUC subjected to given periodic homogeneous displacement boundary condition and the uniformly distributed eigen-strain over the RUC is described. The reduced order model is built up at the offline phase. It consists of clustering process and construction of the cluster-interaction matrix under the assumption of the linear elasticity. In the clustering process, the RUC is divided into a number of the clusters according to values of elemental strain concentration factors, which are obtained from full FEM analysis of the high-fidelity RUC. The RUC is subjected to periodic homogeneous boundary condition and one component of the uniformly distributed eigen-strain vector over the RUC one by one in turn, by k-means clustering. The cluster interaction matrix is constructed with numerical results of the DNS subjected to uniform eigen-strain for each cluster in turn. It represents the interactions between each two arbitrary clusters in the RUC in terms of the uniformly distributed eigen-strain over one cluster and the average stress over another cluster. Its mathematical structures and physical properties are discussed. The online elasto-plastic phase of the reduced order model is performed by the incremental non-linear FE analysis using the constant cluster-interaction matrix, which plays a role in the present work conceptually similar to the initial elastic modular matrix used in the "initial stiffness method" for the traditional incremental elasto-plastic analysis. By doing so, accurate and efficient numerical prediction of effective properties of heterogeneous material in nonlinear range are fulfilled in a consistent way. The performances of the proposed reduced order model and its numerical implementation are studied and demonstrated by several numerical examples. Reference [1] Zeliang Liu, M.A. Bessa, Wing Kam Liu. Comput. Methods Appl. Mech. Engrg. 306 (2016) 319–341.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Efficient Numerical Ice Sheet Simulations over Long Time Spans

Gong Cheng*, Lina von Sydow**, Per Lötstedt***

*Uppsala University, **Uppsala University, ***Uppsala University

ABSTRACT

The full-Stokes models to palaeo-ice sheet simulations have previously been highly impractical due to the requirement on the mesh resolution close to the grounding-line. We propose and implement a new sub-grid method for grounding-line migration in full Stokes equations with equidistant mesh. The beauty of this work is to avoid remeshing when the grounding-line moves from one steady state to another. A new boundary condition is introduced to accommodate the discontinuity in the physical and numerical model. The method is implemented in Elmer/ICE that solves the full Stokes equation with the finite element method. The convergence of the sub-grid method is examined as the mesh is refining and the results are compared with MISMIP benchmark.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Multiscale Mechanical Modeling of Damage Behavior in Drilling of Unidirectional CFRP with Thermo-mechanical Coupling

Hui Cheng*, KunPeng Du**

*Northwestern Polytechnical University, **AVIC Xi'an Aircraft Industry (Group) Company LTD

ABSTRACT

Drilling is one of the most common machining methods for unidirectional carbon fiber-reinforced polymer (UD CFRP) structure, which is a complex thermal-mechanically coupled process. To reveal the deformation mechanism and damage behavior in UD CFRP drilling, a multiscale mechanical modeling for UD CFRP drilling with thermal-mechanical coupling is demonstrated in this paper. which captures the failure modes for fibers, matrix and the interface based on a micro-level RVE and the delamination between different layers in macro-level simulation. Failure models for the fiber, matrix and interface region are applied depending on the material properties of each of these three phases in micro-scale. A modified cohesive element model which can avoid the excessive element distortion in dynamic simulation and propagate the heat is also developed to represent the delamination in macro-scale. Numerical simulations based on the above model with different fiber orientations were performed to predict the damage behaviors. Drilling tests with the conditions as considered in the simulations were carried out to validate the multiscale mechanical modeling. Drilling force get by sensors and damage model measured by scanning electron microscope can match well with the simulation.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Ultrasonic Properties of Polymer Composites with Particle Inclusions

Jian Cheng*, Zhanli Liu**, Zhuo Zhuang***

*Tsinghua University, **Tsinghua University, ***Tsinghua University

ABSTRACT

Glass particles / polyurea composites have great anti-ultrasonic performance and improve a lot at high strain rate / frequency. In order to simulate high strain rate / frequency conditions, many researchers use ultrasonic technology to determine the properties of composite materials, which can easily achieve high-frequency input. In this study, the dynamic mechanical properties of glass particles / polyurea composites were systematically studied by means of ultrasonic test platform, and the glass microspheres were changed to SiO2 nano-particles to observe the performance changes. In addition, a computational model based on random distribution inclusions was established to calculate the mechanical properties of the corresponding composites. The main contributions were as follows: (1) The high-frequency ultrasonic attenuation performance test platform of composite materials was established; (2) The ultrasonic attention properties of glass particles / polyurea composites and SiO2 nano-inclusions / polyurea composites were measured at different frequencies; (3) A computational model for predicting the dynamic mechanical properties of glass inclusions / polyurea composites was established. The experimental platform and calculation model for ultrasonic attenuation performance analysis were established, and several samples were tested and calculated. It can be found that the attenuation coefficient of the polyurea and composites increased rapidly with the increase of the input frequency, and the attenuation performance with the glass inclusions was better than that of the composites with nano-particles. The attenuation performance of the composites with glass inclusions can be increased by 10% (2.5MHz) to 14% (1.5MHz), compared to pure polyurea. The complex modulus also behaved the same law, and the loss modulus was sensitive to the frequency change, and the storage modulus was kept constant. In the calculation, we also found that for the specific sample and input frequency, the composites with higher volume fraction of glass microspheres and the larger inclusion diameter have the better attenuation performance.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Delayed Unstable Expansion of a Gel Balloon

Jian Cheng*, Zheng Jia**, Teng Li***

*University of Maryland College Park, **Zhejiang University, ***University of Maryland College Park

ABSTRACT

The loss of stability, i.e. the burst is commonly observed during the inflation of a rubber balloon. The sudden change in size happens instantaneously once the applied pressure reaches a critical value. However, the inflation of a hydrogel balloon deviates from its better-understood rubber counterpart. In this paper, we demonstrate that when a gel balloon is subject to a pressure even less than the critical value for instantaneous burst, solvent molecules diffuse into the gel network, dilute, and effectively weaken the polymeric network. A hydrogel balloon undergoes a slow and continuous evolution of swollen states. Depending on the material properties and applied pressure the swelling process may either carry the gel balloon to a final equilibrium state, or continues infinitely and eventually results in a sudden burst. We further provide a phase diagram which divides the response of a gel balloon into 3 categories: instantaneous burst, delayed burst, and steady growth, based on the given material properties and applied pressure.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Open Source Package of High Performance Immersed Finite Element Method (IFEM) for Fluid-Structure Interactions

Jie Cheng*, Lucy Zhang**

*Rensselaer Polytechnic Institute, **Rensselaer Polytechnic Institute

ABSTRACT

In this talk, we present a successful refactoring of our existing code, the immersed finite element method (IFEM) and its derivatives, the modified IFEM (mIFEM) for fluid-structure interaction analysis. The algorithm is originally based on the immersed concept, i.e., solid mesh is immersed in the fluid, and the interaction between fluid and solid relies on interpolation between grids. The mIFEM takes advantage of the immersed concept of no-remeshing for the computational domain, and further develops on a volumetric weak form basis where the fluid and the solid solvers can function and evaluate their own dynamics independently. In this work, we utilize open source packages intensively for both the fluid and the solid solvers: the standard finite element ingredients are handled by deal.II, the parallel linear algebra is dealt with by PETSc, the mesh partition relies on p4est, the building process is generated by CMake for cross-platform, and the documentation is done by Doxygen. The source code is written in the object-oriented fashion, automated unit tests and regression tests are deployed. Version-control, peer review and data preservation are carried out. After the refactoring, the number of lines in the code decreases significantly and the performance gain is remarkable. More importantly, with a modern software framework facilitated by open source software, the maintenance is much easier than before, and the life time of the software is expected to last longer. We welcome contributions, including various features to treat interface interpolation, solid material types, fluid solvers for compressible fluid, turbulent flows, etc. from the computational mechanics community.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Fast Process Modeling Based Support Structure Design Optimization for Minimizing Residual Stress and Distortion in Metal Additive Manufacturing

Lin Cheng*, Xuan Liang**, Albert To***

*University of Pittsburgh, **University of Pittsburgh, ***University of Pittsburgh

ABSTRACT

Metal additive manufacturing (AM) as a revolutionary manufacturing technique has been gradually accepted by engineers and applied for rapid manufacturing of functional end-use components. However, there are two key physical phenomena preventing its broad applications, namely the residual stress and large deformation inherent in the melting and solidification processes. These phenomena cause delamination and cracking during the manufacturing process, which can stop the recoater blade from spreading the powder, as well as lead to part warpage after removing from the building tray. To address these issues, a novel design optimization methodology based on fast process modeling is proposed for the design of support structure, in order to reduce residual stress and distortion and ensure manufacturability. First, a modified inherent strain method is proposed and employed for fast prediction of the stress and deformation. It is based on thermo-mechanical modeling at mesoscale and implemented as a one-time static mechanical analysis. Thus, the process modeling can be significantly accelerated and compatible with structural design. Second, a projection scheme is proposed to map the domain of support structure for a given solid component, in which the minimum support area is found for the next step. Third, lattice structure topology optimization is applied to minimize the mass consumption of support structure subjected to yield stress constraint. This not only prevent failure of the AM build by limiting the residual stress below the yield strength, but also reduce material required for support structure. Moreover, the self-support nature of lattice structure, and its ability to provide accurately mechanical representation, makes it a natural design tool for support structure design. Several examples are performed and manufactured to demonstrate the efficiency of the proposed algorithm. Both numerical simulation and experiments prove that the proposed method can significantly reduce residual stress and guarantee the success of metal AM fabrication.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Research on Anti-water Pressure Capability of Railway Tunnel Lining by CDEM (Continuous-Discontinuous Element Method)

Pengda Cheng*, Ping Lu**, Liangtian Peng***, Gang Zhou****, Li Ming Zhang*****, Guo Jun Wang******, Bao Lin Liu*******, Tian Yang********

*Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China, **Sichuan Xu Da Railway Co., Ltd. Luzhou, 646000,China, ***Sichuan Xu Da Railway Co., Ltd. Luzhou, 646000,China, ****Sichuan Provincial Railway Construction Co., Ltd, Chengdu, 610031, China, *****Sichuan Provincial Railway Construction Co., Ltd, Chengdu, 610031, China, ******China Railway Eryuan Engineering Group Co., Ltd(Chongqing), Chongqing 400023, China, *******China Railway Eryuan Engineering Group Co., Ltd(Chongqing), Chongqing 400023, China, ********University of Chinese Academy of sciences, Beijing 100049, China;Institute of Mechanics, Chinese Academy of Sciences, Beijing 100190, China

ABSTRACT

Abstract: The hydrogeological conditions are complex in southwest China, and the anti-water pressure capability of railway tunnel lining is widely regarded in the transportation project. When the drainage conditions are limited, high external water pressure may cause the lining cracking, which is the serious threat to the tunnel safety. Scientifically and rationally assessing the anti-water pressure capability of the lining is very important to the design of the lining structure. In this paper, the research method combine the theoretical analysis and the numerical simulation, the numerical calculation model is established by using the continuous-discontinuous element method (CDEM). Based on that model, the destruction process of tunnel lining under different water pressure conditions is simulated, the stress and strain changes of the initial support, steel-concrete lining and waterproofing board are analyzed. Finally, the development of the cracks and the fracture degree in tunnel lining can be obtained under different water pressure conditions, meanwhile the assessment method can be proposed by using the fracture degree. That has the important practical application value for optimizing the design parameters of the tunnel anti-water lining.
References [1] Li SH, Wang JG, Liu BS, et al. Analysis of critical excavation depth for a jointed rock slope by face-to-face discrete element method. Rock Mechanics and Rock Engineering, 2007, 40(4): 331-348 [2] Itasca Consulting Group Inc. FLAC-3D (Fast Lagrangian Analysis of Continua in 3 Dimensions), Version 3. 0, User's Manual. USA: Itasca Consulting Group Inc, 2005 [3] LI Shihai ZHOU Dong LIU Tianping. Risk analysis method of accumulated landslide based on fracture degree[J]. Chinese Journal of Rock Mechanics and Engineering, 2013, 32:3909-3917.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Turbulence Spectra in the Stable Atmospheric Boundary Layer

Yu Cheng*, Qi Li**, Stefania Argentini***, Pierre Gentine****

*Department of Earth and Environmental Engineering, Columbia University, New York, NY 10027, USA,
**Department of Earth and Environmental Engineering, Columbia University, New York, NY 10027, USA,
***Institute of Atmospheric Sciences and Climate, CNR, Rome, Italy, ****Department of Earth and Environmental Engineering, Columbia University, New York, NY 10027, USA

ABSTRACT

Stratification causes turbulence spectra to deviate from Kolmogorov's isotropic -5/3 power-law scaling in the universal equilibrium range at high Reynolds number. However, a consensus has not been reached with regard to the exact shape of the spectra. Here we propose a theoretically-derived shape of the TKE and temperature spectra that consists of three regimes at small Froude number: the buoyancy subrange, a transition region and isotropic inertial subrange separated by the buoyancy scale and Ozmidov scale through derivation. These regimes are confirmed by various observations in the atmospheric boundary layer. We also show that DNS may not apply in the study of very stable boundary layers as they cannot correctly represent the observed spectral regimes seen in actual boundary layers because of the lack of scale separation. In addition, the spectrum in the transition regime explains why Monin-Obukhov similarity theory cannot entirely describe the behavior of the stable atmospheric boundary.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Controling of Wave Propagation in Composite with Spherical Inclusions in Meso-scale

Luo Chengcheng*, Liu Zhanli**

*+86-15201522105, **18811584467

ABSTRACT

Control of wave of wave propagation is always a hot spot in scientific research, which has also so many applications such as noise reduction and blast wave protection. According to previous studies, the bragger scattering and resonant oscillations are two main principles to control the elastic wave. Based on their theories, we developed a finite element to see the wave propagation in composite particled with spherical inclusions. The distribution of inclusions can be both periodic and casual. By changing the size and volume ratio in composite, we can find the case which gains the most decrease of the wave. The model is generated by abaqus using python and the preprocess and the postprocess can be all automatic. The shape of the particle and the properties of materials can be modified in later research.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

An Improved Contact Detection Algorithm for Dynamic Finite Element Analysis

Chen Chengjun*, Chen Xiaowei**, Liu Ming***

*Institute of Systems Engineering, CAEP, **Frontier Science Research Institute of Beijing Institute of Technology, ***Institute of Systems Engineering, CAEP

ABSTRACT

Contact detection has a significant effect on the efficiency and accuracy of finite element analysis for dynamic contact problems. In this paper, a new contact-pair detection algorithm for dynamic contact simulation in the finite element has been developed and implemented in the transient dynamic finite element code PANDA-IMPACT. The newly developed contact detection strategy composed of: (1) a global search strategy based on the octree algorithm that is used to efficiently find out all the possible candidates for contact and, (2) a robust local search algorithm derived based on the geometric position relationship between the slave segments and the corresponding master segments to determine the actual contact pairs. In the new algorithm, the centroid of the contact segment and its characteristic length (one kind of mean length of contact segment) are employed to represent the segment's true geometry. As a consequence, the contact segments are reduced to a series of discrete points, and the building and updating processes of the octree are very straightforward. The cost of the new global searching is of the order of O(Nlog8M), where N is the number of the slave nodes, M is the number of master segments. In local searching phase, contact point is evaluated analytically based on the principles of force-equivalence and moment-equivalence, and a reverse mapping algorithm. Difficulties associated with the conventional contact algorithms, such as stability and blind zone problems, are resolved. Several numerical simulations of typical benchmarks and physical engineering problems demonstrate that the proposed contact determination strategy is effective and robust, and has good applicability.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Development of an Adaptive Material Point Method Coupled with a Phase Field Model for Analyzing Damage Process and Crack Propagation

Young-Jo Cheon*, Hyun-Gyu Kim**

*Seoul National University of Science and Technology, **Seoul National University of Science and Technology

ABSTRACT

In this study, a new method is developed by combining material point method and phase field method for the analysis of damage evolution and crack propagation in materials. In the conventional finite element method, it is difficult to simulate damage evolution and crack propagation due to meshing a new geometry and the effect of element shape on crack propagation. A background grid of material particles is adaptively refined based on the material damage which is evaluated by solving a phase field model. The characteristic length of material damage and crack propagation is applied to multiscale adaptive material point method and phase field method. The proposed approach is verified through numerical examples of several crack propagation problems.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Dispersive Effective Behaviour of High-contrast Periodic Media

Kirill Cherednichenko*, Alexander Kiselev**, Yulia Ershova***

*University of Bath, **Dragomanov National Pedagogical University, ***University of Bath

ABSTRACT

We prove sharp operator-norm asymptotic equivalence estimates between a family of periodic quantum graphs with rapidly oscillating high-contrast weights and "homogenised'' models with energy-dependent interface conditions. The asymptotic analysis is carried out "on the spectrum'', i.e. it includes order-sharp asymptotic estimates for the eigenfunctions of the mentioned operator families. We show that the above asymptotically equivalent models are equivalent to models for the so-called time-dispersive media, which in the time domain involve memory, and we characterise the corresponding time convolution kernel explicitly.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Statistical Learning Methods and Reduced Order Model for Random Fluid-structure Interaction Problems

Mathilde Chevreuil*, Anthony Nouy**, Erwan Grelier***

*GeM - Université de Nantes, France, **LMJL - Centrale Nantes, France, ***GeM - Centrale Nantes, France

ABSTRACT

The robust design of structures in a fluid environment may involve numerous sources of uncertainties in the model in order to predict their impact on the response. It reveals necessary to develop reliable and efficient tools for the prediction of such responses and in this framework, functional approaches for uncertainty quantification suffer from the highly nonlinear behaviour of the response to the input uncertainties. In order to tackle such problems, we consider statistical learning methods based on least squares minimization for high dimensional problems where the output is approximated in suitable low-rank tensor formats [1]. The storage complexity of these formats grows linearly with the dimension which makes possible the construction of an approximation using only few samples [2]. However the rank of the approximation of the stochastic dynamic response may be high and the method thus loses its efficiency. The key is to propose a suitable functional representation and an adapted parametrization with a new set of variables for the computation of the response so to obtain structured approximations with low complexity. The latter parametrization is determined automatically by coupling a projection pursuit method [2] and low rank approximation. [1] W. Hackbusch. Tensor Spaces and Numerical Tensor Calculus. Springer Berlin Heidelberg, 2012. [2] M. Chevreuil, R. Lebrun, A. Nouy, and P. Rai. A least-squares method for sparse low rank approximation of multivariate functions. SIAM/ASA JUQ, 3(1):897–921, 2015. [3] J. H. Friedman and W. Stuetzle. Projection pursuit regression. Journal of the American statistical Association, 76(376):817–823, 1981.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Stretch-induced Softening and Rupture of DNA

Qingjia Chi*, Xin Lai**, Lisheng Liu***

*Department of Mechanics and Engineering Structure, Wuhan University of Technology, China, **Department of Mechanics and Engineering Structure, Wuhan University of Technology, China, ***Department of Mechanics and Engineering Structure, Wuhan University of Technology, China

ABSTRACT

The mechanical properties of DNA play an important role in its participation in the replication, transcription, recombination and other biological behaviors. But the vast majority of investigations have focused on its biochemical properties based on base sequence. And there are fewer studies on DNA's biomechanical properties, leading to insufficient understanding of some of its mechanical properties. Using unified ideal chain model to investigate force-induced deformations of DNA, we evaluate the softening behavior of DNA. The model can solve the mismatch problem between the models describing force-extension of double-stranded and single-stranded DNA, and can cover the whole force regime. A crossover force is obtained for dsDNA using unified ideal chain model. Moreover, we present results of stretch-induced rupture obtained from peridynamics. Peridynamics provides a reformulation of continuum elasticity theory which is better-suited to model rupture of biopolymers.The governing equation of peridynamics is integral rather than differential, and particles are connected in a non-local manner. Peridynamics can be regarded as an upscaling of molecular dynamics. The application of peridynamics to the investigation of biopolymers is novel and may provide a new inquiry method.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Gradient Reproducing Kernel Collocation Method for High Order PDEs

Sheng-Wei Chi*, Ashkan Mahdavi**

*University of Illinois at Chicago, **University of Illinois at Chicago

ABSTRACT

The Reproducing Kernel approximation in conjunction with the Collocation Method (RKCM)[1] was introduced for solutions of PDEs and engineering problems for some time. Although it offers only algebraic convergence, being less sensitive to the nodal distribution and of compact structure, thus better conditioning, make it an attractive method for engineering applications. However, taking direct derivatives of the reproducing kernel approximation is computationally expensive, in comparison to other commonly used approximations for collocation methods, such as RBFs. In this work, we address the high computational cost in the RKCM while achieving optimal convergence by adopting gradient reproduction kernel approximations for all derivatives involved in a PDE. In contrast to the earlier work in [2], both first order and second order derivatives involved in the approximation for a second order PDE are expressed by gradient reproducing kernels in the present method. We show that the same number of collocation points and source points can be used in the G-RKCM for optimal convergence. The present method is further introduced for problems governed by 4th order PDEs, such as Kirchhoff plate problems and 4th order phase-field model for fracture [3]. The numerical studies show that the present method is much faster and more robust than the RKCM. [1] H. Y. Hu, J. S. Chen, and W. Hu, Weighted radial basis collocation method for boundary value problems, International Journal for Numerical Methods in Engineering 69, p.2736-2757, 2007. [2] S.W. Chi, J.S. Chen, H.Y. Hu, and J.P. Yang, A gradient reproducing kernel collocation method for boundary value problems, International Journal for Numerical Methods in Engineering 93(13), p.1381-1402, 2013. [3] M.J. Borden, T. J.R. Hughes, C. M. Landis, C. V. Verhoosel, A Higher-Order Phase-Field Model for Brittle Fracture: Formulation and Analysis within the Isogeometric Analysis framework, Computer Methods in Applied Mechanics and Engineering, 273, p. 100-118, 2014.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Developing Effective Guidelines Towards Robust Design of Passenger Vehicle Front-ends with Respect to Pedestrian Lower Leg Impact for Early Development Phases

Stefano Chiapedi*, Andreas Koukal**, Fabian Duddeck***

*Technische Universität München, Munich, Germany, **AUDI AG, Ingolstadt, Germany, ***Technische Universität München, Munich, Germany and Queen Mary University of London, UK

ABSTRACT

Pedestrian Protection has gathered lots of attention in academia and industry over the last two decades, aimed at reducing the likelihood of injuries to pedestrians in the event of impact with a car. Research into this discipline has been promoted by the quick evolution of consumer tests requirements, especially in the European market, and has led to a significant redesign of passenger vehicle front-ends. The pedestrian lower leg impact test underwent recently a major consumer test change, as a new legform impactor, the so-called Flexible Pedestrian Legform Impactor (FlexPLI), was introduced [2]. The injury criteria associated with this impactor present a complex link with both geometry and stiffness of the vehicle front-end. Nevertheless, these are usually settled at different design stages, further raising the challenges to be faced in such a cost- and time-consuming product development process. Moreover, practical structural modifications at late stages, such as changes in size and thickness, have limited influence on the injury criteria [1], pointing out the need for early decisions. Effective guidelines towards robust designs, on both geometry and stiffness, delivered in early design stages, are therefore very valuable. CAE tools play an essential role in the vehicle development process. Detailed, high-fidelity FE models of the car front-end enable accurate predictions of the structural response under a great variety of load cases. Nevertheless, the computational effort and the complexity associated with those models are often incompatible with structural optimization methods. In cases where a particular load case, such as the FlexPLI impact, is of interest, simplified, low-fidelity FE models can be derived [3], whose range of validity is restricted to a specific operating region, yet simulation speed and parametrization flexibility are significantly enhanced, thus favoring the application of optimization techniques. In the current work, a method is presented to develop guidelines for early design stages of passenger vehicles concerning requirements for the pedestrian lower leg impact, exploiting the advantages of low-fidelity FE models. References [1] Stefano Chiapedi, Andreas Koukal, and Fabian Duddeck. Sensitivity Analysis for Pedestrian Lower Leg Impact. In 7th GACM Colloquium on Computational Mechanics, pages 408–412. University of Stuttgart, Germany, 2017. [2] Euro NCAP. Pedestrian Testing Protocol. Technical Report 7.1.1, 2014. [3] Simon Mößner, Tim Rudolph, and Fabian Duddeck. Surface Modelling of Vehicle Frontends for Pedestrian Safety with the FlexPLI. International Journal of Crashworthiness, 22(3):243–259, 2017.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

An Adaptive Remeshing Method for Crack Initiation and Propagation Using Cohesive Zone Model

Vincent Chiaruttini*, Eva Borakiewicz**, Noémie Rakotomalala***

*Onera, Université Paris-Saclay, **Onera, Université Paris-Saclay, ***Safran Tech

ABSTRACT

Over the last several decades, a wide range of numerical methods have been developed to efficiently simulate 3D crack propagation: for instance X-FEM, GFEM, BEM or FEM with adaptive remeshing. These approaches have been successful in many situations, yet many issues are still encountered when dealing with complex aspects such as crack lips contact in finite strain, highly non-linear elastic-plastic material behaviors, dealing with both crack initiation and propagation stages... Recent developments have been carried out to address these issues: variational formulation of fracture, phase-field, thick level-set, are some promising strategies to deal with the complete damage to failure problem. Our approach is focused on the capability to mix very complex highly non-linear elastic-plastic material models (for ductile or thermo-mechanical-fatigue failure) with a numerical strategy suitable to simulate a complete scenario from the finite strain plastic deformation of a structure through damage, crack initiation, propagation and up to complete failure. Concerning the material behavior part, a wide range of models can be used, depending on the context (fatigue or critical failure). An important point to remember is the formulation must be independent of the mesh size and orientation as a many adaptive remeshing operations will be performed in order to adapt the computational cost in the zones where non-linearities occur. Thus, in the case of finite strain ductile failure, a regularized formulation of the constitutive model can be required. Sharing some aspects with a previously developed technique [1], we perform local remeshing in identified critical zones where the material dissipation is maximal, and a specific mesh transfer algorithm is applied to ensure further calculation. However, in order to deal with both damage and failure aspects, this new approach aims to insert, in the identified damage zones, a cohesive surface whose size and orientation will be dynamically controlled, in order to satisfy a maximal dissipation during the failure process (using some algorithms previously presented in [2]). To highlight the performance and robustness of this method, various numerical assessments will be presented. This work was performed within the SEMAFOR project funded by the French Agence Nationale de la Recherche ANR-14-CE07-0037 grant). References [1] A new marching ridges algorithm for crack path tracking in regularized media, S Feld-Payet, V Chiaruttini, J Besson, F Feyel, IJSS, 71, 2015, 57-69. [2] An adaptive algorithm for cohesive zone model and arbitrary crack propagation, V Chiaruttini, D Geoffroy, V Riolo, M Bonnet, EJCM/REMN, 21, 3-6, 2012, 208-218.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Superiority of the Bottom Geometry of Surfboard from the Viewpoint of Drag Performance

Kazuhisa Chiba*, Shin-nosuke Ishikawa**

*The University of Electro-Communications, **The University of Electro-Communications

ABSTRACT

We aim at quantitatively clarifying the superiority of the bottom geometry of surfboard which has never been implemented. The bottom geometry of surfboards is an important factor to derive the ability of surfers. Various designs such as flat, vee, and concave have been developed so far, but its performance is decided by the sense of shapers and surfers; it has not been quantitatively evaluated. In this research, we have quantitatively evaluated the performance of the bottom geometry using gas-liquid two-phase flow analysis via the drag value of surfboards as an index when paddling and riding. The drag should be lower at paddling as well as it should be higher at riding; we need the tradeoff performance at between paddling and riding. We prepare three-types bottom geometry: flat, single concave, and double concave (we will focus on long-board, so vee geometry is omitted here). As a result, we confirmed that a single concave geometry has better performance under both paddling and riding conditions with respect to drag and it turned out that there was no tradeoff between those conditions. Moreover, a large amount of curvature (the depth of concave) is better performance, and its physical reasons. When paddling, since the board is positioned parallel to the uniform flow, the deeper concave increases the wetting area and the drag increases. By contrast, when riding, a surfboard has a yaw-angle against uniform flow, so the flow accelerates on the side of the surfboard and the drag drops. We consequently clarified the difference between the depth of concave and the drag value on yaw-angle against uniform flow of surfboard.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Cohesive Polytopal Finite Element Methods for Simulating Dynamic Fracture

Eric Chin*, Joseph Bishop**, Rao Garimella***, N. Sukumar****

*UC Davis, **Sandia National Laboratories, ***Los Alamos National Laboratory, ****UC Davis

ABSTRACT

We present dynamic fracture simulations using cohesive surfaces inserted on inter-element surfaces on polytopal meshes. Cohesive finite elements provide a natural means for modeling nucleating and extending cracks in solids. However, a sufficient network of possible internal crack surfaces is required to insert cohesive elements. An optimal network would both have no preferential direction and be able to accurately follow arbitrary paths. To meet these criteria, we use polytopal elements generated from a maximal Poisson-disk sampled domain. Maximal Poisson-disk sampling provides a means to robustly and rapidly generate a geometry conforming mesh with an optimal fracture network. Elements are convex and can be modified to have good element quality for finite element analysis, while still maintaining an optimal fracture network. Wachspress and maximum entropy basis functions are used to form a finite element basis over the polytopes. Cohesive zone elements are dynamically inserted at facets between the polytopes in the mesh. As the analysis progresses, we track and update the evolving mesh topology using a graph-based approach, which allows mesh operations to be completed robustly and rapidly. Contact is enforced through a penalty method which is applied to both closed cohesive surfaces and general interpenetration of two polytopal elements. Several numerical examples are presented which illustrate the capabilities of the method (capturing large deformation effects, branching cracks, self-contact) and demonstrate convergence of solutions.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Data, Information and Knowledge: A Multiscale Framework

Francisco Chinesta*, Emmanuelle Abisset**, Elias Cueto***

*ENSAM ParisTech, **ECN, ***University of Zaragoza

ABSTRACT

Data-based modeling and simulation appears nowadays as a new pillar of the XXI century engineering. However, making the parallel with the atomic theory, one could expect that data (as atoms) even being at the foundation of the information theory, represent in general a too fine scale for most engineering applications. In mechanics the different scales were addressed using the appropriate representations and models, and all these scales were inter-connected using adequate bridges. Such a multi-scale representation, in the field of data-sciences, could constitute a major accomplishment, and very certainly a real change of paradigm, in data-based science and technology. In this work some proposals concerning the dynamics of data, information and knowledge, covering the micro, meso and macro scales will be discussed, and important questions addressed: which data, when and where for increasing at maximum the knowledge gain. Dynamics of information will be compared with Liouville dynamics and finally the question of probabilistic versus deterministic (with internal variables) dynamics discussed from two very different perspectives, the classical probability theory (Bayes) and its quantum counterpart (where superposition applies), the last opening the possibility of encountering surprising events. This last point is extremely important when putting the human in the loop for creating cognition models to be used for assimilating data (driver assistants or augmented engineers).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Multiphysic and Multiscale Modeling of Additive Manufacturing Processes by Metal Deposition

Michele Chiumenti*, Emilio Salsi**, Miguel Cervera***, Eric Neiva****, Santiago Badia*****

*International Center for Numerical Methods in Engineering (CIMNE), Universidad Politécnica de Cataluña, Campus Norte UPC, 08034 Barcelona, Spain, **International Center for Numerical Methods in Engineering (CIMNE) Universidad Politécnica de Cataluña, Campus Norte UPC, 08034 Barcelona, Spain, ***International Center for Numerical Methods in Engineering (CIMNE), Universidad Politécnica de Cataluña, Campus Norte UPC, 08034 Barcelona, Spain, ****International Center for Numerical Methods in Engineering (CIMNE), Universidad Politécnica de Cataluña, Campus Norte UPC, 08034 Barcelona, Spain, *****International Center for Numerical Methods in Engineering (CIMNE), Universidad Politécnica de Cataluña, Campus Norte UPC, 08034 Barcelona, Spain

ABSTRACT

In this work the framework for the numerical simulation of the Additive Manufacturing (AM) process by Metal Deposition is presented. A fully coupled thermo-mechanical analysis is performed following the actual scanning sequence of the AM machine [1-2]. Hence, the high-fidelity simulation of the fabrication process is achieved, accounting for both precise power source input and the heat loss by convection and radiation mechanisms. The computed thermal field has been proven a remarkable matching with the temperature evolution recorded at different thermocouple locations. Hence, this temperature evolution is used to feed a mesoscale model suitable for computing the kinetics of the microstructure formations. Focusing on Ti64 alloy, the solid state transformations is described by the ???+? diffusion-controlled transformation through JMAK equations, while, in case of faster cooling rates, the martensitic phase is modeled using the empirical Koistinen-Marburger law. During the re-heating phase, the dissolution of the martensitic phase is described by JMAK equation, while the transformation from ? to ? phase is modeled as instantaneous transformation. The predicted microstructure is compared with the experimental evidence

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

POD-ROM for Nonlinear Structural Analysis Based on Co-rotational Finite Element and Parallelized Domain Decomposition

Haeseong Cho*, Haedong Kim**, SangJoon Shin***

*Seoul National University, **Sejong University, ***Seoul National University

ABSTRACT

In this paper, a nonlinear structural analysis based on the reduced-order modeling and proper orthogonal decomposition (POD-ROM) is developed. A procedure for POD-ROM is divided into two stages: offline and online. In the offline stage, a reduced dynamic system is constructed using POD modes [1]. The resulting ROMs are constructed by Galerkin projection of the extracted POD modes into the structural governing equations. In the online stage, the relevant analysis is performed using reduced structural governing equations. However, the computational cost in the offline stage may become significant especially when large-size structural analysis is required. And, the nonlinear analysis may become cumbersome to define accurate ROM due to the linearized characteristics in the ROM based on Galerkin projection. As a result, additional computing algorithm may be required and it is required to be efficient. Hence, relevant computational algorithm is proposed. First, the parallel computing algorithm is proposed to ensure efficiency in the offline stage. In order for parallel computation, domain decomposition using METIS algorithm [2] is used and the parallelized finite element matrix assembling technique is developed. Then, the ROM for nonlinear analysis is developed. In order for that, co-rotational finite elements are developed [3]. And, the ROM is constructed at everyiteration of Newton-Raphson solver. Also, the present parallel computing algorithm is employed in each constructing procedure. Without the parallelization of the ROM, it is found that the computational efficiency in the online stage will be improved up to 68% when compared to that of the FOM. In the future, examinations will be conducted by using the present parallelized POD-ROM. [1] Sirovich L., “Turbulence and the dynamics of coherent structures,” Quarterly of Applied Mathematics, Vol. 45, 1987, pp. 561–590. [2] Karypis, G., “METIS: A software package for partitioning unstructured graphs, partitioning meshes, and computing fill-reducing orderings of sparse matrices ver. 5.1.0,” http://glaros.dtc.umn.edu/gkhome/metis/metis/overview, 2013. [2] Cho, H. S., Kim, H.D., and Shin, S.J., “Geometrically nonlinear dynamic formulation for three-dimensional co-rotational solid elements,” Computer Methods in Applied Mechanics and Engineering, Vol. 328, 2018, pp. 301–320.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Modelling of Polycrystalline Materials Using the Dislocation Dynamics Method

Jaehyun Cho*, Sylvie Aubry**, Athanasios Arsenlis***

*Lawrence Livermore National Laboratory, **Lawrence Livermore National Laboratory, ***Lawrence Livermore National Laboratory

ABSTRACT

The dislocation dynamics method aims at predicting the strength of metals and alloys by modelling the interaction and evolution of dislocations lines. Nearly all dislocation dynamics methods focus on single crystalline materials despite the fact that most engineering materials are polycrystalline and grain boundaries are known to influence plastic behavior. Grain boundary modelling is often neglected because of their complexity. Accurate prediction of the strength of metals and alloys depends on the understanding of the complex interaction between grain boundaries and dislocations that composes their microstructure. In this presentation, we extend the dislocation dynamics method to polycrystalline materials. Grain boundaries are represented by planes from which dislocations can emit. The emission process is accurately modelled through topological operations and is based on a power dissipation criterion. Upon meeting a grain boundary, a dislocation can transmit, reflect, and/or leave a residual dislocation in the grain boundary plane. Several examples of dislocation emission will be presented to illustrate the method.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Multiscale Modeling of Photoresist Fabrication in EUV Lithography Process

Maenghyo Cho*, Muyoung Kim**, Junghwan Moon***, Joonmyung Choi****, Byunghoon Lee*****

*Seoul National University, **Seoul National University, ***Seoul National University, ****SAMSUNG ELECTRONIC CO., LTD, *****SAMSUNG ELECTRONIC CO., LTD

ABSTRACT

Size of wafer has been decreased for improving performance and productivity in semiconductor manufacturing industry, and Extreme Ultraviolet (EUV) light source is one of the most promising candidates to achieve the downsizing. Even though experimental- and theoretical approaches have been suggested to investigate physical mechanism of photoresist (PR) fabrication, technical huddles resulting from complex photochemistry hinder full-description of multiphysics problem such as chemical reaction by electron attachment or diffusion of reactant. From this point of view, we constructed multiscale model having sequential framework of density functional theory (DFT)-molecular dynamics (MD)- finite difference method (FDM). Our newly-developed model provides rigorous description of photo-triggered chemical reaction (acid activation by electron attachment and acid diffusion-deprotection evolution) and also quantification of sub-10 nm PR morphology in atomistic level. This achievement will be the cornerstone of theoretical research which facilitates fundamental understanding on important factors for EUV performance and rational design of the next-generation PR.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Multi-disciplinary Design Optimization for Structure, Dynamic and Flow Characteristic in Subsea By-pass Valve

Su-gil Cho*, Jaewon Oh**, Sanghyun Park***, Cheonhong Min****, Jeonghee Lee*****, Hyungwoo Kim******, Tae Hee Lee*******

*Korea Research Institute of Ship and Ocean Engineering, **Korea Research Institute of Ship and Ocean Engineering, ***Korea Research Institute of Ship and Ocean Engineering, ****Korea Research Institute of Ship and Ocean Engineering, *****Korea Research Institute of Ship and Ocean Engineering, ******Korea Research Institute of Ship and Ocean Engineering, *******Hanyang University

ABSTRACT

A bypass valve, which is used for the safe lifting of mineral resources in deep-sea mining, functions as preventing reverse flow at emergency case. The valve has a simple mechanism, but its design is very difficult because it must guarantee not only structural safety even emergency case but also flow performance at normal operation condition. This equipment should also operate under sludge flow with a mixture of seawater and manganese nodules. Since deep-sea mining system has not been commercialized, the valve is a new attempt and there are many design parameters to consider for design, such as by-pass valve type or size, volume flow rate, leakage hole size, leakage hole position, block type, block shape so on. In this study, fluid dynamics, multi-body dynamics, structure analysis of valves are performed using commercial CAE software. Furthermore, these CAE softwares are linked to the optimization program and multi-disciplinary design optimization is performed for valve design. Finally, a prototype valve was produced and the lab scale valve tests are performed for validation.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Two- and Three-dimensional Crack Path Prediction for Mixed-mode Cohesive Fracture by Using Cohesive Zone Modeling

Habeun Choi*, Moon Kyum Kim**, Kyoungsoo Park***

*Yonsei University, **Yonsei University, ***Yonsei University

ABSTRACT

Cohesive zone models have been one of the most effective tool for representing nonlinear fracture behaviors of materials. For accurate modeling of a displacement discontinuity under mixed-mode conditions, an element splitting scheme [1] is proposed in conjunction with crack initiation criteria, i.e., the maximum strain energy release rate [2]. When the strain energy release rate at a crack tip exceeds the cohesive fracture energy, a continuum element is split and a cohesive surface element is adaptively inserted. Crack propagation direction is identical to an angle which maximizes the strain energy release rate. To accurately approximate strain energy release rate at a crack tip, a virtual mesh grid is generated around a crack tip. The topology-based data structure (TopS) [3] is utilized to update local element connectivities when elements split. A bilinear softening model is used for the constitutive relationship of cohesive concrete fracture. The proposed computational framework is verified and validated by illustrating mixed-mode fracture examples. In a two-dimensional case, four-point shear test and double-edge-notched fracture test in plain concrete are simulated. And also a single edge notched tension test is simulated for a material with microstructure. Multiple crack initiations, crack branching and coalescences are represented using the proposed framework. In three-dimensional case, a mode I crack propagation problem is illustrated to verify the consistency of the element splitting scheme. Then, non-planar crack surface is represented by using the proposed scheme. References [1] H. Choi, K. Park. Removing mesh bias in mixed-mode cohesive fracture simulation using element split and stress recovery. in preparation [2] Bouchard, P. O., Bay, F., & Chastel, Y. (2003). Numerical modelling of crack propagation: automatic remeshing and comparison of different criteria. Computer methods in applied mechanics and engineering, 192(35), 3887-3908. [3] Celes, W., Paulino, G. H., & Espinha, R. (2005). A compact adjacency?based topological data structure for finite element mesh representation. International journal for numerical methods in engineering, 64(11), 1529-1556.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

An ICME Approach for Predicting the Ductility of Thin-Walled High Pressure Die Casting Magnesium

Kyoo Sil Choi*, Erin Barker**, Xin Sun***, Mei Li****, John Allison*****

*Pacific Northwest National Laboratory, **Pacific Northwest National Laboratory, ***Oak Ridge National Laboratory, ****Ford Motor Company, *****University of Michigan, Ann Arbor

ABSTRACT

Mg castings have found increasing applications in lightweight vehicles because magnesium and its alloys are the lightest metallic structure materials. However, a critical technical hurdle hindering the wider applications of Mg castings in vehicle applications is its limited ductility. The factors limiting their ductility can be categorized into two types: intrinsic and extrinsic. Intrinsic factors include features intrinsic to the specific Mg alloy such as the phase composition, grain size, morphology, volume fraction and mechanical properties of its constituent phases. Extrinsic factors come from the external processes applied to the alloy such as casting and heat treatment processes, and they include porosity, segregation, incomplete fill, hot tear and cold shut, etc. In our study, as an integrated computational materials engineering (ICME) approach, we examined the influence of both factors on the ductility of high pressure die castings (HPDC) of Mg alloys based on microstructure-based finite element modeling method. Two different modeling approaches (i.e., intrinsic modeling and extrinsic modeling) were adopted. The lower-length scale intrinsic modeling is to predict the matrix properties based on the grain size-level microstructures and its phase properties extracted from nanoindentation test. The matrix properties predicted from intrinsic modeling can be used as the input properties for the upper-length scale extrinsic modeling. The extrinsic modeling, which is more focused in this presentation, is to predict the macroscopic ductility of the Mg casting which mainly depends on the porosity distributions. For the extrinsic modeling, three-dimensional (3D) microstructure-based finite element models were developed based on actual porosity distributions of some cast Mg samples, measured with CT scanning. The results show that the ductility and fracture locations predicted from simulations agree well with the experimental results. This indicates that the developed 3D extrinsic modeling method may be used to examine the influence of various aspects of pore sizes/distributions as well as intrinsic properties (i.e., matrix properties) on the ductility/fracture of Mg castings.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Isogeometric Optimal Design of Lattice Metamaterials

Myung-Jin Choi*, Hong-Yeon Jung**, Seonho Cho***, Sehyun Kang****, Myung-hoon Oh*****

*Seoul National University, **Seoul National University, ***Seoul National University, ****Seoul National University, *****Seoul National University

ABSTRACT

This paper presents a systematic synthesis of three-dimensional lattice metamaterials having the engineered properties of extremal negative Poisson 's ratio and phononic band-gap size. Along the way, we study several significant issues on the deformation analysis and the design sensitivity analysis (DSA). On the finite deformation of the geometrically exact spatial beams, we discuss the invariance property of spatially discretized problems in the isogeometric analysis (IGA) framework. On the other hand, in the configuration and sizing DSA formulation, the design variations can be expressed by exploiting the kinematics of the beam model, whose material derivatives yield the configuration DSA expressions, and the sizing design of cross-section considers both of the thickness and orientation designs. Importantly, for lattice structures on curved surfaces, like medical stents, the lattice needs to be located on a specified surface, which results in huge number of nonlinear equality constraints and difficulty in parameterization of design variables. To overcome this, lattice structures and their design variables are defined on planar rectangular domains, and the concept of free-form deformation and global curve interpolation are employed to obtain the analytical expressions for the control net of lattice structure on curved surfaces. The material derivative of the analytical expressions eventually leads to design velocity field. The considered applications of design optimizations using the developed methods are two folds: first, synthesis of auxetic structures achieving target Poisson's ratio in both of tensile and compressive loadings. Configuration and sizing designs are simultaneously performed during design optimization in order to sufficiently reduce error between target and actual Poisson 's ratio in finite deformations. The optimal design is manufactured using 3-D printing technology and verified through tension and compression experiments. Second, we find optimal designs of lattice structures for maximizing the phononic band-gap size at low frequency. In the wave propagation analysis, the Bloch theorem is utilized for periodic boundary conditions, and the effects of pre-loading is investigated.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Finite Difference Method for a Conservative Allen-Cahn Equation on Non-flat Surfaces

Yongho Choi*, Darae Jeong**, Seong-Deog Yang***, Junseok Kim****

*Korea University, **Korea University, ***Korea University, ****Korea University

ABSTRACT

We present an efficient numerical scheme for the conservative Allen-Cahn equation on various surfaces embedded in a narrow band domain in the three-dimensional space. We apply a quasi-Neumann boundary condition on the narrow band domain boundary using the closest point method. This boundary treatment allows us to use the standard Cartesian Laplacian operator instead of the Laplace-Beltrami operator. We apply a hybird operator splitting method for solving the CAC equaion. First, we use an explicit Euler method to solve the diffusion term. Second, we solve the nonlinear term by using a ckised form solution. Third, we apply a space-time dependent Lagrange multiplier to conserve the total mass. The overall scheme is explicit in time and does not need iterative step; therefore, it is fast, A series of numerial experiments demonstrate the accuracy and efficiency of the proposed hybrid scheme.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Reduced Order Models and Adaptive Mesh Refinement in Multiple Stress Topology Optimization

Youngsoo Choi*, Daniel Tortorelli**, Cosmin Petra***, Miguel Salazar De Troya****, Daniel White*****

*Lawrence Livermore National Laboratory, **Lawrence Livermore National Laboratory, ***Lawrence Livermore National Laboratory, ****Lawrence Livermore National Laboratory, *****Lawrence Livermore National Laboratory

ABSTRACT

A classical compliance topology optimization problem can result in an optimal solution with stress concentration regions. For more preventive design, stress quantity must be included in topology optimization formulations. Stress topology optimization requires a fine mesh to accurately represent stress quantities, which makes the optimization process slow. To relax the computational burden, but maintain the high accuracy of the stress computation, Adaptive Mesh Refinement (AMR) is useful. Although AMR contributes to relax the computational burden of stress topology optimization process by only refining the part where necessary, a success of AMR heavily depends on error estimates/indicators. There are geometric error indicators and residual-based error estimates (e.g., bounds). Another issue with AMR is that AMR changes mesh resolution throughout the optimization process. This implies that linear solver at each optimization iteration can be affected by potential ill-conditioning due to mesh changes. Additionally, the optimization process cannot avoid multiple expensive physics simulations in design process. Therefore, to further accelerate the procedure without losing much accuracy in stress computations, reduced representation of decision variables is desirable. There are two types of reduced representation: 1. a priori representation and 2. a posteriori representation. A priori reduced representation includes Fourier representation. A posteriori representation includes a data-driven (e.g., POD-based) representation. Data-driven representation performs better than a priori reduced representations in terms of accuracy and speed up. However, a data-driven method requires an offline phase to train data and the performance greatly depends on the quality of data. Additionally, the offline phase can be computationally expensive although it must be done only once. On the other hand, a priori representation does not require any expensive offline phase. We will introduce both approaches and present advantages and disadvantages of each method in terms of accuracy and speed up with multiple-objective stress topology optimization problems.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Unified modeling framework for brittle, quasi-brittle, and ductile failures of pressure-sensitive rocks

Jinhyun Choo*, WaiChing Sun**

*The University of Hong Kong, **Columbia University

ABSTRACT

Rocks display a wide range of failure modes depending on the confining pressure. The failure mode is localized and brittle fracture under a low confining pressure, but it increasingly becomes more diffuse and ductile as the confining pressure increases. Moreover, it has been shown that a rock under tensile loading can show a hybrid fracture mode in which tensile and shear fracture modes are mixed. Nevertheless, existing computational models usually focus on one of these failure modes. This talk will introduce a recently developed computational framework for unified modeling of these different failure modes under a wide range of confining pressure [1]. The framework couples a phase-field approach to fracture and pressure-sensitive plasticity. By doing so, it can capture the brittle failure mode using a phase-field approach, whereas it can simulate the ductile failure mode by plasticity. The coupling of phase-field and plasticity also allows for simulating quasi-brittle shear fracture and hybrid fracture as observed from experiments. The key ideas of this new coupling, such as the use of phase-field effective stress, will be discussed. Reference: [1] Choo, J. and Sun, W. C. (2018). Coupled phase-field and plasticity modeling of geological materials: From brittle fracture to ductile flow. Computer Methods in Applied Mechanics and Engineering, 330, 1–32.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Nitsche-based Approximation of Contact for Explicit Integration of Elastodynamic Problems

Franz Chouly*, Yves Renard**

*Université Bourgogne Franche Comté, **INSA Lyon

ABSTRACT

The dynamic of deformable solids with impact can be approximated numerically using an explicit time-marching scheme. This topic has already been the object of an important literature: explicit schemes for penalized contact, Moreau's NSCD schemes (non-smooth contact dynamics), Paoli-Schatzman scheme, mass redistribution method [3], etc. However, all the difficulties have not been overcome to obtain a method with satisfying properties of stability, monotonicity, accuracy and energy conservation, in the sense that, generally, at least one of these characteristics has a degraded behavior. The purpose of this presentation will be to explore further the properties of the Nitsche-based approximation of contact condition, presented in [1,2] (for the static case and implicit schemes respectively) when it is associated with an explicit time-marching scheme. For this, comparisons will be provided with the aforementioned methods in terms of energy conservation, convergence and occurrence of spurious oscillations. [1] F. Chouly, P. Hild, Y. Renard. Symmetric and non-symmetric variants of Nitsche 's method for contact problems in elasticity: theory and numerical experiments. Math. Comp., 84:1089--1112, 2015 [2] F. Chouly, P. Hild, Y. Renard. A Nitsche finite element method for dynamic contact: 1. Semi-discrete problem analysis and time-marching schemes. ESAIM Math. Model. Numer. Anal., 49:481--502, 2015 [3] H. Khenous, P. Laborde, Y. Renard. Mass redistribution method for finite element contact problems in elastodynamics. Eur. J. Mech., A/Solids, 27(5):918--932, 2008

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Peridynamic Model of Crevice Corrosion

Bufan Chu*, Qiwen Liu**, LIsheng Liu***

*Department of Mechanics and Engineering Structure, Wuhan University of Technology, **Department of Mechanics and Engineering Structure, Wuhan University of Technology, ***State Key Laboratory of Advanced Technology for Materials Synthesis and Processing Wuhan University of Technology

ABSTRACT

A new Peridynamic (PD) model of crevice corrosion is proposed by taking the ion migration and ion diffusion into account based on the dilute solution theory and Nernst-Planck equation. The 304 stainless steel square sample containing a crevice in NaCl solution is studied. Based on the classical diffusion governing equation, the PD formulation is established. Then based on the established PD model , the distribution of metal ion concentration during crevice corrosion was simulated. And the characteristics of the material point are described in terms of its own concentration, the diffusion bond is introduced to describe the connection between the material points. Through the diffusion bond, ions diffuse from the material points with high concentration to that with low concentration. The influences of different solid diffusion coefficients and crevice width on crevice corrosion damage are also analyzed. Finally, the results of the sample simulations and the model verifaction to other simulations are presented.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Study the Dynamic Elastic-Plastic Fracture of Metals Under Strong Shock Loading

Dongyang Chu*, Xiang Li**, Zhanli Liu***

*Department of Engineering Mechanics, Tsinghua University, **Department of Engineering Mechanics, Tsinghua University, ***Department of Engineering Mechanics, Tsinghua University

ABSTRACT

The elastic-plastic fracture mechanism of metals under strong shock loading is quite different from which under quasi-static loading, and the study about it has proven difficult. Under the strong shock loading, the metals undergo complex physical processes such as large deformation and elastic-plastic fracture. These physical processes also have complex coupling with the propagation of strong shock waves and strong sparse waves. In this paper, a computational model has been established based on the framework of thermodynamics to simulate the dynamic fracture of metals with large deformation under strong shock loading. The fracture of material is described based on phase field method. Therefore, this elastic-plastic phase field dynamic fracture model can realize the simulation of the whole process of material failure and crack propagation, and it can also simulate various fracture modes accurately under the propagation of shock wave and sparse wave. We study the dynamic deformation and fracture of a cylindrical steel plate under internal blast loading, and the numerical results is consistent with the experimental results. By simulating, the mechanism of energy transformation and elastic-plastic fracture for steel plate under strong shock loading are studied. This study may contribute to further understanding on the design of explosion containment vessels and can be applied to the engineering field. References: 1 Michael J. Borden et al. (2016), Computer Methods in Applied Mechanics and Engineering. 312: 130–166. 2, Qi Dong et al. (2016), Journal of Pressure Vessel Technology, 138 (6).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

The Mechanical Property and Microstructure of Scaffolds Regulate Differentiation of Annulus Fibrosus-Derived Stem Cells

Genglei Chu*, Bin Li**

*Soochow University, **Soochow University

ABSTRACT

Introduction The current engineered bionic disc tissue is considered as a potential way for treating intervertebral disc degeneration disease, which yet still remains challenging due to the complex radial gradient of natural annulus fibrosus (AF) tissue in cell phenotype, biochemical composition, microstructures, and mechanical properties. Previously, we have found that the differentiation of annulus fibrosus-derived stem cells (AFSCs) could be regulated by the elasticity of scaffold [1]. In this study, we attempted to examine the combined effect of both mechanical and microstructural features on the gene expression of AFSCs. Method AFSCs were cultured on four types of poly(ether carbonate urethane) urea (PECUU) scaffolds with controlled elasticity and fiber diameter: soft, small diameter; stiff, small diameter; soft, large diameter and stiff , large diameter, then incubated for 7 days. Results AFSCs were almost uniformly oriented along the fiber direction of scaffolds. AFSCs on the scaffolds of small diameter were round, while they were spindle-shaped on scaffolds of large diameter regardless of substrate elasticity. Mature focal adhesions were clustered around the periphery of cells on large diameter scaffolds, especially on stiff scaffolds. On the small diameter scaffolds, unmature focal adhesions were distributed in a much diffused manner. Western Blot, immunofluorescence and q-PCR results revealed that when the diameter of scaffold was kept constant, the expression of collagen-I in AFSCs increased with scaffold elasticity, while the expression of collagen-II and aggrecan genes showed an opposite trend. Moreover, when scaffold elasticity was controlled, the gene expression of collagen-I in AFSCs increased with fiber diameter. In contrast, the expression of collagen-II and aggrecan decreased. Such substrate elasticity and microstructure dependent changes of AFSCs were similar to the gradient characteristics of native AF tissue. In addition, increasing elasticity and fiber diameter of scaffolds promoted YAP activation and its nuclear translocation. Disscussion The results illustrate that the mechanical property is a potent regulator of AFSCs differentiation. Moreover, we reveal that microstructure of scaffold affects spreading area, focal adhesion and differentiation of AFSCs. Therefore, both mechanical property and microstructure of scaffold regulate AFSCs differentiation, possibly through a YAP-dependent mechanotransduction mechanism, thus providing a solid foundation for the tissue engineering applications of AFSCs. Reference [1] Zhu C, Li J, Liu C, Zhou P, Yang H, Li B. Modulation of the gene expression of annulus fibrosus-derived stem cells using poly(ether carbonate urethane)urea scaffolds of tunable elasticity. Acta biomaterialia. 2016;29:228-38.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

The Derivation of Heat Conduction Models with Fluctuations

Weiqi Chu*, Xiantao Li**

*Pennsylvania State University, **Pennsylvania State University

ABSTRACT

During the past two decades, there has been rapidly growing interest in modeling heat transport at the microscopic scale. As the size of electrical and mechanical devices is decreased to the micron and sub-micron scales, they often exhibit heat conduction properties that are quite different from the observations familiar at macroscopic level, e.g., Fourier Law. At such scale, the observable quantities also carry substantial fluctuations. In this talk, heat conduction models are derived directly from the many-particle system as a coarse-grained description. By selecting the local averaged energy as the coarse-grained variables, we apply different projection formalisms to derive the reduced models. In sharp contrast to conventional energy transport models, this derivation yields stochastic dynamics models, whose solutions converge to mild solutions of continuous SPDEs as the spacing goes to zero. The model also exhibits non-locality in space and time. We discuss the approximation of the non-local term to ensure the correct statistics of the solution.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Modeling High-strain-rate Responses Brittle Porous Media with Fracture Opening and Closure

Chukwudi Chukwudozie*, SeonHong Na**, WaiChing Sun***

*Columbia University, **Columbia University, ***Columbia University

ABSTRACT

In engineering applications that involves impacts, earthquake, and explosion, geomaterials are subjected to unusually high strain rate loading. This high strain rate leads to material responses significantly different than the quasi-static counterpart. The competition between elastic wave propagation and fracture propagation often leads to complex features, such as multiple fracture branches, coalescence, and closure. These mechanisms in return affect the two-way hydro-mechanical coupling between the fractured solid skeleton and the pore fluid. In this work, we use an implicit function to approximate cracks to dynamic crack growth and closure in brittle porous materials under high-strain-rate loading. To model the crack opening, closing, and slip behaviors under the dynamic conditions, we introduce a homogenization procedure to convert interface plasticity for strong discontinuity to a regularized anisotropic plasticity model with nonlocal plastic flow aligned with the gradient of the phase field. Both the two-field u-p and the three-field u-w-p and u-U-p formulations are implemented. The results are compared in numerical experiments.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Application of Refined Polygon Wall Boundary Model in PNU-MPS Method

Soh-Myung Chung*, Jong-Chun Park**

*Pusan National University, **Pusan National University

ABSTRACT

In order to analyse or solve Engineering problems engaged with fluid flow such as slamming, impact force induced by wave, and sloshing, two methods have been widely used in Computational Fluid Dynamics. One is a grid-based method and the other is a particle-based method. Chiefly, in simulation using particle method, there are several advantages. Since particle method thoroughly meets conservation of mass, it is possible to carry out long-time simulation. Furthermore, it is advantageous to express the motion of a fluid as a movement of particles without making the grid or re-meshing. Even though particle method is good at solving mentioned problems, flow instability issue has been appreciated as being a major obstacle to taking the merits of particle method in simulation. In the present study, in order to impose more precise boundary conditions and suppress the pressure instability derived from imprecise boundary condition including the free-surface, the polygon wall boundary model [1] is employed to the PNU-MPS (Pusan-National-University-modified Moving Particle Semi-implicit) method [2]. The enhanced and refined simulation method called as PNU-MPS-POLY is applied to solve the hydrostatic pressure problems for verifying through the comparison with analytic solution and other simulation result [1]. Moreover, the intensified treatment in boundaries is confirmed for sloshing problem [3] in a rectangular tank and applied to simulate sloshing phenomena in a glass of wine.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Transport Phenomena in Confined Granular Systems with Applications to Pharmaceutical Solids

Pedro Henrique Cidreiro Marints*, Payam Poorsolhjouy**, Marcial Gonzalez***

*Purdue University, **Purdue University, ***Purdue University

ABSTRACT

Imbibition and drainage of water through the pore spaces of granular media play a crucial role in all aspects of their behavior. For example, granular infrastructure materials that experience cycles of rain-freeze-thaw undergo considerable damage to their structural integrity. Of relevance to this presentation, pharmaceutical tablets rely on the process of imbibition into their pore structure for drug dissolution and release processes. In the present study, a three dimensional pore-network model capable of capturing the intricate microstructure of highly confined granular systems, with desired level of accuracy is presented. The model solves mass-transport of wetting and non-wetting fluids through the pore space in a computationally feasible manner. It assumes the two fluids to be incompressible and immiscible. The granular bed microstructure is represented by a random polydisperse packing of spherical particles. The pore space between particles is decomposed into throats that are connected to each other at volumeless pores. Two-phase Poiseuille flow is assumed inside the pore structure and conservation of mass is solved at all throats at every time step calculating the movement of the interfaces between wetting and non-wetting fluids. Entrapment of disconnected phases within the pore-space is allowed by implementing specific rules on interface displacements—these rules use a pore binary status, i.e., whether it is predominantly occupied by the wetting or non-wetting fluid, which is assigned based on the mass flux of incoming pore flows. The hysteresis movement of the interface is captured by using two different values for advancing and receding contact angles between wetting fluid and particles. Finally, a predictor-corrector approach based on flow direction and mass conservation is used in order to derive interface locations at the end of each time step-fixed time steps are used to improve stability and contain the computational cost. The pore structure is decomposed into throats and volumeless pores using a Radical Voronoi tessellation of the poly-disperse. In addition, a Constructive Solid Geometry (CSG) algorithm is used to define the hydraulic parameters of the interconnected throats. Validation of the model with experimental observations of penetration of a sessile drop deposited on a slightly compressed powder bed made of ?-lactose monohydrate, a typical excipient found in pharmaceutical formulations, shows that the developed algorithm captures the behavior of wetting fluids in vicinity of granular media with feasible amount of computational demand with low computational cost, compared to direct numerical simulation of the Navier Stoke equation in the exact pore space geometry.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Isogeometric Manifold Basis Functions with Prescribed Sharp Features and Cracks

Fehmi Cirak*, Qiaoling Zhang**

*University of Cambridge, **University of Cambridge

ABSTRACT

Manifold-based surface construction techniques are well known in geometric modelling and a number of variants exist. Common to all is the concept of constructing a smooth surface by blending together overlapping patches (or, charts) as in differential geometry description of manifolds. We combine manifold techniques with conformal parameterisations and the partition-of-unity method to derive basis functions on unstructured quadrilateral meshes. The obtained basis functions correspond to the vertices of the mesh and have arbitrary prescribed smoothness and approximation order. Each patch on the manifold consists of several elements and has a corresponding planar patch with a smooth one-to-one mapping onto the manifold. On the collection of conformally parameterised planar patches the partition-of-unity method is used for approximation. The smooth partition-of-unity, or blending, functions are assembled from tensor-product b-spline segments defined on a unit square. Polynomials with prescribed degree and continuity are used as local approximants on each patch. Sharp features and cracks are represented with suitably chosen C^0-continuous and discontinuous local polynomials, respectively. As will be demonstrated, the new manifold basis functions have to be carefully constructed in order to be suitable for both geometric modelling and analysis. This is achieved by considering several affine and conformal mappings depending on the local connectivity of the mesh and arrangement of sharp features and cracks. Our numerical simulations indicate the optimal convergence of the resulting approximation scheme for Poisson problems and near optimal convergence for thin-plate and thin-shell problems discretised with structured and unstructured quadrilateral meshes. References: Majeed, M. and Cirak, F. Isogeometric analysis using manifold-based smooth basis functions. Computer Methods in Applied Mechanics and Engineering (2017) 316:547--567. Zhang, Q. and Cirak, F. Manifold-based isogeometric analysis basis functions with sharp features and cracks. Preprint (2018).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Heat Transfer over Super-Hydrophobic and Liquid Infused Surfaces

Umberto Ciri*, Stefano Leonardi**

*The University of Texas at Dallas, **The University of Texas at Dallas

ABSTRACT

Turbulent flows are involved in several engineering fields, such as energy or transport. In many applications, the objective is to reduce the drag that is associated with turbulent motion in order, for instance, to increase the efficiency of air or marine vehicles or oil transport in ducts. In other cases, the strong turbulent mixing is exploited to enhance heat transfer for various applications. In general, heat transfer and drag are closely related in turbulent flows ("Reynolds analogy"), as they are driven by the same physical mechanisms. Recently, super-hydrophobic (SHSs) and liquid-infused surfaces (LISs) have been studied as a means of reducing drag in turbulent flows. These surfaces consist of a micro-texture of posts and cavities, filled with a second fluid, which create a mixed interface solid-fluid with the primary fluid. SHS features have a thin-film hydrophobic coating, that increments the motion of water drops by reducing their contact-angle hysteresis and traps air in the cavities. In LISs, a second liquid (immiscible with the primary fluid) replaces the air pockets in the surface features. Conceptually, the flow over LIS and SHS reproduces a two-layer configuration over a rough surface, where the roughness elements are constituted by the surface textures. Turbulent drag reduction is possible because the second fluid (air trapped in the textures for SHS, and lubricant liquid for LIS) creates a slip interface with the primary fluid, thus reducing friction drag. Experimental and numerical studies have shown great potential for these methods. However, relatively less attention has been dedicated to the heat transfer process over these surfaces. The objective of the present study is to investigate how heat transfer is affected in these configurations, where several factors are at play: the surface texture geometry, the thermodynamic properties of the fluids, as well as the interfacial dynamics. A parametric study will be conducted using direct numerical simulations of turbulent flow and heat transfer over LIS and SHS. The numerical code resolves the dynamics of both fluids with an energy-conserving finite difference scheme. The textures are modeled with the immersed boundary method, and the two-fluid interface is tracked with a level-set method. The simulations will provide data to assess whether LIS/SHS can also be employed in heat transfer enhancement applications, besides drag reduction.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

On the Coupling of Spectral Element Method with Discontinuous Galerkin Approximation for Elasto-Acoustic Problems

Aurélien Citrain*, Hélène Barucq**, Henri Calandra***, Julien Diaz****, Christian Gout*****

*INSA Rouen-Normandie Université LMI EA 3226, Team Project Magique3D (INRIA.UPPA.CNRS), **Team Project Magique3D (INRIA.UPPA.CNRS), ***TOTAL SA, ****Team Project Magique3D (INRIA.UPPA.CNRS), *****INSA Rouen-Normandie Université LMI EA 3226

ABSTRACT

Obtain accurate images of the underground is today the topic of a lot of studies. To do this, the simulations of elasto-acoustic waves has shown is efficiency and several numer- ical methods have been developed with the aim of a gain of accuracy and reducing at best the computational costs. Among them, Discontinuous Galerkin Method (DGM) has demonstrated is efficiency when the use of unstructured grid is necessary to approach complicated geometries. When it comes to structured meshes, Spectral Element Method (SEM) is preferred in particular because it's re- quire a lower computational burden. In this work, we propose to couple these two methods when the propagation media is rep- resentated by an hybrid mesh composed of unstructured and structured cells, with the aim of reducing the computational costs. For example, when the medium include a layer of water and the use of unstructured grid is not necessary. Here, we're interested with time-dependent problem, so we have a need of doing stability analysis in order to find the optimal CFL condition. In this presentation, we will describe the methodology of coupling DG-SEM and establish the stability of the method using various time scheme. Then, some numerical results will be presented to show the efficiency of the method in particular we will made a comparison of the computational costs between the ones of DG-SEM and those of DGM and SEM.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Migrating a Production Multiphysics Finite Element Code to Next-generation and Heterogeneous Architectures Using the Kokkos Abstraction Layer

Jonathan Clausen*, Victor Brunini**, Mark Hoemmen***, David Noble****, Christian Trott*****

*Sandia National Laboratories, **Sandia National Laboratories, ***Sandia National Laboratories, ****Sandia National Laboratories, *****Sandia National Laboratories

ABSTRACT

High-performance computer architectures have increasingly fine-grained and heterogeneous forms of parallelism. This makes the traditional approach to parallelism in scientific applications, using the Message Passing Interface (MPI) for coarse-grained distributed-memory parallelism with no threads within MPI processes, may no longer give best performance on many future computers. The SIERRA Aria thermal/fluid application has a large, complex production codebase developed in C++ over the past few decades. Aria's core computational kernels rely on C++ features like dynamic polymorphism, which are good for software productivity, but take some care to work correctly and perform well on some computer architectures. Key to managing the complexities associated with programming for many-core and heterogeneous architectures is the use of Kokkos (http://github.com/kokkos/kokkos), an abstraction layer for shared-memory parallel programming and thread-scalable data structures that supports a variety of back ends including openMP and CUDA. In this talk, we discuss the strategies used to provide portable performance on newer architectures while maintaining a clean, sustainable codebase in the Aria production code. "Portable performance" means we can write computation kernels once and have these kernels run efficiently on different architectures. Accordingly, we present work on the use of Kokkos data structures and parallel constructs, Single Instruction Multiple Data (SIMD) instructions, as well as other code structures within prototype and production applications to demonstrate their impact. Application performance when running on CPU architectures such as Intel Sandy Bridge, Haswell and Knights Landing processors, as well as GPU-based architectures is shown. Also, the relative merits of threading, hyperthreading, and SIMD vectorization on Intel platforms are discussed. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Tailoring VMS-based FEM for Different Boundary Value Problems

Ramon Codina*

*Universitat Politècnica de Catalunya

ABSTRACT

The Galerkin finite element approximation of many boundary value problems may suffer instabilities arising from different origins. The main two groups are those appearing in singularly perturbed problems, such as plates with small thickness or convection-diffusion problems with small diffusion, and those in which there is a compatibility condition in the interpolation spaces for the unknowns, such as the Stokes or the Darcy problems. Furthermore, instabilities may arise for a given problem just by changing the space where the solution is sought. The power of the VMS approach is demonstrated by the fact that it has served us to design stabilized finite element methods in all cases we have tried, ranging from flow problems (incompressible, compressible, low Mach, viscoelasticity) to solid mechanics problems (damage, plasticity, plates) and waves and electromagnetism. There are of course may aspects that deserve improvement, the most important being the design of the stabilization parameters, but definitely experience has shown that VMS is certainly a paradigm in computational mechanics.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Immersed Boundary Hierarchical B-spline Method for the Numerical Simulation of Nano-Scale Electromechanical Transduction

David Codony*, Onofre Marco**, Sonia Fernández-Méndez***, Irene Arias****

*Universitat Politècnica de Catalunya, **Universitat Politècnica de Catalunya, ***Universitat Politècnica de Catalunya, ****Universitat Politècnica de Catalunya

ABSTRACT

Continuum modeling of physical phenomena at the micron- and sub-micron scales requires high-order continuum theories in order to take into account size or length-scale effects. This is the case of relevant micronscale electromechanical transduction mechanisms such as flexoelectricity: a two-way electromechanical coupling between strain-gradient and electric polarization fields. To this end, we consider the generalized continuum model in [1], which describes the flexoelectric coupling as a fourth order partial differential equation, with displacements and electric potential as the only mechanical and electrical unknowns. The high-order nature of the PDE requires C1-continuous solutions, so the standard Finite Element Method (FEM) is not suitable, and advanced discretization methods are required such as the Meshfree Method [1] and the Mixed FEM [2]. These methods are relatively expensive, the former uses C∞ smooth basis functions with expensive evaluation and integration, whereas the latter increases the number of unknowns to circumvent the smoothness requirement. Here, we propose an alternative numerical method based on an Immersed Boundary HB-spline approach. (Hierarchical) B-spline basis functions provide high-order continuity of the original unknowns and are efficiently evaluated and integrated. Since they are globally defined on a Cartesian parametric space, we consider a regular Cartesian mesh and make use of the Immersed Boundary concept to permit simulations on arbitrary domain shapes, which can be exactly represented. High-order numerical integration is specifically performed on each cut cell [3]. Boundary and interface conditions are weakly enforced by means of the Nitsche 's method. This high-order method is particularly attractive, since it can capture the exact geometry of the domain, can easily handle material inclusions and interfaces, considers spatial resolution adaptivity, can be easily extended to shape optimization and permits parallel computation. We present the particularization of the Nitsche 's method to the formulation in [1] and show numerical examples of electromechanic transduction at small scales, including conductive inclusions and multi-material setups of particular engineering interest. References [1] A. Abdollahi, D. Millán, C. Peco, M. Arroyo, and I. Arias. Phys. Rev. B, 91:104103 (2015) [2] S. Mao, P. K. Purohit, and N. Aravas, Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences, 472(2190) (2016) [3] O. Marco, R. Sevilla, Y. Zhang, J. J. Ródenas, and M. Tur, International Journal for Numerical Methods in Engineering, 103(6): 445468 (2015)

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Strength-oriented Design of Periodic Microstructures Using Topology Optimization

Pedro Coelho*, José Guedes**, Hélder Rodrigues***, João Cardoso****

*UNIDEMI-UNL Portugal, **IDMEC Portugal, ***IDMEC Portugal, ****UNIDEMI-UNL Portugal

ABSTRACT

Topology optimization problems with stress based criteria are of special interest in engineering practice because they provide not only very efficient designs but also ones where the material strength is not compromised [1]. However, contributions from topology optimization in material microstructure design with stress criteria have been scarce. The present work addresses topology optimization of a material unit-cell mixing void and solid phases taking into account and controlling the induced stress distribution. The optimal topology is defined on the top of a finite element mesh with the help of density based design variables. However, due to the highly non-linear stress distribution verified in most cases it is required an appropriate finite element discretization. With that purpose one pursues here the h-refinement method. Finally, a level of mesh discretization is selected balancing stress predictions accuracy with computational time cost. The stress-design singularity problem in topology optimization with stress constraints is solved through relaxation techniques such as the epson-approach and the qp-approach [2]. The local nature of the stress constraint implies that the optimization problem number of constraints is the same order of the total number of the problem design variables. The computational cost of this "point-wise" control of stresses is then significant but softened in the scope of the present work through the application of parallel computing techniques. The topology optimization problem is formulated as the material volume minimization on the density variables subject to stiffness and stress constraints. The unit-cell response to an external applied load is obtained through homogenization [3]. Simple load cases (biaxial and shear) are considered leading to symmetries both in density and stress distributions. The obtained strength-oriented optimal lay-outs are compared to results published in the literature for validation.
Acknowledgements: This work was partially supported by the Portuguese Foundation for Science and Technology, FCT-Portugal, through the projects UID/EMS/00667/2013, UID/EMS/50022/2013 and PTDC/EMS-PRO/4732/2014.
[1] Duysinx P, Bendsøe MP (1998) Topology optimization of continuum structures with local stress constraints. Int J for Num Meth in Engng 43(8): 1453-1478 [2] Bruggi M, Duysinx P (2012) Topology optimization for minimum weight with compliance and stress constraints. Struct Multidisc Optim 46: 369-384 [3] Guedes JM, Kikuchi N (1990) Preprocessing and postprocessing for materials based on the homogenization method with adaptive finite element method. Comput Meth Appl Mech Engng 83: 143-198

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Impacts of Topology Optimization Method Choice on Designing for Prescribed Structural Frequency Response

Peter Coffin*, Tyler Schoenherr**

*Sandia National Lab, **Sandia National Lab

ABSTRACT

Density methods for topology optimization typically rely on the interplay between objective and constraints that are penalized differently to minimize intermediate material. This presentation will discuss fundamental method choices as applied to the problem of fixture design, where the objective is to generate fixture geometry that has structural frequency response matching that of a prescribed next level assembly. In this design problem, a volume or mass constraint may not be desired or active, impacting the effectiveness of common density methods. The Solid Isotropic Material with Penalization (SIMP) density method and an explicit Level-Set Conformal Decomposition Finite Element Method (LS-CDFEM) will be compared for this design problem. Additionally, regularization via quantities such as static response and common geometric measures will be investigated. The advantages and disadvantages of these different methods will be discussed regarding generating the most useful and physically realizable designs.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Sensitivity Analysis and Uncertainty Quantification of a 1D Fluids Model of the Pulmonary Circulation

Mitchel Colebank*, Mette Olufsen**, M. Umar Qureshi***, Naomi Chesler****, Dirk Huismeier*****

*Biomathematics Graduate Program, North Carolina State University, Raleigh, NC, USA, 27695-8205, **Department of Mathematics, North Carolina State University, Raleigh, NC, USA, 27695-8205, ***Department of Mathematics, North Carolina State University, Raleigh, NC, USA, 27695-8205, ****Department of Biomedical Engineering and Madison, University of Wisconsin at Madison, WI, 53706-1609 USA, *****School of Mathematics & Statistics, University of Glasgow, Glasgow, G12 8QQ, U.K.

ABSTRACT

For decades fluid dynamics models have been used to predict flow and pressure wave propagation in the cardiovascular system [1]. More recently focus has shifted to fitting these measured waveforms to data and on obtaining geometries from imaging [2]. However, little work has been done to understand how error in image segmentation impacts fluid dynamics. This is of particular importance in network models, since at each bifurcation the vessel dimensions change significantly. In the pulmonary vasculature, networks branch rapidly and hence the dimensions of each vessel change in concert. While vascular networks are similar from organism to organism, connectivity of the vessels may vary drastically. This study addresses uncertainty in blood flow and pressure predictions from 1D networks extracted from micro-CT images together with flow and pressure measurements from control mice. 1D Networks are extracted from micro-CT images from C57BL6/J mice (Jackson Laboratory, Bar Harbor, ME) using global thresholding techniques, where smoothness and lower threshold limits in the network segmentation are varied. To obtain the rendered networks, we fix the number of steps for a semi-automated contour evolution algorithm. The 1D network is obtained by calculating centerlines, connected at the barycenter of each junction. All vessel segments are assumed straight with a radius defined as the mean over the vessel, calculated away from the junction. Fluid dynamic predictions are obtained by solving the 1D Navier-Stokes equations combined with a linear constitutive equation relating pressure and area [2-4]. At junctions, pressure is assumed continuous and flow is conserved. A measured flow profile is applied at the inlet and a three element Windkessel boundary condition is attached at each terminal vessel. Similar to previous studies [3] nominal parameter values were calculated using imaging data and available flow and pressure data. Each simulation is computed using a variable geometry, where the variance of each vessel's dimensions comes from 20 a priori segmentations of one micro-CT image. Since a measured inflow is attached at the inlet, the main variations are associated with predictions of pressure and vessel area. Results reveal significant variation within the network, emphasizing model sensitivity to geometric parameters. Uncertainty is also associated with outflow boundary conditions, vessel stiffness, and the inflow profile [4]. [1] van de Vosse et al. (2011) Annu Rev Fluid Mech, 43:p467 [2] Qureshi et al, (2014) Biomech Model Mechanobiol 13: p1137 [3] Qureshi et al. (2017) arXiv:1712.01699 [physics.flu-dyn] [4] Paun et al. (2017) Stat Neerl, in press.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Nonreciprocal Elastodynamical Waves Using Programmable Metacomposite

Manuel Collet*, Sami Karkar**, Kaijun Yi***

*LTDS, CNRS, Ecole Centrale de Lyon, **LTDS, CNRS, Ecole Centrale de Lyon, ***LTDS, CNRS, Ecole Centrale de Lyon

ABSTRACT

Research activities in smart materials and adaptive structures are of a great interest for many years. In order to implement new vibroacoustic functionalities inside complex coupled metacomposite, new technologies are now available which allow integration of dense and distributed set of smart materials, electronics, chip sets and power supply systems for implementing distributed control strategies. It is also possible to develop the next generation of smart “composite” structures also called adaptive metacomposite. By using such an integrated distributed set of electromechanical transducers, one can imagine to control vibroacoustic flow in a large frequency band and implement unconventional behavior such as non-reciprocal wave propagation. Time-space modulated structures (or dynamic structures) possess properties modulated both in time and space that can be program inside adaptive metacomposite with suitable technologies. This contribution gives a comprehensive understanding of the behaviors induced by dynamic structures and proposes some technological implementations. Reflection and transmission of elastic waves incident on dynamic structures are numerically studied using a specific using of multiple scattering theory. It is shown that the scattering matrix directly describes all the unconventional wave propagation phenomena induced by time-space modulated metacomposite in specific situations. Results show that multiple Bloch modes are stimulated in dynamic structures by incident harmonics, these modes lead to the observed unusual wave conversion phenomena. Practical implementations are also discussed and mechanical diodes are proposed.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Mesoscale Multiphysics Modeling of Ablation in Composite Thermal Protection System Materials Using the Conformal Decomposition Finite Element Method

Lincoln Collins*, Scott Roberts**

*Sandia National Laboratories, **Sandia National Laboratories

ABSTRACT

Thermal protection systems (TPS) for aerospace applications are commonly used to protect vehicles from intense heat fluxes experienced during flight. These TPS materials are typically comprised of a fibrous fabric encompassed in a phenolic resin. When exposed to the heat fluxes of atmospheric re-entry, heat is dissipated through the ablation of the resin by pyrolysis, causing its recession through the fiber matrix and the release of products that react with the remaining charred porous material. The performance of these systems is dictated by the microstructural features of the composite governing its behavior in a complex multi-physical system coupling thermal transport, reactive fluid transport, mechanical stress formation, and re-radiation. At the mesoscale, modeling the ablation requires an accurate description of surface recession and tracking the changing interface of the resin phase coupled with the gas-phase transport of product gases. Using a simplified description of the resin decomposition chemistry, we focus on the mesoscale modeling of this process. Multiple level-set formulations are used to describe the various phases: a stationary background mesh generated using either analytical parameterizations or tomographic data describes a representative woven fabric, and a dynamic, conformal mesh describes the receding resin domain. The Conformal Decomposition Finite Element Method (CDFEM) is used to dynamically decompose a background tetrahedral mesh into conformal material domains. This conformal interface treatment is required to characterize the pyrolysis surface chemistry. Effective thermal-mechanical properties and ablation rates are calculated for the domain as a function of recession. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy 's National Nuclear Security Administration under contract DE-NA0003525.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Simulation of Geomechanical Processes Using Viscoelastoplastic Models for Solid Mechanics with Large Deformations

Oriol Colomés*, Guglielmo Scovazzi**, Nabil Abboud***, Nabil Atallah****

*Duke University, **Duke University, ***Duke University, ****Duke University

ABSTRACT

In this work we propose a quasi-static formulation for the solid mechanics problem to simulate buoyant instabilities of salt layers under rock formations. We consider visco-elasto-plastic constitutive models to characterize the mechanical properties of the rock and salt formations. Our approach enables the characterization of materials with different constitutive models, one for each layer. A variational multiscale (VMS) approach is used to stabilize the numerical instabilities that appear when incompressible materials are considered. With this method, simple linear tetrahedral Finite Elements can be used. To accurately characterize large deformations of the soil, an Arbitrary Lagrangian-Eulerian (ALE) formulation is used, together with a remeshing strategy. The different layers of the salt and rock are modelled using an embedded approach with explicit interfaces, in which the layer surfaces are embedded in a background mesh, avoiding the need of generating meshes of complex geometries. The interfaces between different materials are defined by a given surface mesh, which is then advected according to the material motion. With the explicit treatment of the interfaces, less numerical dissipation is introduced, having a more accurate definition of the interface position than, for instance, level set methods.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

On Characterizing the Viscous and Porous Effects in Human Brain Tissue

Ester Comellas*, Silvia Budday**, Jean-Paul Pelteret***, Paul Steinmann****

*University of Erlangen-Nuremberg (FAU), **University of Erlangen-Nuremberg (FAU), ***University of Erlangen-Nuremberg (FAU), ****University of Erlangen-Nuremberg (FAU)

ABSTRACT

Adequate characterization of human brain tissue rheology is crucial to obtaining meaningful computational predictions within a clinical context. Experimental evidence shows that the essential features of brain tissue are nonlinearity, preconditioning, hysteresis, and tension-compression asymmetry [1]. Past work in our group has characterized brain tissue using a finite viscoelastic material model [2]. The obtained results support the hypothesis that brain tissue behaviour is characterized by at least two different time scales. Herein, the longer time scale seems to be associated with the poroelastic interaction of fluid flowing within the solid network of cells and extracellular matrix in the tissue. The shorter one seems to be attributed to the viscoelastic nature of the solid skeleton itself, primarily due to fluid flow inside the cells. The monophasic viscoelastic model can only implicitly capture the porous effects of the longer time scale. To address this shortcoming, we have developed a biphasic nonlinear poro-viscoelastic model to further explore the role of viscous and porous effects in human brain tissue. Within the framework of the theory of porous media, we treat the material as an immiscible aggregate of a nonlinear viscoelastic solid skeleton saturated with pore fluid. Using the deal.II finite element library [3], the governing equations are linearised with automatic differentiation techniques, and a monolithic scheme is used to solve for the unknown solid displacements and fluid pore pressure values. Numerical examples are presented to verify and validate our results with the experimental data available. Our work serves to further elucidate the rheology of brain tissue. We anticipate the insights gained in the characterization of the poro-viscoelastic behaviour of brain tissue will contribute to the future development of clinically relevant predictive and preventive computational approaches to treat trauma-related brain pathologies. References [1] S. Budday, G. Sommer, J. Haybaeck, P. Steinmann, G.A. Holzapfel and E. Kuhl, Rheological Characterization of Human Brain Tissue. Acta Biomater., 60:315–329, 2017. [2] S. Budday, G. Sommer, G.A. Holzapfel, P. Steinmann and E. Kuhl, Viscoelastic parameter identification of human brain tissue. J. Mech. Behav. Biomed. Mater., 74:463–476, 2017. [3] D. Arndt, W. Bangerth, D. Davydov, T. Heister, L. Heltai, M. Kronbichler, M. Maier, J.-P. Pelteret, B. Turcksin and D. Wells, The deal.II Library, Version 8.. J. Numer. Math., 25(3):137–146, 2017.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Improvements for Structural Model Interfacing between Non-conforming Meshes

Simone Coniglio*, Christian Gogu**, Joseph Morlier***

*Airbus\ISAE\Université de toulouse, **UPS\Université de Toulouse, ***ISAE\Université de Toulouse

ABSTRACT

The interfacing of non-conforming meshes arises in several practical situations in both structural and multi-disciplinary finite element analysis. In Structural finite element analysis this communication can pose some difficulties. In fact using a simple collocation scheme (i.e. imposing the kinematic continuity between interface surfaces trough interpolation [1]) artificial interface stiffening, gap openings or stress concentrations localized near the interface arise eventually. Hence in literature several methods were developed to alleviate these problems, for instance, by imposing kinematic continuity in an integral or weak. The mortar approach [2] is maybe one of the most popular approaches in this context. Nevertheless its computational burden and implementation complexity can be a limit for practical implementation. In the Fluid-Structure Interaction field a new approach, the Internodes [3], was proposed to achieve accuracy similar to Mortar, on the other hand reducing implementation and computational effort. This promising technique has been studied from a theoretical point of view and tested on patch tests and Fluid-Structure Interaction applications. This work will first compare on academic benchmark problems several approaches for interfacing non-conforming meshes, including the Mortar and Internodes approach. These approaches are compared according to several metrics: balance of forces and moments, displacement field error and displacements continuity, stress field error. Moreover a new approach that tries to achieve similar performance to Mortar but is simpler to implement is presented. Finally we note that most existing techniques can have issues with the non-satisfaction of Moment equilibrium at the interface. This problem is enhanced and quantified through several numerical experiences on the benchmark problems. A further contribution is proposed to satisfy “apriori” the mechanical moment equilibrium equation at non-conforming interface. This technique consists in a correction that can be applied to every technique tested in this work. After the proposed moment correction all techniques show better performance at a very small computational cost. 2. REFERENCES [1] Barlow John. Constraint relationships in linear and nonlinear finite element analyses. International Journal for Numerical Methods in Engineering. 1982;18(4):521–533. [2] Bernardi, Christine. "A new nonconforming approach to domain decomposition: the mortar element method. " Nonlinear partial equations and their applications (1989). [3] Deparis Simone and Forti. INTERNODES: an accurate interpolation-based method for coupling the Galerkin solutions of PDEs on subdomains featuring non-conforming interfaces. Computers & Fluids. 2016;141:22–41.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Higher-Order Asynchronous Coupling for Fluid-Fluid Interaction

Jeffrey Connors*

*University of Connecticut

ABSTRACT

The distribution of energy across space and time scales is quite different between the atmosphere and ocean. Therefore, codes for air-sea interaction are constructed by coupling together atmosphere and ocean components, each highly optimized using different numerical methods, by passing fluxes of conserved quantities between the components in the form of boundary conditions at the air-sea interface. For efficiency, the fluxes are usually asynchronous, meaning they are calculated using data extrapolated from previous times for at least one component. Moreover, these extrapolations are low-order accurate in terms of the time step size associated with the coupling interval. The accuracy may be improved via iteration, but this is expensive. In some cases, higher-order extrapolation in time may suffice to improve accuracy and circumvent or reduce iteration costs, but then stability considerations arise. For a simplified, model problem of fluid-fluid interaction, a rigorous stability analysis is performed for higher-order extrapolation of fluxes. A scaling analysis provides some intuition regarding the use of high-order extrapolation methods for climate or regional forecasting applications. Some computations are provided to illustrate different coupling configurations; that is, using low- versus high-order extrapolations and with or without iterations to tighten the coupling.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Quadrilateral Bi-cubic Conforming Finite Elements for Plates and Shells

Loredana Contrafatto*, Leopoldo Greco**, Massimo Cuomo***

*University of Catania - Italy, **University of Catania - Italy, ***University of Catania - Italy

ABSTRACT

In this work, we present a new formulation for a class of quadrilateral conforming finite elements for pure bending Kirchhoff plate problems and its extension to general shells. The rational enrichment of the cubic Bezier's basis, proposed by J. Gregory in 1974 for obtaining G1 continuous surfaces, is the starting point of the formulation. The element presents 20 degrees of freedom and can be generalized in the context of isogeometric analysis including the knot insertion operation and polynomial degrees different than 3. The rational interpolation is modified in order to obtain a formulation able to reproduce states of constant curvature that pass the patch test. Examples demonstrate that the proposed element presents optimal rate of convergence and presents high robustness with respect to mesh distortion even when non-structured meshes are considered.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Biomolecular Electrostatics Calculations Using Polarizable Force Fields in a Continuum Ionic Solvent, with Algorithmic and Hardware Acceleration

Christopher D Cooper*

*Universidad Técnica Federico Santa María

ABSTRACT

Rather than treating the solvent degrees of freedom explicitly, implicit-solvent models use continuum electrostatic theory to compute the mean-field potential in biomolecular systems. This yields a coupled system of partial differential equations, with the Poisson equation in the protein region (enclosed by the molecular surface), and the Poisson-Boltzmann equation in the exterior domain. The charge distribution inside the protein, due to the atomic charges, is modeled by force fields that usually place fixed point charges at the locations of the atoms. However, more elaborate force fields have emerged lately, which consider higher order multipoles, and polarizability. One popular force field of this type is AMOEBA, which describes the charge distribution with permanent point monopoles, dipoles, and quadrupoles, and allows for the dipole component to react to an external field. In this work, we present an implementation of the Poisson-Boltzmann solver PyGBe, that is compatible with the AMOEBA force field. PyGBe uses a boundary integral formulation of the system of partial differential equations, and solves it numerically with a boundary element method. Moreover, it uses a treecode algorithm to accelerate a quadratically scaling matrix-vector product to O(NlogN), and offloads the most computationally intensive parts to a GPU card. To account for polarizability, we solve for the electrostatic potential with self-consistent iterations, so that the induced dipole component converges. The boundary integral formulation treats the point multipoles inside the protein analytically, which is an important advantage compared to volumetric solvers, where the multipolar charge distribution needs to be interpolated to a mesh. Furthermore, preliminary results show that the multipolar representation of the protein has a small effect on the mesh sizes required to correctly resolve the electrostatic potential, making a boundary integral formulation ideal for implicit-solvent calculations using AMOEBA. For the conference, we will present details of our implementation in PyGBe, and validation results using analytical expressions and small molecules. Also, we will show calculations with larger biomolecules, assessing the performance of the boundary integral formulation in a polarizable and multipolar description of the charge distribution.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Adaptive Simulation of Plates and Shells with Hierarchical B-Splines

Luca Coradello*, Annalisa Buffa**, Rafael Vázquez***

*École Polytechnique Fédérale de Lausanne, **École Polytechnique Fédérale de Lausanne, ***École Polytechnique Fédérale de Lausanne

ABSTRACT

The novel paradigm of Isogeometric Analysis (IGA) [1] applied to the Finite Element Method (FEM) has been a thriving area of research in recent years, aiming at closing the gap between design and analysis. In Computer Aided Design (CAD) the standard representation of shapes is obtained via the so-called Boundary Representation (B-rep), which eases the integration between CAD and dimensionally-reduced models such as plates and shells. Additionally, thanks to the higher inter- element regularity achievable with B-Splines compared to standard finite elements, fourth-order Partial Differential Equations (PDEs) (i.e. the governing equations of plates and shells) can be discretized in a straight-forward manner without the need of additional degrees of freedom. However, due to the tensor product nature of IGA, local refinement is a pivotal area of research in the IGA community. Moreover, how to properly capture sharp features in the solution and how to trigger an adaptive algorithm to resolve those features, are still wide open questions in mechanical problems.[2] In this work, we propose a new a-posteriori error estimator for plates and shells, which is com- putationally cheap and does not require the evaluation of the residual in a strong form. This is a crucial advantage, since the evaluation of the residual requires the computation of derivatives of shape functions up to order four (on a surface in case of a shell). Specifically, starting from the work of [3], we develop an adaptive algorithm for fourth-order PDEs, which is simple and performs well in steering adaptive simulations. Through several numerical examples on both smooth and singular benchmarks we show the reliability and efficiency of the proposed method. References: [1] Hughes, T.J.R., Cottrell, J.A. and Bazilevs, Y. “Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement”, Computer methods in applied mechanics and engineering, page 4135-4195, (2005) [2] Buffa, A. and Giannelli, C. “Adaptive isogeometric methods with hierarchical splines: error estimator and convergence”, Mathematical Models and Methods in Applied Sciences, page 1-25 (2017). [3] Bank, R.E. and Kent Smith, R. “A Posteriori Error Estimates Based on Hierarchical Bases”, Society for Industrial and Applied Mathematics, page 921-935 (1993).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Evaluation of Residual-based Turbulence Models on the Drag and Lift Computations of Risers with Helical Strakes

Adriano M. A. Cortes*, Erb F. Lins**, Paula A. Sesini***, Renato N. Elias****, Alvaro L. G. A. Coutinho*****

*Federal University of Rio de Janeiro, **Federal University of Para, ***Federal University of Rio de Janeiro, ****Federal University of Rio de Janeiro, *****Federal University of Rio de Janeiro

ABSTRACT

Risers are one of the most critical structures in the offshore production of Oil and Gas. Due to hydrodynamics loads and Vortex-induced vibrations (VIV) caused by sea currents, they suffer intense material fatigue, possibly implying severe damage to them. To avoid this setback, different strategies have been applied by the O&G industry to reduce such vibrations (VIV). One of those strategies, classified as passive VIV suppressors, consists of attaching helical strakes to the riser surface. To evaluate the efficiency of the strakes addition becomes mandatory to estimate and predict the drag and lift forces. Besides experimental investigations, for example [1], numerical simulations are successful tools to tackle such challenge. An additional issue regarding the numerical investigations, in this case, is the turbulent regime of the flow. To address this matter, we used the residual-based variational multiscale (RB-VMS) framework, an implicit LES scheme with a scale separation given a priori by a proper decomposition of the fields ' spaces [2,3]. Based on the considerations in [2] we investigate different eddy viscosities within the RB-VMS framework and evaluate their influence in the drag and lift forces computations. The simulations are done with our in-house incompressible flow solver, EdgeCFD [3], a hybrid MPI+OpenMP parallel edge-based implementation of the RB-VMS method. [1] Y. Gao, J. Yang, Y. Xiong, M. Wang and G. Peng, Experimental investigation of the effects of the coverage of helical strakes on the vortex-induced vibration response of a flexible riser. Applied Ocean Research, 2016. [2] A. A. Oberai and T. J. R. Hughes, A palette of fine-scale eddy viscosity and residual-based models for variational multiscale formulations of turbulence. Computational Mechanics, 2016. [3] E. F. Lins, R. N. Elias, G. M. Guerra, F. A. Rochinha and A. L. G. A. Coutinho, Edge-based finite element implementation of the residual-based variational multiscale method. Int. J. Numer. Meth. Fluids, 2009.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

An HDG Formulation for the Two-phase Flow through Porous Media Simulations

Albert Costa-Solé*, Eloi Ruiz-Gironés**, Josep Sarrate***

*Universitat Politècnica de Catalunya, **Barcelona Supercomputing Center - BSC, ***Universitat Politècnica de Catalunya

ABSTRACT

Two-phase flow through porous media problems are commonly solved in petroleum reservoir simulation, specifically, during the secondary phase of the oil recovery process. This stage starts when the natural pressure difference between the reservoir and the surface is not high enough to move the hydrocarbons upward. In order to mobilize the oil (non-wetting phase) to the production wells and to keep the flow rate, water (wetting phase) is injected through the reservoir, [1]. We assume that both phases and the rock are incompressible and phases are inmiscible and occupy the reservoir porosity. The governing equations are obtained from combining, for each phase, mass conservation with Darcy's law, leading to a coupled non- linear system of transient PDE's, [2]. Oil companies are interested in using unstructured meshes to obtain a better representation of the reservoir geometry complexity and also to obtain high-accuracy solutions, [2]. All of these requirements are achieved by high-order continuous Galerkin formulations. Nevertheless, local mass conservation can also be achieved by using a discontinuous and hybridizable Galerkin formulation (HDG) [3]. One of the main advantages of this method, is that when a time integration algorithm of order p+1 is used in conjunction with element-wise polynomials of degree p ? 0, the scalar unknowns and their fluxes converge with order p+1 in the L2-norm, [3]. Moreover, the scalar unknowns can be post-processed in order to obtain a convergence rate of p+2 in the L2-norm. We present a novel high-order HDG formulation to solve the two-phase flow problem in a heterogeneous porous media, taking into account all the mentioned assumptions. In particular, we apply a high-order HDG formulation in the spatial discretization, combined with a DIRK method for the time discretization. This leads to an implicit scheme for both the pressure and the saturation unknowns. Finally, we assess the efficiency and the main features of the proposed HDG formulation showing several 2D and 3D simulations with homogeneous and heterogeneous material properties. [1] Z. Chen, G. Huan and Y. Ma, Computational methods for multiphase flows in porous media, Siam, Vol. II, 2006. [2] Y. Epshteyn, B. Rivière, Fully implicit discontinuous finite element methods for two-phase flow, Appl. Numer. Math. 57 (2007), no. 4, 383– 401. [3] N.C. Nguyen, J. Peraire and B. Cockburn, An implicit high-order hybridizable discontinuous Galerkin method for nonlinear convection- diffusion equations, J. Comput. Phys. 228 (2009), no. 23, 8841–8855.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Influence of Material Heterogeneity on the Stability of Explicit High-Order Spectral Element Methods

Regis Cottereau*, Ruben Sevilla**

*CNRS, CentraleSupélec, Université Paris-Saclay, **Swansea University

ABSTRACT

Summary: The paper proposes several stability estimates for wave propagation in random heterogeneous media with high-order spectral elements, generalizing classical CFL conditions. This talk [1] describes precisely the influence of material heterogeneity on the stability of explicit time marching schemes for the high-order spectral element discretisation of wave propagation problems. Two different types of heterogeneity are considered. In a first part, it consists in a periodic fluctuation of the density and stiffness parameters, whose period is related to the characteristic element size of the mesh. A new stability criterion is derived analytically for quadratic and cubic one dimensional spectral elements in heterogeneous materials, which may in some situations replace the current rule of thumb. The analysis presented reveals the origin of instabilities that are often observed when the stability limit derived for homogeneous materials [2] is adapted by simply changing the velocity of the wave to account for the material heterogeneity. In a second part, a more complete heterogeneity is considered and precise stability estimates are obtained based on Irons and Treharne theorem [3] and general eigenvalue bounds. Finally, in a third part, very simple estimates are obtained for rapidly fluctuating media. Several extensions of the results are discussed, including higher order approximations, higher dimensions and random media. Extensive numerical results demonstrate the validity of the new stability estimates. REFERENCES [1] R. Sevilla and R. Cottereau, Influence of material heterogeneity on the stability of explicit high–order spectral element methods. Submitted for publication in Comput. Phys., 2017. [2] G. Cohen, Higher-order numerical methods for transient wave equations, Springer, 2001. [3] A. J. Wathen. An analysis of some element-by-element techniques. Comput. Meth. Appl. Mech. Engr. 74, pp. 271-287, 1989.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Structural Optimization of Jackets for Offshore Wind Turbines under Dynamic Loading

Iván Couceiro*, Raquel Guizán**, José París***, Fermín Navarrina****, Xesús Nogueira*****, Ignasi Colominas******, Manuel Casteleiro*******

*Universidade da Coruña, **Universidade da Coruña, ***Universidade da Coruña, ****Universidade da Coruña, *****Universidade da Coruña, ******Universidade da Coruña, *******Universidade da Coruña

ABSTRACT

The design of bottom fixed steel substructures as supports for offshore wind turbines is a very demanding task in terms of computational resources. The analysis of the structural behavior is not straightforward nor conventional and also hard to be assessed with the required accuracy. And the complexity of the problem rises to a much higher level when the optimization of the structure is simultaneously addressed. For this reason, most of the approaches that have been proposed so far require important simplifications of the structural model, the loading conditions or the dynamic response, what gives rise to a significant loss of accuracy in the results. In this work we present a methodology for the dynamic response shape and sizing optimization of offshore jackets under Ultimate Limit Stress, Fatigue Limit State and frequency constraints. The structural analysis takes into account the rotation of the blades, and the whole structure -including the jacket, the tower, the rotor-nacelle assembly and the blades- is modeled as a whole, in order to capture the coupled dynamic behavior. Time integration is based on the Non-Linear Newmark algorithm. Wave and wind loading are considered and fatigue damage is assessed in terms of S-N curves [1] by means of the Palmgren-Miner rule and the Rainflow algorithm for counting stress cycles. The optimization process is addressed by means of a Sequential Linear Programming type algorithm, which requires performing the first order full sensitivity analysis. The sensitivities are obtained through Direct Differentiation, which is clearly more efficient than the Adjoint State Method in this case [2]. The optimization results show fair robustness of the algorithm when facing different problems, and substantial reductions in the weight of the steel jackets are obtained. The optimized designs are strongly conditioned by all the types of imposed constraints. As a general rule, the structural sizing is mostly determined by the fatigue constraints, while the frequency constraints have a major impact on the final shape and how the design is driven through the optimization process. [1] DNV-RP-C203 Fatigue design of offshore steel structures. Det Norske Veritas, 2011. [2] F. Navarrina, S. López-Fontán, I. Colominas, E. Bendito, M. Casteleiro, High order shape design sensitivity: a unified approach. Computer Methods in Applied Mechanics and Engineering, 188: 681-696, 2000.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Implicit Boundary and Anisotropic Mesh Adaptation, Immersed Method and Stabilized Finite Element for Multiphase Flow Simulation

Thierry Coupez*, Elie Hachem**, Hugues Digonnet***, Luisa Rocha Da Silva****

*MINES ParisTech, **Mines ParisTech, ***Ecole Centrale de Nantes, ****Ecole Centrale de Nantes

ABSTRACT

A wider use of numerical simulation is still depending on meshing and adaptive meshing capabilities when complex geometry, multi-domain, moving interface and multiphase flow are involved. This task becomes more and more difficult when it is combined with a posteriori adaptive meshing or/and dealing with moving interfaces and boundary layers and also when running on massively parallel computers. In order to overcome the lack of flexibility of the common body fitted method, the alternative proposed here, is based on an implicit representation of the interfaces by a local distance function using a hyperbolic tangent filter. Therefore, the geometries can be interpolated and contribute to the numerical error which is detected by an a posteriori error estimator technique. This approach favors the full usage of anisotropic adaptive meshing techniques providing an optimal capture of the interfaces within the volume mesh, whatever is the complexity of the geometry involved. From the flow solver side, unstructured meshes with highly distorted elements (however solution aligned) need to rely on a robust solution framework. The interface condition transfer is enforced by following the immersed boundary/volume (IVM) methodologies for fluid/fluid and or fluid/structure interaction. The proposed multiphase flow solver, including a related local level set technique is based on a stabilized finite element method (VMS) that can afford with anisotropic meshing with high aspect ratio elements. For transient flow a complete stabilization approach including the interface stabilization term and the dynamic of the subscales will be proposed with a quasi-optimal calculation of the stabilization parameter. The error estimation and the metric calculation will be presented and various application examples will be proposed. [1] T. Coupez, E. Hachem, “Solution of high Reynolds Incompressible Flow with Stabilized Finite Element and Adaptive Anisotropic Meshing”, Comp. Meth. in App. Mech. and Engng Vol. 267, pp. 65-85, (2013) [2] T. Coupez, L. Silva, E. Hachem, Implicit boundary and adaptive anisotropic meshing, SEMA SIMAI Springer Series, Vol. 5, pp. 1-18, (2014) [3] L Silva, T Coupez, H Digonnet, Massively parallel mesh adaptation and linear system solution for multiphase flows, International Journal of Computational Fluid Dynamics 30 (6), 431-436, (2016) [4] E Hachem, S Feghali, T Coupez, R Codina 2015 ‘A three?field stabilized finite element method for fluid?structure interaction: elastic solid and rigid body limit’, International Journal for Numerical Methods in Engineering 104 (7), 566-584

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Integrating In-Situ Data Analysis and Visualization on libMesh Library

Alvaro Coutinho*, Patrick Valduriez**, Jose Camata***, Vitor Silva****, Daniel de Oliveira*****, Marta Mattoso******

*COPPE/UFRJ - Brazil, **Inria and LIRMM - France, ***DCC/UFJF - Brazil, ****COPPE/UFRJ - Brazil, *****IC/UFF - Brazil, ******COPPE/UFRJ - Brazil

ABSTRACT

In situ data analysis and visualization have been used successfully in large-scale computational simulations to extract and visualize scientific data of interest. Such data are obtained from partial (or final) simulation results, and typically stored in raw data files. However, existing In Situ Data Analysis and Visualization (ISAV) solutions have limited online query processing and no support for dataflow analysis. The latter is a challenge for exploratory raw data analysis. In this work, we propose a solution that integrates a dataflow analysis tool, DfAnalyzer, with ParaView Catalyst for performing ISAV and monitoring dataflow from simulation runs. DfAnalyzer contributes with dataflow analyses to monitor the simulation evolution by grouping parameters, associating input data and parameters to solver convergence data, all coupled to ParaView visualizations. We validate our approach solving particle-laden flows using an adaptive mesh refinement and coarsening (AMR/C) solver built on top of the libMesh library. The model involves solving the Navier-Stokes equations coupled to a transport equation for the sediment concentration. The Navier-Stokes equations are discretized by a finite element residual-based variational multiscale formulation, while the transport equation uses a stabilized finite element formulation with discontinuity capturing. The online dataflow query support helps to investigate the effects on the physics of the problem when exploring different input parameter values. Queries can track the sediment concentration (e.g. should be less or equal to 1) at different time steps. This analysis requires relating them to the input parameters, such as time adaptivity control method, AMR/C parameters and the nonlinear tolerance for the flow and sediments solvers. Another example is monitoring the flow and transport sedimentation solver convergence (final linear and nonlinear residuals), and relate them to the images generated by Catalyst visualization pipeline for each time step. Our experimental results show that our approach yields a rich data analysis support with negligible overhead.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Numerical Simulation of Pipeline Flotation in Liquefied Sand

Massimiliano Cremonesi*, Federico Pisanò**, Gabriele Della Vecchia***

*Politecnico di Milano, Italy, **TU Delft, Netherlands, ***Politecnico di Milano, Italy

ABSTRACT

Submarine pipelines are widely employed to transport hydrocarbons through the ocean from wells to production and distribution plants. Pipelines are usually laid in trenches, either left open or filled with sand. Pipelines in trenches are typically exposed to soil liquefaction. This phenomenon can be triggered by wave action, earthquakes or tidal fluctuations leading to very large pipeline displacements. The present work aims to present a numerical technique to analyze the pipeline flotation and sinking in liquefied sand. The Particle Finite Element Method has been adapted and extended to tackle this kind of problems [1,2]. The approach is based on the assumption of soil fully liquefied at the inception of pipeline flotation, which justifies the use of a one-phase fluid model [2]. A non-Newtonian Bingham-like constitutive law has been calibrated to describe the liquefied soil behavior. A simplified, soil mechanics based approach has been also introduced to include reconsolidation effects[3]. Soil-pipe interaction is reproduced via a staggered scheme. The numerical approach has been validated against experiential tests to show the effectiveness and robustness of the proposed techniques. [1] Cremonesi M., Frangi A., Perego U. (2010) A lagrangian finite element approach for the analysis of fluid-structure interaction problems. International journal for numerical methods in engineering 84, No. 5, 610-630 [2] Della Vecchia G., Cremonesi M., Viti A., Pisanò F. (2018) On the use of the dam breaking test for the rheological characterisation of liquefied sands. Géotechnique Letters, submitted for publication. [3] Pisanò F., Cremonesi M., Bortolotto F., Della Vecchia G. (2018) Feeding soil mechanics into the CFD analysis of pipeline flotation in liquefied sand Géotechnique, submitted for publication.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Modeling Size Effects in the Strength Statistics of Nanoindentation

Joshua Crone*, Jaroslaw Knap**

*US Army Research Laboratory, **US Army Research Laboratory

ABSTRACT

Nanoindention experiments reveal that the onset of plastic deformation occurs over a wide range of indenter loads when the indenter size approaches the mean dislocation spacing. Under these conditions, it has been shown that plastic deformation is due to the activation of pre-existing dislocations, rather than homogeneous dislocation nucleation. Quantifying the effect of dislocation density on the mean and variance of the critical indenter force has remained a challenge with current experimental capabilities. In the present work, we use discrete dislocation dynamics (DDD) simulations of indentation to quantify the effect of dislocation density and indenter size on the mean and variance of the critical force to induce plasticity. Furthermore, we employ DDD to identify the underlying dislocation mechanisms that lead to the onset of plastic deformation and pop-in. To include free surface effects and the highly varying stress field induced by the indenter, we couple the bulk DDD simulator, ParaDiS, with a parallel finite element solver. Simulations are carried out for multiple randomly seeded dislocation configurations at several dislocation densities in order to obtain a statistically relevant measure on both the mean and standard deviation of the critical force. Our results suggest a power law scaling for both the mean and standard deviation with respect to the dislocation density, which is in good agreement with the limited experimental work on quantifying this effect.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Multiscale Designer: Efficient Multiscale Simulation at the Structural Scale with Minimal Testing

Robert Crouch*, John Kytasty**, Jacob Fish***

*Altair Engineering, **Altair Engineering, ***Columbia University

ABSTRACT

Development of accurate computational models for composite materials presents two challenges for industry practitioners. Challenge one: the computational expense of homogenization based multiscale models make simulation at structural scales infeasible, often even when high performance computing capabilities are used. Multiscale Designer addresses this difficulty with a unique multiscale, reduced order modelling technique that maintains the physically meaningful parameters of multiscale models based on computational homogenization, while greatly reducing the computational burden. Challenge two: the input parameters of a multiscale models for a composite material are the properties of the constituent materials, e.g. carbon fiber and epoxy, and it is often not possible to fully characterize a complex constituent material such as carbon fiber by performing experiments on the constituent in isolation. Even if such experiments are possible, manufacturing processes often result in different in situ properties. Multiscale Designer addresses these difficulties by providing a multiscale calibration procedure that requires a minimum number of experimental tests to specify the material parameters. This approach to determining the parameters is based on rigorous inverse calibration, and within Multiscale Designer, this inverse calibration is automated and highly accessible to practicing engineers. In particular, stochastic approaches provide crucial insight into the reliability of the inverse solution, and can inform the analyst when the lack of a particular experimental observation negatively impacts the solution. The salient features of Multiscale Designer are: (i) arbitrary numbers of spatial scales, (ii) a unique model reduction scheme that reduces the computational cost of complex n-scale material systems, (iii) stochastic reverse engineering procedures that reliably identify material properties at multiple spatial scales, and (iv) seamless integration in major commercial finite element codes. We demonstrate the capabilities of Multiscale Designer by showing how to calibrate the constituent material parameters for a non-crimp fabric used in the automotive industry and then validating the model on structural scale component subjected to bending. The calibration and validation experiments were performed at General Motors, and the validation simulations were conducted using the Multiscale Designer plugin for the explicit finite element code Radioss.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Valve-Seat Contact Analysis in Internal Combustion Engine in Order to Predict and Reduce the Wear Level

Martial Crozet*, Benyebka Bou-Saïd**, Yves Berthier***, David Jones****, Mark Fowell*****

*INSA de Lyon/LaMCoS/Volvo, **INSA de Lyon/LaMCoS, ***INSA de Lyon/LaMCoS/CNRS, ****Volvo, *****Volvo

ABSTRACT

The valve / valve seat contact plays a significant role in determining the sealing of the combustion chamber as well as the flow of intake and the exhaust of gases, in an internal combustion engine. Any changes of this contact may lead to a reduction in engine performance and an increase in emissions, which can lead to increased maintenance cost and therefore reduced freight efficiency. Due to the continuous requirement to increase engine performance (i.e. increased cylinder pressure, reduce pollutant content and increased durability), the valve / valve seat contact may become a significant factor in future engine development. The aim of the current work is to improve the understanding of the factors affecting the wear of the valve / valve set contact and to enable better optimization of the system at the design stage, using both computational modelling and experimental measurements. To achieve this, a rigid body dynamic model coupled with finite element analysis has been developed in order to assess, the global valve motion as a function of the engine operating conditions, the vibration response of the system, and the local contact conditions at the valve / valve seat interface. Four distinct phases of relative valve / valve seat motion have been identified: 1. Impact between the valve and the seat. Impact speed is supposed to be controlled by the camshaft geometry. However, in the current study using measured camshaft geometry the impact velocity was shown to be underestimated by currently used industrial tools; 2. Macro scale sliding of valve in valve seat. Due to any geometrical misalignment, the valve can slide against the seat insert creating interfacial shear stress which may cause plastic deformation and 3rd body transformation; 3. Valve vibration during steady state, which can induce a fretting motion within the contact area; 4. Elastic deformation of the valve due to combustion pressure, resulting in sliding at the valve / valve seat contact interface. From this work, it has been possible to identify and correlate wear behaviour observed using SEM, with each of these distinct phases. From this it has been possible to highlight geometric parameters which may be adapted in the design process to reduce the severity of the contact conditions while maintaining a sufficient gas seal.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

An Adaptive Fixed-Mesh ALE Formulation for Free Surface Problems: Numerical Model and Experimental Validation

Marcela Cruchaga*, Ernesto Castillo**, José Flores***, Joan Baiges****

*Departamento de Ingeniería Mecánica, Universidad de Santiago de Chile, **Departamento de Ingeniería Mecánica, Universidad de Santiago de Chile, ***Departamento de Ingeniería Mecánica, Universidad de Santiago de Chile, ****Departamento de Ingeniería Civil y Ambiental, Universidad Politécnica de Cataluña

ABSTRACT

A free surface flow formulation is presented and applied to model a proposed experiment of an oil sloshing problem. The numerical technique encompasses an adaptive remeshing technique and an arbitrary Lagrangian-Eulerian stabilized fixed mesh finite element methodology. A level set approach is used to capture the moving interface. A sloshing experiment is reported with the aim to provide valuable data to validate the numerical model. The experiment consists of a rectangular tank filled with vegetable oil subjected to controlled vibrating motions. The free surface evolution is captured using a motion capturing technique. The study includes different filling depths and motion conditions, i.e., amplitudes and frequencies. The numerical results obtained with the proposed model are satisfactorily compared with experimental data.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Finite Viscoelasticity Model in Curvilinear Coordinates for the Nonlinear Dynamic Analysis of Cable Structures

Miquel Crusells-Girona*, Filip Filippou**, Robert Taylor***

*University of California, Berkeley, **University of California, Berkeley, ***University of California, Berkeley

ABSTRACT

This paper presents the formulation and validation of a finite viscoelastic material model in curvilinear coordinates that is suitable for the nonlinear dynamic analysis of cable structures under large displacements. The formulation is based on a general multiplicative decomposition of the deformation gradient in multiple viscous strains, and uses a quadratic evolution law in terms of the Kirchhoff axial force and of the Lie derivative of the left Cauchy-Green strains [1]. This material model is used with a mixed variational formulation of the catenary problem that allows a continuous and a discontinuous axial force distribution, and is thus capable of representing the axial force jump under concentrated forces [2]. The proposed finite viscoelastic material model is first used to represent the physical internal mechanisms and the air resistance that dissipate the high-frequency compression waves in flexible cables with different sag-to-span ratios [3]. The analyses of three simply-supported cables from the literature under large-amplitude free vibration [3] and one simply-supported cable under earthquake excitation show that a small relaxation time is effective in removing the undesired high-frequency contributions to the dynamic response. A model with multiple viscoelastic strains and large relaxation times is implemented in the mixed element to model the overall decay of the dynamic cable response. The same examples show that, for small displacements, results reduce to the infinitesimal approximation, while the nonlinear inelastic components account for the more general decaying behavior of the response with phase transitions and 3d coupling. In conclusion, the proposed viscoelastic material model and its numerical implementation constitute a generalization of existing cable formulations to curvilinear coordinates and large displacements. The resulting element and its numerical implementation are characterized by consistency, accuracy and numerical robustness. [1] S. Reese and S. Govindjee, “A theory of finite viscoelasticity and numerical aspects”, International Journal of Solids and Structures, 35, 3455-3482 (2013). [2] M. Crusells-Girona, F.C. Filippou and R.L. Taylor, “A mixed formulation for nonlinear analysis of cable structures”, Computers & Structures, 186, 50-61 (2017). [3] M. Crusells-Girona, F.C. Filippou and R.L. Taylor, “Nonlinear static and dynamic analysis of mixed cable elements”, Proceedings of the 14th International Conference on Computational Plasticity – Fundamentals and Applications. Barcelona, 2017.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Parametric Numerical Modelling of Thermally-bonded Nonwovens: Effect of Manufacturing Parameters

Vincenzo Cucumazzo*, Emrah Demirci**, Memis Acar***, Behnam Pourdeyhimi****, Vadim Silberschmidt*****

*Loughborough University, **Loughborough University, ***Loughborough University, ****North Carolina State University, *****Loughborough University

ABSTRACT

Nonwovens are engineered polymer-based materials with a microstructure made of randomly distributed fibres bonded together with mechanical, thermal or chemical techniques. Due to an anisotropic and nonlinear nature of their mechanical behaviour, modelling their mechanical performance is challenging. This becomes particularly complex for thermally-bonded nonwovens, since their mechanical response is not only influenced by material properties, but also by manufacturing parameters (e.g. shape, orientation and pattern of bond points and calendering temperature). In order to account for these effects, a novel subroutine-based parametric finite-element (FE) model was proposed in this research. Such a method allows automated modelling of nonwoven materials considering variability of their material and design parameters. The FE modelling approach was conducted within a continuous domain and incorporated an elastic-plastic constitutive material model to capture strain-hardening effects, large deformations and rotations. The obtained numerical results of these simulations were compared with experimental data obtained from tensile tests performed in various loading directions, namely, machine and cross directions. The developed numerical scheme will be improved further to include a damage model capable of describing various damage scenarios.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Thermodinamically Sound Data-driven Computational Mechanics

Elías Cueto*, David González**, Francisco Chinesta***

*Universidad de Zaragoza, **Universidad de Zaragoza, ***ENSAM ParisTech

ABSTRACT

In the paradigm of data-intensive science, automated, unsupervised discovering of governing equations for a given physical phenomenon has attracted a lot of attention in several branches of applied sciences. In this work we propose a method able to avoid the identification of the constitutive equations of complex systems, and rather work in a purely numerical manner by employing experimental data. In sharp contrast to most existing techniques, this method does not rely on the assumption on any particular form for the model (other than some fundamental restrictions placed by classical physics such as the second law of thermodynamics, for instance) nor forces the algorithm to find among a pre-defined set of operators those whose predictions fit best to the available data. Instead, the method is able to identify both the Hamiltonian (conservative) and dissipative parts of the dynamics while satisfying fundamental laws such as energy conservation or positive production of entropy, for instance. The proposed method is tested for some examples of discrete as well as continuum mechanics, whose accuracy demonstrate the validity of the proposed approach.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Perspective on New Generation Stent-graft by Metamaterial Design and Computational Optimization

Fangsen Cui*, Yucheng Zhong**, Gideon Praveen Kumar***, Gongfa Chen****, Jackie Pei Ho*****, Hwa Liang Leo******, Chang Shu*******

*Institute of High Performance Computing, A*STAR, **Institute of High Performance Computing, A*STAR, ***Institute of High Performance Computing, A*STAR, ****Guangdong University of Technology, *****National University of Singapore, ******National University of Singapore, *******Fuwai Hospital, Chinese Academy of Medical Sciences

ABSTRACT

Aortic pathologies such as aneurysm and dissection can be treated by less invasive method – the endovascular aortic repair (EVAR). It provides a lower operative mortality and morbidity solution compared to conventional open surgery repair. The key medical device used for EVAR is called stent-graft (SG) and has been successfully used for abdominal aortic aneurysm repair as well as straight thoracic aorta. For aortic arch with sharp curve variations, it is challenging to minimize complications such as endoleaks with thoracic endovascular aortic repair (TEVAR). The other challenging issue with the aortic arch is to preserve the three supra-aortic branches blood flow which usually requires hybrid repair, chimney repair, and even custom-made fenestrated or branched devices with high morbidity and cost. To design new generation stent-graft, the new design concept such as origami structure and auxetic materials can play a key role in improving the performance and minimizing complications. However, such metamaterial stent-graft must be well tailored so its mechanical performance can be better utilized. In addition, computational solid mechanics, computational fluid dynamics, and multi-objective optimization can be used for the development of new generation stent-graft. In this paper, first we review recent progress on developing metamaterial stent-graft. The benefits of such design incorporated with our previous proposed design are then discussed. Furthermore, simulations on the evaluation of mechanical performance of stent-graft are presented. The optimization methodology of stent-graft design is also discussed. References 1. W Wu, X Song, J Liang, et al. Mechanical properties of anti-tetrachiral auxetic stents, Composite Structures, online Nov 20, 2017 2. Z You, Folding structures out of plate materials, Science 2014;345(6197):623?645 3. G. Alaimo F. Auricchio M.Conti, M. Zingales, Multi-objective optimization of nitinol stent design, Medical Engineering & Physics, Volume 47, September 2017, Pages 13-24

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

New Insights in Dislocation Behaviors under Shock Loading

Yinan Cui*, Giacomo Po**, Nasr Ghoniem***

*UCLA, **UCLA, ***UCLA

ABSTRACT

Understanding the mechanical behavior of metallic solids under extreme conditions of high strain rate is of great interest to engineering applications. However, until recently little understanding of the effect of the elastodynamic stress field emission by dislocations on dislocation behaviors has been achieved. In all the available three dimensional discrete dislocation dynamics (DDD) method, dislocations are treated in a quasi-statically way, even though the time-dependent nature is found to be very important when the strain rate is higher than 10^6/s. This work presents the first 3D DDD method, based on a fully time-dependent elastodynamic description of the elastic fields of discrete dislocations. The fundamental time-dependent solutions and its numerical implementation are presented. New insights on dislocation interactions during shock loading are revealed.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Novel Fatigue Strength Prediction Method for Optical Fibers with Initial Flaws

Yuxuan Cui*, Yunxia Chen**, Jingjing He***

*Beihang University, **Beihang University, ***Beihang University

ABSTRACT

The dynamic fatigue behavior of optical fiber is strongly affected by the surface defects generated during manufacture and handling. Crack initiation and propagation due to stress concentration would result in catastrophic failure of optical fibers. In this work a physics-based model is presented to quantify the effect of initial flaws. Artificial triangle indentations are introduced with indentation method to represent the natural flaws of optical fiber caused by material uncertainties or manufacture procedure. Two geometry parameters, the diametrical length of the indentation impression and the diametrical flaw length, are chosen to describe the influence of initial flaws. Both cases for indentation with or without radial cracks are included in this study. Experimental studies are used to validate the proposed method and a good agreement is observed between the model predictions and experimental data.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Uncertainty Quantification in the Brazilian Outbreak of Zika Virus

Americo Cunha Jr*, Eber Dantas**, Michel Tosin***

*Universidade do Estado do Rio de Janeiro, **Universidade do Estado do Rio de Janeiro, ***Universidade do Estado do Rio de Janeiro

ABSTRACT

Several instances of Zika virus epidemic have been reported around the world in the last 20 years, causing Zika fever to become a disease of international concern. The use of mathematical models for epidemics in this context very important, once they are useful tools to predict the outbreaks underlying numbers, and allow one to test the effectiveness of different strategies to combat associated diseases. This work deals with the development and calibration of an epidemic model to describe the Zika virus outbreak in Brazil. The modeling and quantification of the initial conditions uncertainties is also of interest. In order to calibrate the model, two inverse problems (one deterministic and another one stochastic) are formulated and solved. A consistent stochastic model of uncertainties is constructed by means of a parametric probabilistic approach, which employs Monte Carlo method to compute the propagation of uncertainties.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Continuum Damage and Plasticity Model for Higher Gradient Materials

Massimo Cuomo*, Loredana Contrafatto**, Leopoldo Greco***

*University of Catania, **University of Catania, ***University of Catania

ABSTRACT

Continuum Damage and Plasticity Model for Higher Gradient Materials M. Cuomo, L. Contrafatto, L. Greco Department of Civil Engineering and Architecture University of Catania - ITALY Complex materials, among which those usually referred to as metamaterials, exhibit different, often independent, mechanisms for the evolution of anelastic phenomena at the micro- and at the macro-scale. Gradient plasticity, originally introduced for geomaterials, has been extended to a large variety of non local materials, see e.g. [1]. Similarly, continuum damage has been extended to micromorphic and higher gradient models, introducing internal damage variables and their gradient. Damage evolution is determined by rate equations depending upon the thermodynamic conjugate forces, related to the local value of the damage variables and to its gradient. An additional field differential equation is then obtained for damage compatibility, that has to be solved simultaneously with the equilibrium equations. In this work is proposed a new continuum damage model for strain gradient materials characterized by two independent damage internal variables, each evolving with its own law. In this way no additional field equation for the damage variable is needed. The derivation has been obtained within a thermodynamic framework, introducing suitable functionals for the internal energy and for the rate of dissipation. Specific objectives of the work are: - to present a damage model for strain gradient materials that does not need the solution of additional differential equations; - to analyze a simpler version of the model, in order to compare it with local damage models - to study whether also in this case, similarly to what has been found by the author with non local softening plasticity models, the presence of strain gradients is able to avoid strain localization and consequently mesh dependency in the numerical simulations. Numerical simulations of a strain gradient mode with damage, eventually couple with plasticity, will be discussed. [1] Forest, S., Micromorphic Approach for Gradient Elasticity, Viscoplasticity, and Damage, Journal of Engineering Mechanics ASCE, 2009, vol. 135, 3, 117-131.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Dislocation Cross-slip in FCC Metal Alloys

William Curtin*, W.G. Noehring**

*EPFL, **EPFL

ABSTRACT

Cross-slip of screw dislocations is the thermally-activated dislocation process that influences dislocation structuring, work hardening, fatigue, and ductility. Cross-slip has been widely studied in elemental fcc alloys, where the cross-slip energy barrier scales inversely with the stacking fault energy. This thermally-activated phenomenon has been incorporated into various studies of mesoscale plasticity using discrete dislocation dynamics to demonstrate its role in plasticity. Most engineering materials are alloys with some elements in solid solution, yet the cross-slip in alloys has typically been considered to depend only on the stacking fault energy of the alloy. Here, we report on atomistic studies of the cross-slip process in a wide range of fcc random solid solution alloys and demonstrate that the cross-slip energy barrier itself is statistically distributed so that the stacking fault alone does not reflect the operative barriers in a real alloy. The standard deviation of the distribution of cross-slip barriers can be computed knowing only the solute/dislocation and solute/solute interaction energies. The cross-slip of long dislocation segments typical of real materials (1000b or larger) then involves both nucleation at locally favorable (low activation energy) regions of solutes and propagation (lateral extension) that is driven by either Escaig or Schmid stresses. A random walk model in the presence of local fluctuations in cross-slip energy difference is developed to predict the operative distribution of energy barriers as a function of solute concentration, dislocation length, and applied stress levels, with excellent quantitative success. These results demonstrate that the cross-slip barriers in alloys are much smaller than those in the pure metals, making cross-slip much more frequent in alloys. The resulting models are suitable for incorporation into dislocation-level models and may inform crystal plasticity models, while the consequence on various macroscopic plasticity phenomena are discussed.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Computational Mechanics Intelligence: How to Teach Continuum Mechanics to an Artificial Intelligence Using Computer Simulations

Christian Cyron*, Roland Aydin**

*Hamburg University of Technology, **Technical University of Munich

ABSTRACT

Over the last years, we have witnessed several groundbreaking advances in artificial intelligence (AI) that were based on a simple strategy: a virtual training environment was created by setting up some general rules. Subsequently, an AI, typically represented by an artificial neural network (ANN), was placed in this training environment and allowed to practice a certain kind of activity until it reached a superhuman level of mastery. The rules of the training environment were, for example, the rules of the board game Go in the AlphaGo project. Other research projects rely on virtual environments as used in computer games in order to train an AI to perform intelligent actions within such environments or solve certain problems. All this research has in common so far that it uses training environments defined by rules whose complexity is far below the one of real physics. With physically more realistic training environments one could train AIs to solve problems, for example, from mechanical engineering that require so far intense human interactions. Creating physically realistic models of systems and processes in mechanical engineering is the main objective of computational mechanics. It is thus natural to combine computational mechanics and machine learning to create what one may refer to as “computational mechanics intelligence”, that is, a kind of artificial/computational intelligence that is endowed with an accurate understanding of a certain mechanical problem and which is trained in a virtual environment created by methods from computational mechanics. It this talk we will discuss fundamental aspects of the idea of computational mechanics intelligence. We will discuss how to combine ANNs with finite element simulations in order to provide physically realistic and accurate training environments to ANNs. In particular we will address a key question: how can one achieve an acceptable computational cost of such a set-up for AI training despite the necessity of numerous computational simulations, each of which can be associated with a substantial computational cost when trying to model a complex physical system accurately. The strategy is based on a smart coupling of the learning progress of the AI with the resolution of the computational models that provide the training environment for the AI. We demonstrate advantages of our strategy using some simple examples from continuum mechanics in one and higher dimensions.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Shock Structure in Porous Metals: The Interplay of Material Strain Rate Dependency with Micro-inertia Effects

Christophe Czarnota*, Sébastien Mercier**, Alain Molinari***

*LEM3 - UMR CNRS 7239, Université de Lorraine - 7 rue Félix Savart BP 15082 - 57073 METZ Cedex 03 - FRANCE, **LEM3 - UMR CNRS 7239, Université de Lorraine - 7 rue Félix Savart BP 15082 - 57073 METZ Cedex 03 - FRANCE, ***LEM3 - UMR CNRS 7239, Université de Lorraine - 7 rue Félix Savart BP 15082 - 57073 METZ Cedex 03 - FRANCE

ABSTRACT

The present work proposes to examine the combined influence of micro-inertia and material rate dependency on the shock structure in porous metals. Porosity is assumed to be moderate and voids are not connected. Beyond some propagation distance from the shock initiation site (few times the effective plastic shock width), steady plastic shock waves are formed. As the shock wave is traveling in the porous medium, voids are facing a rapid collapse. Material particles located in the vicinity of voids are subjected to very high acceleration. Owing to the mass density of the matrix, the local acceleration induces local inertia effects, called micro-inertia. Micro-inertia effects are embedded in the overall constitutive response of the porous material following the work of [Molinari and Mercier, 2001] and [Czarnota et al., 2017]. The overall response of porous materials is obtained by a dynamic homogenization approach where the static part is determined from a GTN viscoplastic flow potential. The present talk will enlighten the influence of the material strain rate sensitivity on the shock structure and the interplay between the material viscosity and micro-inertia effects. One of the major finding of the present study concerning shock wave structures is the relationship connecting the plastic strain rate within the shock to the shock amplitude. The [Swegle and Grady, 1985] power law relationship will thus be revisited for porous metals. Acknowledgement: The research leading to these results has received funding from the European Union 's Horizon2020 Programme (Excellent Science, Marie-Sklodowska-Curie Actions) under REA grant agreement 675602 (Project OUTCOME). REFERENCES: Czarnota, C., Molinari, A., and Mercier, S., 2017, "The structure of steady shock waves in porous metals ", to appear in J. Mech. Phys. Solids. Molinari, A. and Mercier, S., 2001, "Micromechanical modelling of porous materials under dynamic loading ", J. Mech. Phys. Solids 49, 1497–1516. Swegle, J. W. and Grady, D. E., 1985, "Shock viscosity and the prediction of shock wave rise times", J. Appl. Phys., 58(2), 692-701.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Determination of Effective Cross-Section Properties by Chemo-Mechanical Simulations

Lisa-Marie Czernuschka*, Ioannis Boumakis**, Jan Vorel***, Marco Marcon****, Roman Wan-Wendner*****

*Christian Doppler Laboratory LiCRoFast, Institute of Structural Engineering, University of Natural Resources and Life Sciences, Vienna, Austria, **Christian Doppler Laboratory LiCRoFast, Institute of Structural Engineering, University of Natural Resources and Life Sciences, Vienna, Austria, ***Christian Doppler Laboratory LiCRoFast, Institute of Structural Engineering, University of Natural Resources and Life Sciences, Vienna, Austria, ****Christian Doppler Laboratory LiCRoFast, Institute of Structural Engineering, University of Natural Resources and Life Sciences, Vienna, Austria, *****Christian Doppler Laboratory LiCRoFast, Institute of Structural Engineering, University of Natural Resources and Life Sciences, Vienna, Austria

ABSTRACT

The safety and sustainability of state of the art bridge structures is a crucial task in modern civil engineering practice. The long-term behavior of concrete is complex and influenced by many different phenomena such as aging, shrinkage, creep and their interactions. As widely known, the main source of these phenomena is the hydration of concrete, which is strongly influenced by the boundary conditions, the mix design, as well as the geometry of the structure. Hence, careful consideration of these effects is required especially for large concrete structures. The latter show significant spatial gradients in reaction degree, temperature and humidity, consequently also being visible in material properties. In order to be able to capture the behavior as accurately as possible, a strong numerical tool is of great importance. This study presents the determination of effective cross-section properties by utilization of chemo-hygro-thermal simulations coupled with mechanical analysis in a multi-physics framework [1,2]. This framework is calibrated and validated based on an extensive experimental campaign, comprising temperature and humidity evolution measurements, as well as calorimeter, shrinkage and modulus data. Specifically, effective cross section properties of different practically relevant types under different boundary conditions are derived. Influences of environmental boundary conditions and cross-section characteristics on thermal strains, shrinkage and their interaction with creep are analyzed and discussed in detail. [1] Di Luzio, G. and Cusatis, G., Hygro-thermo-chemical modeling of high performance concrete - I: Theory, Cement and Concrete Composites, 2009; 31:301-308. [2] Di Luzio, G. and Cusatis, G., Hygro-thermo-chemical modeling of high performance concrete - II: Numerical implementation, calibration and validation, Cement and Concrete Composites, 2009; 31:309-324.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Enhancing Alya Multiphysics Code with WSMP Solver and Solving Large Scale Ill-Conditioned Problems

Paula Córdoba*, Guillaume Houzeaux**, Seid Koric***, Anshul Gupta****

*Barcelona Supercomputing Center, **Barcelona Supercomputing Center, ***National Center for Supercomputing Applications & University of Illinois, ****IBM Watson Research Center

ABSTRACT

The discretization of partial differential equations of complex physical problems involves solving linear systems of equations with a great number of unknowns. The resultant matrix obtained from this discretization is often sparse and ill-conditioned. In many cases problems are solved in fine structured meshes with irregular geometries yielding ill-conditioned matrices, where using implicit methods together with preconditioned iterative solvers often diverge or the preconditioned system can be computationally more expensive than using direct methods. This work aims at improving the parallel scalability and robustness of the hybrid MPI/OpenMP high performance computational code Alya developed at BSC-CNS by using the parallel linear solver WSMP solver from IBM Watson. In this framework WSMP, a direct linear solver developed at IBM Watson has been integrated into Alya code to study and improve the performance of such problems. To do so, Alya's parallel structure and matrix format has been adapted to the one required by WSMP and WSMP has been integrated into Alya workflow for symbolic and numerical factorization as well as solution steps. Finally WSMP has been validated and compared with Alya's internal solvers performing scalability and convergence studies on several real life cases of heat transfer and solid mechanic problems. The results of this collaboration will improve Alya's numerical robustness and open the door for the high-fidelity multiphysics modeling of complex processing real scale. M. Vázquez, G. Houzeaux and S. Koric et al., Alya: Multiphysics engineering simulation toward exascale, Journal of Computational Science, 2016, In Press, doi:10.1016/j.jocs.2015.12.007 S. Koric and A. Gupta, "Sparse Matrix Factorization in the Implicit Finite Element Method on Petascale Architecture, " Computer Methods in Applied Mechanics and Engineering, 2016 v.32,281-292, 2016

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Locally Refined Isogeometric Analysis of Trimmed Shells

Davide D'Angella*, Luca Coradello**, Massimo Carraturo***, László Kudela****, Stefan Kollmannsberger*****, Ernst Rank******, Alessandro Reali*******

*Technische Universität München, TUM Institute for Advanced Study, **École polytechnique fédérale de Lausanne, ***Università degli Studi di Pavia, ****Technische Universität München, *****Technische Universität München, ******Technische Universität München, TUM Institute for Advanced Study, *******Università degli Studi di Pavia, TUM Institute for Advanced Study

ABSTRACT

The Isogeometric B-Rep analysis of shells allows to perform computations on the exact geometry, reducing the gap between analysis and design [1]. However, how to properly handle trimmed surfaces is still a frequently discussed question. Moreover, small geometric features or localized mechanical responses demand for higher accuracy in selected areas. In this work we present how different techniques can be successfully combined to perform efficient Kirchhoff-Love shell analysis. In particular, we present how the trimming can be dealt with at the integration level by means of an immersed boundary method like the Finite Cell Method (FCM) [2]. Conforming integration domains are adaptively produced to accurately capture the geometry [3], while the element shape is kept regular and not distorted. This is used together with local hierarchical refinement to efficiently adapt the mesh locally. In conclusion, we show how these methodologies can create a powerful tool for the integration of design and analysis of B-Rep shell models. [1] Breitenberger, M., et al. "Analysis in computer aided design: Nonlinear isogeometric B-Rep analysis of shell structures, " Computer Methods in Applied Mechanics and Engineering, 284, 2015. [2] Rank, E., et al. A. "Geometric modeling, isogeometric analysis and the finite cell method, " Computer Methods in Applied Mechanics and Engineering, 249-252, 2012. [3] Kudela, L., et al. "Efficient and accurate numerical quadrature for immersed boundary methods, " Advanced Modeling and Simulation in Engineering Sciences, 2: 10, 2015.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Optimization-based Coupling Strategy for Local and Nonlocal Elasticity Problems

Marta D'Elia*, Pavel Bochev**, Mauro Perego***, David Littlewood****

*Sandia National Lab.s, **Sandia National Lab.s, ***Sandia National Lab.s, ****Sandia National Lab.s

ABSTRACT

Nonlocal continuum theories such as peridynamics and nonlocal elasticity can capture strong nonlocal effects due to long-range forces at the mesoscale or microscale. For problems where these effects cannot be neglected, nonlocal models are more accurate than classical Partial Differential Equations (PDEs) that only consider interactions due to contact. However, the improved accuracy of nonlocal models comes at the price of a computational cost that is significantly higher than that of PDEs. The goal of Local-to-Nonlocal (LtN) coupling methods is to combine the computational efficiency of PDEs with the accuracy of nonlocal models. LtN couplings are imperative when the size of the computational domain or the extent of the nonlocal interactions are such that the nonlocal solution becomes prohibitively expensive to compute, yet the nonlocal model is required to accurately resolve small scale features. We propose an optimization-based coupling strategy for the solution of a nonlocal elasticity problem. Our approach formulates the coupling as a control problem where the states are the solutions of the nonlocal and local equations, the objective is to minimize their mismatch on the overlap of the nonlocal and local domains, and the controls are virtual volume constraints and boundary conditions. We present the implementation of our coupling strategy using Sandia 's agile software components toolkit, which provides the groundwork for the development of engineering analysis tools. We show that our method passes linear and quadratic patch tests and we present numerical convergence studies. Using three-dimensional geometries, we also show that our approach can be successfully applied to challenging, realistic, problems.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Fast Helmholtz Solvers on Multi-Threaded Architectures

Ruiyang DAI*, Jean-François Remacle**, Christophe Geuzaine***

*Université catholique de Louvain (UCL), **Université catholique de Louvain (UCL), ***Université de Liège

ABSTRACT

Solving the Helmholtz equation in the high frequency regime is a notoriously difficult problem. In this paper, we aim at solving Helmholtz problem in heterogeneous media in the frequency domain. A high order continuous finite elements is thus used. Because of the high frequency, a large number of unknowns is required to obtain accurate solutions of the problem (typically 4 elements per wavelength for a polynomial order of 4). Linear systems arising at high frequency are indefinite and iterative methods fail to converge. The large number of unknowns forbids to use direct methods as well. Thus, a Domain Decomposition Method (DDM) with a double sweep preconditionner has been developed and implemented in parallel on modern Intel Knight's landing architectures. Both the assembly of the system and the resolution have been parallelized with reasonable success. We will discuss optimal strategies that are specific to the KNL: fast finite element assemblies using AVX512 extensions, size and number of sub-domains, multiple right hand sides, efficiency of linear solves... Extension to hybrid parallelism i.e. using several KNL's will be discussed as well.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Seismic Assessment of Existing Structures: Contribution of In-Situ Measurements by Ambient Vibrations in the Design of Numerical Models

Cedric DESPREZ*

*IFSTTAR, Université Paris-Est Marne-la-Vallée 14-20 bd Newton, cité Descartes, 77447 Marne la vallée

ABSTRACT

Seismic assessment of existing structures is a major issue of civil engineering. Indeed, many constructions built before seismic requirement codes are located in moderate or important seismic areas. Expectations are high regarding the preservation of human life, strategic installations, economic activities and cultural heritage. The numerical modeling is often used to perform an advanced vulnerability assessment. In this context, the level of precision sought highly depends on the knowledge got on the considered construction; this knowledge being often lacunars. Based on several case-studies, this paper highlights the value of structural measurements by ambient vibrations in the design of a numerical mock-up and the resulting analysis. The first case study concerns a reinforced concrete building built in the 1960s for which a vulnerability analysis was carried out on the basis of a multifibre beam finite element model. The second case concerns the evaluation of a hydroelectric concrete gravity dam before and after retrofitting work. The modeling was carried out with finite three-dimensional elements. The third case focuses on the application of this type of measures in the context of the simplified modeling of masonry heritage monuments. For each of these cases, datas obtained from the in-situ measurements were particularly interesting since they notably allow accessing the modal characteristics of the structures or sub-structures; high value factor in the response of a structure. The application of this technology to various typologies of constructions demonstrates its robustness and the associated perspectives in terms of representativeness in numerical modeling.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A New Solid-shell Finite Element Dedicated to Non-linear Thin-to-thick Structures - Application to Energy Production Facilities and Safety Structures

Mouhamadou DIA*, Nahiene Hamila**, Anthony Gravouil***, Dzifa Kudawoo****

*Energie de France (EDF), **Univ Lyon, INSA Lyon,CNRS, Lamcos 5259, France, ***Univ Lyon, INSA Lyon,CNRS, Lamcos 5259, France, ****Energie de France (EDF)

ABSTRACT

Thin or thick shell like structures are naturally present in most industrial structures and particularly in nuclear power plants such as pipes, tanks, reactor-buildings, to name just a few. Their mechanical modeling imply to describe properly shell kinematics and to capture accurately through-thickness phenomena, as the calculations to be carry out can be highly non-linear. To satisfy those requirements, solid-shell elements are a good option. In the present contribution the solid-shell element initially formulated in small deformation [1] is extended to large deformations adapted for modeling non-linear effects combined with contact and elastic-plastic behavior. This solid-shell element has nine nodes: eight located at the vertex and the ninth placed at the element center. The middle-node is endowed with only one degree of freedom, in the thickness direction, allowing the assumption of a quadratic interpolation of the transverse displacement. Unlike solid-shell finites elements reported previously in the literature [2] and formulated under the hypothesis of plane stress, the new solid-shell element here mentioned uses a complete three-dimensional constitutive law [3], thanks to the middle-node. Moreover, to handle the various locking problems that usually arise on solid-shell formulation, the reduced integration technique is used as well as the assumed shear strain method. Finally to assess the effectiveness and performance of this new formulation, we will investigate a set of popular benchmark problems, involving geometric non-linear analysis as well as elastic-plastic behavior. [1] Bassa, B., Sabourin, F., & Brunet, M. (2012). A new nine?node solid?shell finite element using complete 3D constitutive laws. International Journal for Numerical Methods in Engineering, 92(7), 589-636. [2] Abed-Meraim, F., & Combescure, A. (2001, June). SHB8PS a new " intelligent" assumed strain" continuum" mechanics shell element for impact analysis on a rotating body. In 1srt MIT Conférence. [3] Sansalone, M., Sabourin, F., & Brunet, M. (2011). A new shell formulation using complete 3D constitutive laws. International Journal for Numerical Methods in Engineering, 86(6), 688-716.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Simulation of a Dam Behaviour with a Damage Model

Sébastien DOMITILE*, Romain TAJETTI**

*EDF - CIH, **EDF - CIH

ABSTRACT

The Brévières dam is located in French Alps and at immediate downstream of Tignes dam. It represents one of the closure structures of Malgovert water intake. This dam is a movable weir made in concrete and masonry of 24 meters height and 17 meters wide above the foundation. It's composed of three passes equipped with gates and bounded by four piles put on concrete slab. The foundation on dam lies on rock on its sides and on a breach made of crushed materials in the center. Displacements of the rock sides cause valley tightening bringing important displacements of dam and significant forces. This situation led to dam collapse mechanisms reflected by very important cracks. The dam has been auscultated by topography since 1994. The dam behavior is characterized by a shortening of bank in bank and an elevation of right bank compared to the left. The set of these phenomena are involved to the difficulties to operate gates for flood releases. Number of studies have been developed to understand tightening mechanisms and to find solutions to ensure the operation of the spillways without success in the long term. Thus, we have decided to model the dam and its surrounding to simulate its passed behavior until 2016 and predict its evolution with the aim to integrate some reparation solutions in the model to evaluate them and to ensure efficiency at long term. The works were modelled with a hexahedral volumetric mesh through Nx V9 and performed with ASTER. The movements of foundation are traduced by imposed displacements of nodes. A first model was based on linear elastic approach coupled with contact law. It showed a good representation between the model and auscultations. Stresses analysis explained the disorders observed on dam. Nevertheless the range of actual stresses couldn't ensure the validity of elastic model for predicting behavior of dam. We have decided to use a damage model to simulate future behavior in relation to the solutions for remedial works. The constitutive law used is the damage concrete law developed by EDF-CIH and LMDC of Toulouse University. The results of this simulation were better in comparison with elastic model. They gave predicting displacements of fixed supports of gates for different scenarios of civil works. This study provides an example of damage models use to improve decision aid.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Multiscale Topological Design of Heterogeneous Materials and Structures without Scale Separation

Daicong Da*, Julien Yvonnet**, Liang Xia***, Min Vuong Le****, Guangyao Li*****

*Université Paris-Est, **Université Paris-Est, ***Huazhong University of Science and Technology, ****Université Paris-Est, *****Hunan University

ABSTRACT

Most existing literature on multiscale topology optimization, e.g. tailoring the topology of material microstructures for the concurrently designed macrostrucutres in terms of structural stiffness, using the classical homogenization method to bridge the microscopic and macroscopic scales. However, the classical homogenization method assumes separation between two scales, i.e., the material microstructures are assumed to be infinite small, resulting the optimally designed microscopic structures by this scheme can't be manufactured. To this end, this work put forward a new multiscale topology optimization framework in a context of non-separated scales to obtain the optimal material microstructures with manufacturable details. A nonlocal filter-based homogenization approach capable of dealing with the heterogeneous materials and structures without scale separation is adopted to perform the multiscale computations. The constitutive relationship at the higher scale is derived by a fully microscopically-based framework to account the heterogeneous details, and the effective local fields can be reproduced by solving the structural problem at higher scale on a coarse mesh only, resulting the degree of freedom greatly reduced. On the other hand, a computationally efficient sensitivity formulation with all information of local fields is derived to perform the topology optimization design. Finally, several numerical benchmark examples are presented to demonstrate the effectiveness of the proposed method. The presented work then provides a very promising tool to design manufacturable microscopic structures within multiscale topology optimization framework. [1] J. Yvonnet, G. Bonnet, A consistent nonlocal scheme based on filters for the homogenization of heterogeneous linear materials with non-separated scales, Int. J. Solids. Struct (2014) [2] A. Tognevi, M. Guerich and J. Yvonnet, A multi-scale modeling method for heterogeneous structures without scale separation using a filter-based homogenization filter, Int. J. Numer. Meth. Engng (2016)

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Virtual Manufacturing and Performance Coupling for Endless Fibre Reinforced Plastics – A General Concept

Patrick Da Luca*, Andé Berger**

*ESI Group, **Dr.

ABSTRACT

Due to their superior strength to density ratio fibre reinforced plastics (FRP) provide a high performance for energy dissipating parts and are consequently ideal for lightweight design for crashworthiness. However, due to the complex inner structure of FRP parts the prediction of the mechanical behaviour in simulation under crash loading is still challenging. Using multi-scale approaches taking into account different level of information, like micro-scale and meso-scale offer new possibilities but also provide new challenges. How to get a proper virtual model of the complex fibre architecture on meso-scale? How to identify predictive mechanical properties on micro-scale? Therefore, this presentation will demonstrate a general modular concept for the derivation of the complex inner fibre structure of FRP based on manufacturing simulation and the determination of fracture curves using virtual testing on micro-scale. The latter is subsequently used to determine the parameters of PUCK's law for inter-fibre fracture. Finally, the two approaches are combined to demonstrate the potential of a multi-scale-approach for a filament wound tube under axial crash loading by comparing the results obtained by simulation with experimental data. In addition, it will be shown how the approach can be used to represent various manufacturing processes i.e. braiding or different base materials.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Adaptive Inexact Semismooth Newton Methods for the Contact Problem between Two Membranes

Jad Dabaghi*, Martin Vohralik**, Vincent Martin***

*Inria Paris & CERMICS (ENPC), **Inria Paris & CERMICS (ENPC), ***Université technologie de Compiègne (UTC)

ABSTRACT

We propose an adaptive inexact version of a class of semi-smooth Newton methods. As a model problem, we consider the system of variational inequalities describing the contact between two membranes and its conforming finite element discretization. Any iterative linearization algorithm like the Newton-min, Newton-Fisher Burmeister is taken into account, as well as any iterative linear algebraic solver. We prove an a posteriori error estimate between the exact solution and the approximate solution which is valid on any step of the linearization and algebraic resolution. Our estimate is based on flux reconstructions in discrete subspace of $\textbf{H}(\mathrm{div},\Omega)$ and on potential reconstructions on discrete subspaces of $H^1(\Omega)$ satisfying the constraints. The estimate distinguishes the discretization, linearization, and algebraic components of the error and allows us to formulate adaptive stopping criteria for both solvers. Under these criteria, the local efficiency of our estimates is also established. Numerical experiments for the semi-smooth Newton-min algorithm in combination with the GMRES solver confirm the efficiency of the method.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

High Order FEA of Proximal Humeri – Mechanical Response and Yield Prediction Validated by Experiments

Gal Dahan*, Zohar Yosibash**

*Tel Aviv University, **Tel Aviv University

ABSTRACT

While a major part of proximal humerus fractures are classified as non-displayed and can be treated non-operatively, the management of the displaced fractures remains a controversial matter. In such cases, the orthopedic surgeon is required to assess the fracture 's stability, to determine if surgical intervention is needed. Nowadays, such clinical diagnoses are based on X-ray examination of the fracture and surgeon 's personal experience. With the high incidence of proximal humerus fractures in the elderly, and the growing incidence of surgically treated fractures and revision surgeries [1], there is a need for a biomechanical-based quantitative tool that can assist the surgeons in the clinical decision-making process and in particular, in stability assessment. The first step towards this solution is obtaining a verified and validated high order FE (p-FE) model, compared to experimental observations of the mechanical response and fracture of proximal humeri. In [2] verified and validated p-FE models of humeri were presented, using empirical-based isotropic inhomogeneous material properties derived originally for the femur. In the in-vitro experiments used for validation, the humeri were also loaded to obtain fracture, and yield loads were compared to p-FE predictions using a maximum strain criterion. Since bone is known to be anisotropic, the p-FE models are enhanced to include orthotropic material properties. According to [3], based on voxel average rules for X-ray attenuation coefficient, and representing the bone by means of continuum micromechanics (MM), the orthotropic effective stiffness tensor can be calculated and a failure criterion at the trabecular level may be considered. REFERENCES [1] Bell J., Leung B.C., Spratt K.F., Koval K.J., Weinstein J.D., Goodman D.C. and Tosteson A. & quot;Trends and Variation in Incidence, Surgical Treatment, and Repeat Surgery of Proximal Humeral Fractures in the Elderly ". The Journal of Bone and Joint Surgery-American Volume, 93, 121–131, 2011. [2] Dahan G., Trabelsi N., Safran O. and Yosibash Z., "Verified and validated finite element analyses of humeri ", Journal of Biomechanics, 49,1094-1102, 2016. [3] Hellmich C., Kober C., and Erdmann B. & quot;Micromechanics-based conversion of CT data into anisotropic elasticity tensors, applied to FE simulations of a mandible ". Annals of Biomedical Engineering, 36:1, 108-122, 2008.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Calibration and Factor Analysis of Particle Sandpile Process for Additive Manufacturing via Discrete Element Simulation

Ling Dai*

*Scientist

ABSTRACT

For modern additive manufacture, particle pouring and piling process at micron size scale is the fundamental procedure. Traditionally, at macro scale, the particle sandpile has been calibrated via measuring the bulk properties, such as repose angle, mechanical test, etc. Nowadays, the discrete element simulation tool shows strong power to provide deep understanding for the process and mechanism, significantly help to enhance our understandings for the modern additive manufacture technology. Here, we carried out a serial of discrete element simulations to model the particle dynamic process from pouring to sandpile formation under various conditions of friction, material property, damping and particle size. The results were calibrated with the sandpile geometry and packing density, aiming to the functional performance for additive manufacture. Through our investigation, we found that in order to obtain satisfactory piling morphology for following additive manufacturing process, we need to dominantly control both the sliding friction and rolling friction. The material property and damping conditions didn't much affect the pile morphology, but led to some side effects on the cost of computational aspects. The distribution of particle size presented charming mechanism, based on which extraordinary packing density could be achieved, which was significantly beneficial to the functional performance. In summary, our works provides an overall understanding of process and mechanism for particle pouring and piling procedure, which makes the fundamental contribution to the modern additive manufacture.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Application of the Haar Wavelet Method to Dynamic Stability Analysis of Truncated Conical Shells

Qiyi Dai*, Qingjie Cao**

*Harbin Institute of Technology, **Harbin Institute of Technology

ABSTRACT

In this paper, the Haar wavelet method is employed to analyze the parametric instability of truncated conical shells under static and time dependent periodic axial loads. The present work is based on the Love first-approximation theory for classical thin shells. The displacement field is ex-pressed as the Haar wavelet series in the axial direction and trigonometric functions in the circum-ferential direction. Then the partial differential equations are reduced into a system of coupled Ma-thieu-type ordinary differential equations describing dynamic instability behavior of the shell. Using Bolotin's method, the first-order and second-order approximations of principal instability regions are determined. The correctness of present method is examined by comparing the results with those in the literature and very good agreement is observed. The difference between the first-order and second-order approximations of principal instability regions for tensile and compressive loads is also investigated. Finally, numerical results are presented to bring out the influences of various pa-rameters like static load factors, boundary conditions and shell geometrical characteristics on the domains of parametric instability of conical shells.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Implications of Mode of Control and Loading Rate on the Determination of Concrete Fracture Properties

Gilda Daissè*, Christian Carloni**, Roman Wan-Wendner***

*University of Natural Resources and Life Sciences, Vienna, Austria, **University of Bologna, Bologna, Italy, ***University of Natural Resources and Life Sciences, Vienna, Austria

ABSTRACT

Among all the parameters that characterize the concrete behavior, the fracture energy is one of the most crucial for the (numerical) investigation of damage propagation and failure in reinforced concrete members. Currently no standards exist that provide guidance to the characterization of concrete fracture properties. The experimental evaluation of fracture energy is influenced by different laboratory limitations, such as specimens' size [1] and mode of control during the fracture test. In order to investigate the differences between specimen geometries and evaluate the effect of mode of control on the fracture test, a numerical analysis supported by an experimental campaign and digital image correlation (DIC) is presented. The Lattice Discrete Particle Model (LDPM) [2] has been used to simulate concrete and to provide realistic crack patterns and crack widths. In the first part of the study the relationship between load point displacement rate, opening rate at the position of a surface-mounted extensometer, and actual strain rate at the crack tip are established for a number of specimen geometries and sizes by means of calibrated numerical simulations. For this purpose, the position of the crack tip is identified through an energetic approach. It is well-known that concrete is a visco-elastic material with strain-rate dependent fracture properties [3]. The potential influence of differences in loading rate on the determined fracture energy owing to these two phenomena is investigated in the second part, based on simulated three-point bending tests of differently sized specimens with two notch depths, loaded at different rates. The simulations are supported by an experimental campaign including Digital Image Correlation (DIC) data of the ligament area of beams loaded at different rates. The latter study has relevance both for the determination of a recommended loading rate and for permitting an acceleration range in the post-peak to shorten the test duration. References: [1] Bazant Z. and Kazemi M: Size dependence of concrete fracture energy determined by RILEM work-of-fracture method, International Journal of Fracture, 1991; 51(2):121-138. [2] Cusatis, G.; Pelessone, D.; Mencarelli, A. Lattice Discrete Particle Model (LDPM) for failure behavior of concrete. I: Theory. Cem. Concr. Compos. 2011,33, 881–890. [3] F. P. Zhou (1992). Time dependent crack growth and fracture in concrete. Ph.D thesis, Lund Univ. of Technology, Lund, Sweden.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Nonlinear Mechanical Model for Soft Robot Arms

Francesco Dal Corso*, Costanza Armanini**, Diego Misseroni***, Davide Bigoni****

*University of Trento, **University of Trento, ***University of Trento, ****University of Trento

ABSTRACT

The key to the mechanical design of soft structures lies in the development and use of nonlinear models, among which, the Kirchhoff rod which allows for the description of large deflection of elastic one dimensional structures. With reference to a planar setting, a basic model of soft robot arm is presented as a cantilever beam, with its free end subject to a dead load, and constrained by a continuously rotating clamp. The problem is addressed through new theoretical, numerical, and experimental developments providing design principles to be exploited towards the achievement of targeted positions for the load and the realization of snap mechanisms. More specifically, the considered system behaves as an elastica compass, so that smooth transitions of the deformed shape are observed and the free end traces a closed curve, which approaches a circle as the stiffness of the rod is increased. Differently, when the load is higher than that leading to buckling, an unstable configuration is reached at a specific value of the clamp angle and the rod displays a snap back instability. An analytical model is developed to predict the critical clamp angle for which the snap back occurs, while the subsequent dynamic motion is simulated through a specific numerical model. The reliability of the theoretical predictions is finally validated through experimental tests performed on physical models. Acknowledgements: Support from the ERC Advanced Grant Instabilities and non-local multiscale modelling of materials 340561-FP7-PEOPLE-IDEAS-ERC-2013-AdG (2014-2019) is gratefully acknowledged.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Multi-body Moving Mesh Approach to Efficiently Handle Large Displacements of Immersed Complex Geometries

Wafa Daldoul*, Elie Hachem**, Youssef Mesri***

*MINES ParisTech - CEMEF - CFL research group, **MINES ParisTech - CEMEF - CFL research group, ***MINES ParisTech - CEMEF - CFL research group

ABSTRACT

The CFD simulations involving moving bodies undergoing large displacements represent a real challenge. These simulations, which combine the difficulties, related to instability, meshing and Fluid-Structure Interaction are generally difficult to perform and have a high computational cost. In this work we propose an efficient "r-to-h" adaptation algorithm for moving boundaries problems using only vertex displacements and local h-adaptation operations. It is based on the Inverse Distance Weighting (IDW) interpolation method combined with a selective h-adaptation. It involves local mesh modifications such as edge flipping, local refinement and local coarsening for only badly-shaped elements. The developed approach is tested and validated on multi-body simulations with turbulent flows interactions.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Patient-Specific Bicuspid Aortic Valve Finite-Element Models with Raphe

Jérémy Dallard*, Michel Labrosse**, Benjamin Sohmer***, Carsten Beller****, Munir Boodhwani*****

*Department of Mechanical Engineering, University of Ottawa, Canada, **Department of Mechanical Engineering, University of Ottawa, Canada, ***Division of Cardiac Anesthesiology, University of Ottawa Heart Institute, Canada, ****Department of Cardiac Surgery, University of Heidelberg, Germany, *****Division of Cardiac Surgery, University of Ottawa Heart Institute, Canada

ABSTRACT

Introduction: The aortic valve is normally composed of three cusps. However, in one common lesion, two cusps are fused together, generating closure malfunction and back-flow. In such bicuspid aortic valves (BAV), the conjoined area of the fused cusps is termed raphe. There is a need to better understand BAV biomechanics, with direct applications in surgery. However, the geometry and material properties of the raphe, and the mechanical influence of the raphe on BAV function have not been studied, nor has the patient-specific modeling of BAV been considered [1,2]. The present study aims to propose improvements on both aspects. Methods: Three patient-specific FE models of BAVs (average age 60 yrs) were created based on measurements obtained from 3D trans-esophageal echocardiography and assuming age-dependent material properties [3]. The FE models were run assuming that the raphe material properties were identical to the cusps'. The unpressurized valve geometry was determined by an iterative shrink-pressurize algorithm to minimize the error between seven measured vs. computed geometrical parameters [3]. Two levels of model validation were used: 1) the pressurized computed geometry of the BAV was compared to that observed from medical imaging (anatomical validation); 2) measured vs. computed geometric parameters used in clinical routine were compared to validate the BAV function in terms of its dynamics and pathology mechanism (functional validation). Finally, rigid raphe were also tried to assess the impact of the raphe's stiffness on the cusps ' motion. Results: The pathology was successfully reproduced in the FE models of all three patients. The combined average errors for the three cases were 1.5% for the anatomical validation, 11.6% for the functional validation of cusps motion based on 12 different measurements, and 34.5% for the functional validation based on the quantification of the valve opening area. Mechanical stress transmission from the fused cusps to the aortic wall was observed through the raphe. As measured from geometric parameters used in clinical routine, a rigid raphe decreased cusp motion along the valves axis by 77% and was not consistent with observations from medical imaging. Conclusion: The first age-dependent BAV patient-specific models with raphe were created and analyzed. The findings support the use of material properties for the raphe that are identical to the cusps '. References: [1] Conti CA et al. (2010) The Journal of thoracic and cardiovascular surgery 140(4):890-896. [2] Fedak PW et al. (2002) Circulation 106(8):900-904. [3] Labrosse MR et al. (2015) Medical image analysis 20(1):162-172.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Mathematical Model of Extravascular Platelet Aggregation

Nicholas Danes*, Karin Leiderman**

*Colorado School of Mines, **Colorado School of Mines

ABSTRACT

Platelet aggregation is an essential part of hemostasis, the process to stop bleeding in response to a vascular injury. The local hemodynamics and the nature of the injury can affect size, structure and formation time of a platelet aggregate. Our previous models were restricted to study intravascular clot formation, which is confined to the interior of a single vessel. Here, we develop a mathematical model of extravascular platelet aggregation that has been iteratively developed with an experimental microfluidic device. Our previous model of platelet aggregation is extended to include a transiently bound platelet species and a new description for the limited transport of platelet densities using the finite element method. The setup includes two channels in parallel, a blood and a wash channel, connected by an “extravascular” injury channel. Separate flow rates are imposed at the inlets of the two parallel channels to force blood through the injury channel and exit through the outlet of the wash channel. The injury channel is coated with small proteins that initiate platelet aggregation. Under various shear rates, hematocrits and platelet counts, computational estimates of occlusion times, flow fields, and platelet aggregate porosities are compared to experimental measurements. We find that the timing and spatial distribution of extravascular platelet aggregates are sensitive to these variations.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

An Adaptive hp-Refinement Strategy with Inexact Solvers and Computable Guaranteed Bound on the Error Reduction Factor

Patrik Daniel*, Alexandre Ern**, Martin Vohralík***

*Inria Paris & Université Paris-Est, CERMICS (ENPC), **Université Paris-Est, CERMICS (ENPC) & Inria Paris, ***Inria Paris & Université Paris-Est, CERMICS (ENPC)

ABSTRACT

In this work we extend our recently proposed adaptive refinement strategy for hp-finite element approximations of elliptic problems by taking into account an inexact algebraic solver. Namely, on each level of refinement and on each iteration of an (arbitrary) iterative algebraic solver, we compute guaranteed a posteriori error bounds on the algebraic and the total errors in energy norm. For the algebraic error upper bound, we crucially exploit the nested hierarchy of hp-finite element spaces created throughout the adaptive algorithm, whereas the total error bound is computed using the finest space only. These error bounds allow us to formulate adaptive stopping criteria for the algebraic solver ensuring that the algebraic error does not significantly contribute to the total error. Next, we use the total error bound to mark mesh vertices for refinement via Dörfler 's bulk-chasing criterion. On patches associated with marked vertices only, we solve two separate primal finite element problems with homogeneous Dirichlet boundary conditions, which serve to decide between h-, p-, or hp-refinement. Altogether, we show that these ingredients lead to a computable guaranteed bound on the ratio of the total errors of the inexact approximations between successive refinements (the error reduction factor), when the stopping criteria are satisfied. Finally, in a series of numerical experiments, we investigate the practicality of the proposed adaptive solver and the accuracy of our bound on the reduction factor.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

High-Order Finite Element Methods for Efficient High-Rate Lumped-Mass Explicit Modeling

Kent Danielson*, Mark Adley**, Neil Williams***, Eric Lynd****

*Geotechnical & Structures Laboratory, U.S. Army Engineer Research and Development Center, **Geotechnical & Structures Laboratory, U.S. Army Engineer Research and Development Center, ***Geotechnical & Structures Laboratory, U.S. Army Engineer Research and Development Center, ****Geotechnical & Structures Laboratory, U.S. Army Engineer Research and Development Center

ABSTRACT

This presentation discusses the recent advances in higher-order finite elements for lumped-mass explicit approaches typically needed for high-rate weapons effects modeling. Topics include benefits of 2nd order tetrahedral, wedge, and hexahedral element formulations for both compressible and nearly incompressible materials as well as at higher orders, superconvergence and variable extraction, and efficient explicit time solution methods. These technologies are included in ERDC-GSL in-house meshing (ProMesher), parallel analysis (ParaAble), and visualization (PenView) codes as well as implementations into popular meshing (Cubit), parallel analysis (EPIC), and visualization (ParaView) software freely and readily available to DoD and other government agencies. These elements have also been linked with several integration schemes to the ERDC-GSL PENCURV cavity expansion-based penetration resistance functions for deformable penetrator trajectory simulation within both the ParaAble and EPIC codes. These capabilities are also incorporated into comprehensive and seamless modeling capabilities, computed serially or by launching massively parallel Linux/Unix jobs, all within the PENCURV+ Windows GUI and framework. The benefits for shape optimization and large tradespace analyses are also demonstrated.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Tunable Seat Belt Behavior in Nanocomposite Interfaces Inspired from Bacterial Adhesion Pili

Kerim Dansuk*, Sinan Keten**

*Northwestern University, **Northwestern University

ABSTRACT

A challenging problem in designing nanocomposites is to engineer nanoparticle interfaces that have tunable cohesive strength and rate-responsive behavior, for which inspiration can be taken from biological systems. An exemplary bio-interface is the Chaperone-Usher (CU) pili, such as type 1 expressed by bacteria Escherichia coli. The pili have unique biomechanical properties that enhance the ability of bacteria to sustain attachment to surfaces under large stresses, such as constant force extensibility, logarithmic velocity-uncoiling force dependence, and adhesive tips with catch bond behavior that exhibit longer bond life-times at greater force levels. Although biophysics of the pili under strain/stress is well-studied for anti-infective applications that aim to compromise pili adhesion, utilizing the biomechanical properties of the pili in material design applications is yet to be explored. In this work, we have modeled the elongation of a single CU pilus with catch bond tip adhesin and examined its toughness response using Monte Carlo simulations. We showed that thepilus can act as a “molecular seat belt” that exhibits low toughness when pulled slowly and high toughness when pulled rapidly. Furthermore, we found that systematically varying the catch bond and shaft parameters leads to tunable seat belt behavior at the interface, where the sharpness of the transition from the low toughness to the high toughness regime and the velocity at the start of the transition can be dictated by molecular design parameters. Lastly, we test the performance of CU pilus in slowing down a fast particle, and reveal that pili can effectively stop micron size projectiles with high initial velocities. The molecular seat belt mechanism presented here provides insight into how nanocomposite interfaces can be engineered to create molecular networks with linkers that switch on or off depending on strain rate.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Modeling Uncertainty and Propagation of Data in Rigid Musculoskeletal Simulation: Unavoidable Best Practice for Translating Models to Clinical Routine Practice

Tien Tuan Dao*, Marie Christine Ho Ba Tho**

*Université de technologie de Compiègne, France, **Université de technologie de Compiègne, France

ABSTRACT

Rigid musculoskeletal simulations have been intensively investigated to estimate joint kinematics, loading, and muscle forces for clinical decision support [1]. However, the use of these simulation outcomes in clinical routine practice remains a challenging issue. Data uncertainty due to human variabilities, differences in experimental protocols and measuring techniques is one of the possible causes affecting on the reliability of simulation outcomes. In this talk, current knowledge, limitations and future challenges related to this important issue will be presented. In particular, we will present recent achievements from our group using precise and imprecise probabilities to model data uncertainties related to segmental and muscle properties [2]. Advanced data fusion has been also developed to reduce data uncertainties [3]. Data uncertainty of dependent parameters has been taken into consideration using copulas. Model uncertainty has been also quantified. Demonstrations of developed methodologies will be focused on rigid musculoskeletal models of the lower limbs. Propagation of data uncertainties on the joint loading and muscle force estimation will be also presented. In fact, accounting data and model uncertainties become unavoidable best practice for translating the developed models and associated simulation outcomes into clinical routine in the framework of in silico medicine. Keywords: Data uncertainty, model uncertainty, uncertainty modeling, uncertainty propagation, rigid musculoskeletal modeling, reliable simulation outcomes.
Acknowledgements This work was carried out in the framework of the Labex MS2T, which is funded by the French Government. References [1] TT Dao, F Marin, P Pouletaut, P Aufaure, F Charleux, M C Ho Ba Tho (2012). Estimation of Accuracy of Patient Specific Musculoskeletal Modeling: Case Study on a Post Polio Residual Paralysis Subject. Computer Method in Biomechanics and Biomedical Engineering 15 (7): 745-751. [2] TT Dao, MC Ho Ba Tho (2015). Assessment of Parameter Uncertainty in Rigid Musculoskeletal Simulation using a Probabilistic Approach. Journal of Musculoskeletal Research, Vol. 18, No. 3 (2015) 1550013. [3] TT Dao, MC Ho Ba Tho (2017). A Consistent Data Fusion Approach for Uncertainty Quantification in Rigid Musculoskeletal Simulation. Journal of Mechanics in Medicine and Biology. 17(4), 1750062

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Simulation of Dynamic Damage Evolution due to Micro-cracking in Quasi-brittle Materials

Nitin Daphalapurkar*, Darby Luscher**, Daniele Versino***

*Los Alamos National Laboratory, **Los Alamos National Laboratory, ***Los Alamos National Laboratory

ABSTRACT

Simulations incorporating micro-cracking-based damage model are used to elucidate dynamic compressive response of a quasi-brittle material permeated by spatially evolving wing-cracks. Effective elastic compliance considers mechanism of wing-crack activation from pre-existing flaws, which are characteristic of flaw-sensitive quasi-brittle materials (e.g. energetic and geological materials). Increment in macroscale compliance due to growth of a single planar wing-crack is used for calculation of damage strain. Constitutive model incorporates evolution of effective compliance and tensorial damage, which is in turn driven by the growth of planar wing-cracks. Model is demonstrated by comparing results predicted from simulations with measurements from high-rate experiments.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Scattering Problem at an Interface Using Bloch Wave Theory: Application to Seismic Metamaterials

Michaël Darche*, Denis Aubry**, Fernando Lopez-Caballero***, Bing Tie****

*CentraleSupelec, Paris-Saclay University, **CentraleSupelec, Paris-Saclay University, ***CentraleSupelec, Paris-Saclay University, ****CentraleSupelec, Paris-Saclay University

ABSTRACT

To assure the stability of constructions to a seismic perturbation or vibration, there are a lot of different types of waves that should be suppressed or at least reduced, for example the surface waves induced by a railway. Instead of the traditional systems installed on existing construction, there is an increasing interest for para-seismic protections modifying the soil around the area where the waves have to be attenuate with barrier or periodic inclusions. Different methods have been used to study these problems (e.g. finite elements, Floquet theory, etc.). We want to propose an alternative approach based on Bloch wave theory. This approach uses the periodicity of a physical lattice to give periodic transformed responses on Bloch mode from any solution. Contrary to a fully simulation using finite element among others, we need only to identify the eigenvalues and the eigenmodes on a primitive cell to evaluate the behavior on the whole lattice due to its periodicity. It allows to reduce considerably the size of the numerical model. With the analysis of the dispersion curves, some frequency bandgaps could appear depending on the lattice parameters and the medias properties. These gaps provide informations on the diffraction of the wave through the inclusions. Moreover the scattering problem which appears at the boundary between the periodic media and the homoge- neous one has also been treated as well because Bloch theorem usually works for infinite medias. On account of the complexity of this part, the problem is applied to acoustic wave propagation through a plane interface between the semi-infinite medias. Analytical results are shown considering some basic arrays. To validate the model, some cases will be tested and compared with existing numerical and experimental results. A parametric study concerning the effect of the number of inclusions and the contrast of rigidity between the soil and the inclusion on the bandgaps apparition is done.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Convolved Action Principles and Space-Time Finite Element Methods for Elastodynamics

Gary Dargush*, Georgios Apostolakis**

*University at Buffalo, SUNY, **University of Central Florida

ABSTRACT

The appearance of temporal convolutions in the reciprocal theorem for dynamical problems leads naturally to the development of mixed convolved action principles (Dargush and Kim, 2012), as an extension of work by Gurtin, Tonti and Oden and Reddy (1984). For linear continuum elastodynamics, the governing equations written in terms of displacements and stress impulses display an elegant symmetry that can lead to the formulation of stationary action principles, similar to those associated with Hamilton, except using temporal convolution rather than an inner product over the time interval. As a result, the issues with Hamilton's principle relating to end point constraints and dissipative phenomena are resolved. Remarkably, the stationarity of the mixed convolved action provides not only the governing partial differential equations, but also the specified boundary and initial conditions, as its Euler–Lagrange equations. Thus, the entire elastodynamic initial/boundary value problem is encapsulated in a scalar mixed convolved action functional written in terms of displacements and stress impulses. Furthermore, the convolved action provides the foundation for the development of true space-time finite element methods (Dargush et al., 2015). In this presentation, our previous work is extended to formulate a minimum principle for the discretized convolved action, along with an interesting maximum principle for discretized complementary convolved action. New finite element methods are developed for each of these two principles and several prototype examples are examined and compared. Oden JT, Reddy JN (1983) Variational Methods in Theoretical Mechanics. Springer, Berlin. Dargush GF, Kim J (2012) Mixed Convolved Action. Phys. Rev. E 85, 066606. Dargush GF, Darrall BT, Kim J, Apostolakis G (2015) Mixed Convolved Action Principles in Linear Continuum Dynamics, Acta Mechanica, 226(12), 4111-4137.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Goal-Oriented hp-Adaptivity Using Unconventional Error Representations

Vincent Darrigrand*, David Pardo**, Théophile Chaumont-Frelet***, Ignacio Muga****, Serge Prudhomme*****

*Basque Center for Applied Mathematics (BCAM), **University of the Basque Country (UPV-EHU), ***Basque Center for Applied Mathematics (BCAM), ****Pontifcia Universidad Católica de Valparaíso (UPCV), *****École Polytechnique de Montréal

ABSTRACT

An increasing number of engineering applications require a good accuracy of a given quantity of interest. The design of a mesh that provides the desired precision is therefore crucial. Goal-oriented adaptive methods provide such meshes. To represent the error in the quantity of interest with local and computable indicators, one computes the influence function by solving the adjoint problem with the (continuous linear) quantity of interest as the source. Errors in the primal and adjoint solutions applied to the adjoint operator provide the error representation. We introduced in [1, 2, 3] an alternative error representation with the use of an alternative operator that allows us to compute a Riesz representation of the error of the adjoint problem. If the alternative operator is select as the original operator of the adjoint problem, we recover the classical method. This method can be applied to a wide range of problems of any dimension. While we previously studied a purely p-adaptive process, the topic of this presentation will focus on applying the alternative error representation to h- and hp-adaptive processes. Mesh coarsening will also be considered during the adaptive process. Numerical examples will be drawn from multi-dimensional (2D) problems such as the Helmholtz or convection-dominated diffusion problems. References: [1] V. Darrigrand, D. Pardo, and I. Muga. Goal-oriented adaptivity using unconventional error representations for the 1D Helmholtz equation. Computers & Mathematics with Applications, 69(9):964–979, 2015. [2] V. Darrigrand, A. Rodriguez-Rozas, I. Muga, D. Pardo, A. Romkes, and S. Prudhomme. Goal-oriented adaptivity using unconventional error representations for the multi-dimensional Helmholtz equation. International Journal for Numerical Methods in Engineering, 113(1):22–42, 2018. [3] V. Darrigrand, A. Rodriguez-Rozas, D. Pardo, and I. Muga. Goal-oriented p-adaptivity using unconventional error representations for a 1D steady-state convection-diffusion problem. Procedia Computer Science, 108:848–856, 2017. International Conference on Computational Science, ICCS 2017, 12-14 June 2017, Zurich, Switzerland.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Real-space Electronic Structure Studies on the Energetics of Dislocations in Al-Mg Materials System and Its Connection to Mesoscale Models

Sambit Das*, Vikram Gavini**

*University of Michigan, **University of Michigan

ABSTRACT

We study the dislocation core in Aluminum and Magnesium using a local real-space formulation of orbital-free density functional theory, implemented using finite-element discretization. The framework enables direct calculation of isolated dislocation core energetics. So far our studies on edge [1,2] and screw [3] dislocations in Aluminum, and ongoing studies in Magnesium, suggest that the core size—region with significant contribution of electronic effects to dislocation energetics—is around seven to ten times the magnitude of the Burgers vector. This is in stark contrast to estimates based on atomic displacments. Interestingly, our study further indicates that the core-energy of the dislocations are strongly dependent on external macroscopic strains. Role of such core-energetics behaviour towards the low ductility of Magnesium in the c-axis is currently being investigated. Next, we use the electronic structure core energetics information to inform higher scale models. In particular, we develop a continuum energetics model for a discrete dislocation network, which accounts for the core energy dependence on macroscopic deformations, and from the variations of the core energy with respect to the nodal positions of the network, we obtain the nodal core force [3] which can directly be incorporated into discrete dislocation dynamics frameworks. This nodal core force includes contributions that are not accounted for in currently used discrete dislocation dynamics models which assume the core energy to be a constant excepting for its dependence on the dislocation line orientation. Using static case studies involving simple dislocation structures, we demonstrate that these additional contributions can be significant in comparison to the elastic Peach-Koehler force even up to distances of 10-15 nm between dislocation structures. Furthermore, we have incorporated the nodal core force into a 3-D dislocation dynamics implementation, where we are investigating the influence of core effects on elementary mechanisms of dislocation enabled hardening in Aluminum such as structure and strength of various dislocation junctions, critical passing stress around obstacles etc. [1] Iyer, M., Radhakrishnan, B., Gavini, V., 2015. Electronic-structure study of an edge dislocation in Aluminum and the role of macroscopic deformations on its energetics. J. Mech. Phys. Solids 76, 260–275. [2] Das, S., Iyer, M., Radhakrishnan, B., Gavini, V., 2016. Corrigendum to [1]. J. Mech. Phys. Solids 95, 428–429. [3] Das, S., and Gavini, V., 2017. Electronic-structure study of a screw dislocation in Aluminum and the role of macroscopic deformations on its energetics. J. Mech. Phys. Solids 104, 115–143.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Finite-Strain Homogenization Models for Multi-Scale Porous Viscoplastic Polycrystals and Applications

Shuvrangsu Das*, Dawei Song**, Pedro Ponte Castañeda***

*University of Pennsylvania, **University of Pennsylvania, ***University of Pennsylvania

ABSTRACT

We formulate constitutive models for the finite-strain macroscopic response of porous viscoplastic polycrystals using the recently developed iterated second-order homogenization method [1]. The model is then used to estimate the effective behavior under various types of loadings, with special attention to simple shear and pure shear strain loadings. The porous polycrystal is modeled as a two-scale composite, where large voids are distributed randomly in a fine-grained polycrystalline matrix with the grains described by single-crystal viscoplasticity. The method constructs a linear comparison composite (LCC) with material properties chosen via a suitable variational statement and the same sub-structure as the actual nonlinear composite. In turn, the macroscopic response of the two-scale LCC is derived by means of a sequential homogenization procedure, utilizing the self-consistent estimates for the effective behavior of the polycrystalline matrix and the Willis estimates for the effective behavior of the porous composite. The iterated homogenization improves over the non-iterated estimates, especially at low porosities, high nonlinearities and high triaxialities, by allowing a finer “discretization” of the matrix and, thereby reproducing the matrix behavior accurately. In addition, consistent homogenization estimates for the average strain rate and spin fields in the voids and grains are used to develop evolution laws for the sub-structural variables, including the porosity, void shape and orientation, as well as the “crystallographic” and “morphological” textures of the underlying matrix. The model then is used to generate estimates for both the instantaneous effective response and the evolution of the microstructure for porous FCC and HCP polycrystals under simple shear and pure shear strain loadings. The effect of macroscopic vorticity is deduced by comparing the evolutions of sub-structural variables and macroscopic response for simple shear with corresponding results for pure shear loading (no macroscopic rotation). The effects of textures on the effective behavior are demonstrated by comparing with the effective response of porous isotropic materials. The textures have hardening effects and the vorticity has softening effects on the macroscopic response, and their interactions result in complex behavior of the effective response. In addition, more general loading conditions, involving combined tension and shear, are considered to explore the effect of the stress triaxiality on the macroscopic hardening or softening for the porous polycrystals. Reference: [1] Song, D. and Ponte Castañeda, P., 2017. A finite-strain homogenization model for viscoplastic porous single crystals: I–Theory. Journal of the Mechanics and Physics of Solids, 107, pp.560-579.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

New Bounds on Tangential Constitutive Elasticity Matrix for Non-Linear Elastic Materials: A Multiscale Approach

Sonjoy Das*, Sourish Chakravarty**

*University at Buffalo, **Massachusetts Institute of Technology

ABSTRACT

A novel multiscale framework is proposed in this work to determine two matrix-valued bounds on the macroscopic tangential constitutive elasticity matrix for nonlinear elastic materials. The two bounds reflect the effects of underlying heterogeneous microstructures and are obtained by considering a small mesoscopic material volume element that is smaller than the classical representative volume element. This small mesoscopic material volume element not only includes multiple phases of materials but may also contain multiple microcracks which can be potentially dangerous and lead to catastrophic structural calamities or poor structural performance if not detected in time since they merge together to form macro-level cracks. The theoretical argument given in a previous work [1] for small deformation linear elasticity theory is extended in the present work. Two special uniform incremental boundary value problems on the small mesoscopic material volume element, that is finitely deformed and assumed to be in a state of uniform macroscale deformation gradient, are proposed to construct the matrix-valued bounds on the macroscopic tangential constitutive elasticity matrix. Micromechanical analyses based numerical procedure is outlined to evaluate the matrix-valued bounds for the macroscopic material property. The proposed method is demonstrated by the evaluating the bounds for a small material volume element with nonlinear elastic microstructures and several microcracks that induce heterogeneity and anisotropy in the macroscopic tangential constitutive elasticity matrix. It will be useful to characterize the heterogeneous nonlinear elastic materials such as metals, composites, and polymers that may include microcracks. Bibliography [1]. Huet, C., 1990. Application of variational concepts to size effects in elastic heterogeneous bodies. J. Mech. Phys. Solids 38 (6), 813–841.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Computationally Effective Lubrication Theory Based Modeling of Cerebrospinal Fluid in Brain Mechanics during Impact on Head

Sonjoy Das*, Abhishek Venketeswaran**

*University at Buffalo, **University at Buffalo

ABSTRACT

Finite element head models (FEHM) are increasingly used to gain insights into the mechanisms of traumatic brain injury (TBI). An important component in this context is the realistic modeling of the flow of cerebrospinal fluid (CSF) at the interface of the skull and brain. The CSF is contained in a chamber known as sub-arachnoid space (SAC). One vital function of the CSF is to absorb some energy during head impact and protect the brain inside the skull. Existing FEHM in the literature characterizes the CSF as a nearly incompressible solid with low shear modulus, to bypass the challenges and computational cost associated with the coupling between a solid mechanics solver (for skull and brain) and a fluid mechanics solver (for CSF). The present work develops a theoretical framework to characterize the CSF flow and the dynamics of the brain and skull motion resulting from an impact to the skull. A simplified geometry of the head is adopted, constituting of the brain, CSF and skull, each being represented by spheres of their representative diameters. The CSF flow in the SAC (thickness is about less than 3 mm) is modeled as a flow through thin gap using the lubrication theory. The inertial component of the Navier-Stokes equation, which is typically ignored in classical lubrication model, is retained in the present formulation. The velocity flow field of the CSF is represented by relying on stream functions. The resulting governing equation for the CSF flow turns out to be a fourth order linear partial differential equation (PDE) [1]. It has been experimentally reported in literature [2] that both the brain and skull solely undergo rigid body motions during the time duration of the impact (~10-2 s). Accordingly, the brain and skull are modeled as rigid bodies during this duration of the impact. The rigid body dynamics of the brain is found to be governed by an integro-differential equation (IDE) in terms of the CSF pressure, skull and brain accelerations. The IDE and the PDE form the governing equations for the fluid structure interactions. These equations are solved numerically using the finite element (FE) approach and the associated computational scheme is found to be superior and more effective than the simulation of the fluid structure interaction based full-scale FE model. The result of CSF flow is validated against the predictions from the fluid structure interaction module of Abaqus© (v 6.14-5). References [1]. Exact and approximate solutions for transient squeezing flow. Lang, Ji, Santhanam, Sridhar and & Wu, Qianhong. 10, 2017, Physics of Fluids, Vol. 29, p. 103606. [2]. Separating brain motion into rigid body displacement and deformation under low-severity impacts. Zou, Hong, Schmiedeler, James P and & Hardy, Warren N. 6, 2007, Journal of Biomechanics, Vol. 40, pp. 1183-1191.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

New Positive-Definite Random Matrix Ensembles and their Applications in Mechanics

Sonjoy Das*

*University at Buffalo

ABSTRACT

The scientific community has seen an increasing surge of applications of positive-definite random matrix ensembles in the fields of mechanics and multiscale mechanics in recent years. These ensembles are employed to directly model several positive-definite matrix-valued objects, e.g., mass matrices, stiffness matrices, small-deformation constitutive elasto-plasticity tensor, finite-deformation constitutive non-linear elasticity tensor, etc. Matrix variate distributions, e.g., Wishart/Gamma distribution, Beta Type 1 distribution, Kummer-Beta distribution, or distributions derived from them, are currently used for this modeling purpose. These distributions are, however, parameterized such that they induce specific mean and covariance structures that do not allow sufficient flexibility in modeling high level of uncertainties. The current work will discuss two new positive-definite random matrix ensembles that are likely to provide more flexibility in modeling high level of uncertainties. Applications of the new ensembles will be illustrated through examples from mechanics.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Two-scale Modeling of Thermo-mechanical Dynamic Damage in Brittle Solids

Cristian Dascalu*, Kokouvi Gbetchi**

*Université de Lorraine, Laboratoire d'Etude des Microstructures et de Mécanique des Matériaux, Metz, France,
**Université de Lorraine, Laboratoire d'Etude des Microstructures et de Mécanique des Matériaux, Metz, France

ABSTRACT

Under impact mechanical loadings or thermal shocks, structural components made of brittle materials may be exposed to dynamic failure. The appropriate modeling of the failure mechanisms at different scales of observation and the prediction of the corresponding thermo-mechanical damage evolution in such materials are essential for structural reliability predictions. Over the last decades, it has been established that thermo-mechanical coupling plays an important role in the proper description of the dynamic fracture. Although the thermo-elastic coupling has been often neglected in the dynamic fracture studies, it was shown experimentally that these effects are not negligible under transient conditions. For instance, Rittel (1999) reported experiments showing significant temperature drops at the crack tip during the initiation phase of mode I dynamic fracture in PMMA samples. The aim of the present contribution is to show that the observed thermo-elastic effects associated with the rapid failure can be successfully predicted using a two-scale dynamic damage model. For this, a new theoretical model able to assess the interplay between micro-cracking and thermo-mechanical evolutions during dynamic fracture processes is proposed. In the last years, we developed a two-scale damage model (Keita et al. 2014, Dascalu 2018) for the dynamic failure of brittle materials. In the present context, the model is extended to account for the thermo-elastic coupling at microscopic and macroscopic scales. The evolution law for damage is deduced using asymptotic developments homogenization from small-scale descriptions of mode I dynamic propagation of micro-cracks. The crack-tip heating process and the bulk thermo-elasticity are considered at the micro scale. The resulting homogenized model is sensitive to the size of the microstructure through a length parameter present in the damage law. Finite Elements simulations have been performed to characterize local and structural responses predicted by the new model. In particular, the impact test on compact compression PMMA specimens was reproduced and the obtained results are in good agreement with those reported in the experiments (Rittel, 1999). Keywords: Micro-cracks, two-scale damage model, dynamic brittle failure, thermo-mechanical coupling, microstructural size effects, finite-element simulations. References: Rittel, D. 1999. Thermomechanical aspects of dynamic crack initiation. Int. J. Fracture. 99, 199-209. Keita O., Dascalu, C., Francois B., 2014. A two-scale model for dynamic damage evolution. J. Mech. Phys. Solids. 64, 170-183. Dascalu, C., 2018. Multiscale modeling of rapid failure in brittle solids: Branching instabilities. Mechanics of Materials. 116, 77-89.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Computational Modeling of 2D Materials and their Heterostructures for Sustainable Energy Storage: Opportunities and Challenges

Dibakar Datta*, Vidushi Sharma**, Kamalika Ghatak***

*New Jersey Institute of Technology (NJIT), **New Jersey Institute of Technology (NJIT), ***New Jersey Institute of Technology (NJIT)

ABSTRACT

Because of the low gravimetric capacity of conventional graphite anode (theoretical value of 372 mAh/g), and massive structural changes and volume expansion of silicon anode (on the order of 300%) extensive research has been carried out during last few decades to develop anode materials that can yield much higher capacity. We, therefore, examined the possibility of 2D materials for application of high-capacity anode materials. By first-principle calculations based on density functional theory (DFT), we investigated the adsorption of lithium (Li), sodium (Na), and calcium (Ca) on graphene with divacancy and Stone-Wales defects. We find that with controlled defect topology, we can achieve a maximum storage capacity of approximately 1675, 1450 and 2900 mAh/g for Li-, Na-, and Ca-ion batteries respectively. Our results indicate a new paradigm of 2D materials based energy storage. However, despite enormous opportunities, we need to concern about several challenges such as adatom trapping at the defect sites, the effect of defects on adatoms diffusivity, microstructural changes, e.g., mechanical degradation at defect sites, etc. Besides graphene, several other 2D materials such as graphene allotropes, Transition Metal Dichalcogenides (TMD), etc. Moreover, by building heterostructures made by stacking of different 2D materials, it is possible to combine the advantage and eliminate the disadvantages of the individual materials. However, we need a computational genome to identify the optimal heterostructures for the energy storage. In this talk, we will provide a detailed overview of opportunities and challenges of modeling of 2D materials and its heterostructures for sustainable energy storage applications.

13th World Congress on Computational Mechanics (WCCM XIII) and 2nd Pan American Congress on Computational Mechanics
(PANACM II), July 22 - 27, 2018, New York City, NY, USA

ROBUST TARGET DESIGN FOR COMPLEX SYSTEMS USING MULTI-OBJECTIVE OPTIMIZATION

MARCO DAUB* **AND FABIAN DUDDECK***,†

* Technische Universität München
Arcisstraße 21, 80333 Munich, Germany
e-mail: {marco.daub, duddeck}@tum.de

† Queen Mary University of London
Mile End Road, London E1 4NS, UK

Keywords: Robust design, interval uncertainties, lack of knowledge, complex systems, multi-objective optimization.

Abstract. *During complex systems development, various uncertainties occur. Designs chosen at an early stage often turn out to be non-permissible at a later stage because of uncertain or currently unknown conditions. Therefore, a specific type of robust design is desirable which is insensitive to such conditions. Though, a challenge is that many uncertainties are not quantifiable at an early stage of development due to lack of knowledge. To overcome this, Hendrix et al. (1996) proposed to target the "most interior" design in the region of permissible designs which is then called a "robust design". This design centering method mainly addresses errors in manufacturing. However, other sources of uncertainties like changing operation conditions or model uncertainties, compare (Beyer, Sendhoff, 2007), are not considered with this approach. Hence, the method proposed in this work includes these uncertainties by using multi-objective optimization. Here, an optimal or robust design maximizes both tolerances in (controllable) design variables, tolerances in uncontrollable model parameters, and distances between the system performances and their threshold values.*

1 INTRODUCTION

In complex system design, uncertainties can be classified according to where they occur and how they are modeled mathematically. Depending on this classification, an overview is given in [1], how a robust design which is resistant to the uncertainties that are considered can be calculated. However, in real-world applications the information on the uncertainties is often limited, especially at an early design phase. This is due to imprecise or incomplete knowledge which is also referred to as epistemic uncertainties in literature. To overcome this problem, a method to find robust designs was proposed in [3] where maximal possible deviations of the design variables are sought by still satisfying all requirements. In [4] and [5] the method was slightly adapted and applications to complex systems design were given. Nevertheless, all considerations focused only on uncertainties in the controllable design variables.
In this work, the method of [3] is generalized by including uncertainties in uncontrollable parameters, the system responses and its threshold values in order to account for a non-reducible lack-of-knowledge situation in early design phase. Here, robust target designs are obtained by using multi-objective optimization. In chapter 2, definitions and uncertainties that occur in complex system design are considered before an enhanced method to calculate robust target designs is introduced. In chapter 3, the method is then applied to a simple crash design problem and results are visualized.

2 METHODOLOGY

2.1 Definitions

For complex systems, the goal is to find a suitable design. The corresponding design variables $x_i \in \mathbb{R}$, $i = 1, \ldots, d$ are collected in a d-dimensional vector $x \in \mathbb{R}^d$ with $x = (x_1, \ldots, x_d)$. Each design variable is lower bounded by $x^{\mathrm{l}}_{\mathrm{ds},i} \in \mathbb{R}$ and upper bounded by $x^{\mathrm{u}}_{\mathrm{ds},i} \in \mathbb{R}$, i.e. $x^{\mathrm{l}}_{\mathrm{ds},i} \leq x_i \leq x^{\mathrm{u}}_{\mathrm{ds},i}$ or $x_i \in [x^{\mathrm{l}}_{\mathrm{ds},i}, x^{\mathrm{u}}_{\mathrm{ds},i}]$ for $i = 1, \ldots, d$. As the design variables can be chosen by a decision maker within these bounds, they are also called controllable variables. The Cartesian product of the intervals $[x^{\mathrm{l}}_{\mathrm{ds},i}, x^{\mathrm{u}}_{\mathrm{ds},i}]$ form the design space Ω_{ds} with $\Omega_{\mathrm{ds}} \subset \mathbb{R}^d$.
In complex systems design, there are also quantities that cannot be controlled. These are the uncontrollable parameters $p_l \in \mathbb{R}$, $l = 1, \ldots, q$ which are collected in a q-dimensional vector $p \in \mathbb{R}^q$. For given x and p, the responses of the system can be determined uniquely. The responses $z_j \in \mathbb{R}$, $j = 1, \ldots, m$ are collected in in a m-dimensional vector $z \in \mathbb{R}^m$. The relationship between x, p and z can be expressed by using a system performance function $f : \mathbb{R}^d \times \mathbb{R}^q \to \mathbb{R}^m$ with

$$z = f(x, p). \tag{1}$$

In general, there are requirements in complex systems design that bound the system responses. Without loss of generalization, only upper thresholds $f_{\mathrm{c}}(p) \in \mathbb{R}^m$ are considered in the following as a multiplication of an inequality with lower thresholds will yield upper thresholds. Together with the restrictions of the design space, these requirements form a set of permissible

designs which is

$$\Omega_{\mathrm{c}} = \{x \in \Omega_{\mathrm{ds}} : \ f_j(x,p) \leq f_{\mathrm{c},j}(p),\ j = 1,\dots,m\}. \tag{2}$$

It shall be remarked that x and p can be responses of subsystems, and their values depend on lower level design variables or parameters. Here, this is included by the uncertainty consideration.

2.2 Uncertainties

In reality, the values of the selected design variables, the uncontrollable parameters, the system responses and their thresholds are usually uncertain, compare [1]. Inaccurate manufacturing or uncertainties propagated from a lower system level can affect the values of design variables or a priori chosen uncontrollable parameters for example. The values of uncontrollable parameters can also depend on changing environmental or operating conditions. Approximation errors inherent to the chosen model give rise to uncertainties in the system responses including their thresholds.
In early phase of complex systems design, there is only limited data about the uncertainties due to imprecise or incomplete knowledge. This complicates a proper mathematical quantification. In the following, it is assumed that the real values are symmetrically distributed around nominal values. Furthermore, they can be found within intervals where the interval bounds are unknown and only tolerance bands for the real values are given. The nominal values are marked with a check and express the selected variables in the case of design variables. It holds

$$x_i \in [\check{x}_i - \delta, \check{x}_i + \delta] \tag{3}$$

for $\delta \geq 0$, $\check{x}_i - \delta \geq x^{\mathrm{l}}_{\mathrm{ds},i}$, $\check{x}_i + \delta \leq x^{\mathrm{u}}_{\mathrm{ds},i}$, $i = 1,\dots,d$,

$$p_l \in [\check{p}_l - \gamma, \check{p}_l + \gamma] \tag{4}$$

for $\gamma \geq 0$, $l = 1,\dots,q$, and

$$f_j(x,p) - f_{\mathrm{c},j}(p) \in [(\check{f}_j(x,p) - \check{f}_{\mathrm{c},j}(p)) - \varepsilon, (\check{f}_j(x,p) - \check{f}_{\mathrm{c},j}(p)) + \varepsilon] \tag{5}$$

for $\varepsilon_j \geq 0$, $x \in \Omega_{\mathrm{ds}}$, $p \in \mathbb{R}^q$, $j = 1,\dots,m$ where δ, γ, and ε are the maximal tolerances.

2.3 Robust target design

In [3], a design is said to be robust, if possible deviations do not lead to a non-permissible design, i.e. $x \notin \Omega_{\mathrm{c}}$. A method is proposed how the tolerances for the design variables can be maximized by allowing only permissible designs. This is a design centering problem, see [2]. However uncertainties in uncontrollable parameters, the system responses and its thresholds, are not incorporated. Thus, a method which generalizes the one in [3] is proposed here that

maximizes all tolerances by using multi-objective optimization. For given nominal values of the uncontrollable parameters, the problem statement reads

$$\begin{aligned} \underset{\check{x},\delta,\gamma,\varepsilon}{\text{maximize}} \quad & (\delta,\gamma,\varepsilon) \\ \text{subject to} \quad & \delta,\gamma,\varepsilon \geq 0, \\ & x^{\mathrm{l}}_{\mathrm{ds},i} \leq x_i \leq x^{\mathrm{u}}_{\mathrm{ds},i},\ i=1,\ldots,m, \\ & \check{f}_j(x,p)+\varepsilon \leq \check{f}_{\mathrm{c},j}(p),\ j=1,\ldots,m \\ & \forall x_i \in [\check{x}_i-\delta,\check{x}_i+\delta],\ i=1,\ldots,d, \\ & \forall p_l \in [\check{p}_l-\gamma,\check{p}_l+\gamma],\ l=1,\ldots,q. \end{aligned} \tag{6}$$

Problem (6) is a multi-objective optimization problem with three objective functions. The nominal values for the design variables as part of a Pareto optimal solution are called a robust target design which considers various uncertainties. Pareto optimal solutions are solutions where it is impossible to improve in any of the objectives without degrading in another one.
In general, it is not easy to obtain Pareto optimal solutions of problem (6) because the optimization constraints must be satisfied for all possible x and p. In chapter 3, it is shown how problem (6) can be solved for a simple crash design problem.

3 APPLICATION TO CRASH DESIGN

3.1 A simple problem

An example of a complex system that must fulfill requirements is a vehicle. Regarding crash tests like the USNCAP crash load case where the vehicle is driven against a rigid wall with a velocity v_0, specific requirements can be set. The maximal acceleration, the energy absorption, and the order of deformation of the relevant components are system responses which have to be bounded. They can be calculated from the force-deformation characteristics of the components where their degrees of freedom are the design variables. In general, force-deformation characteristics cannot be designed as they are responses of the components' lower level design variables. Therefore, this selection must follow a second step, which is not part of this paper.
In figure 1, a simple example for a vehicle front structure which is modeled as two components is shown, see [5]. It shall be remarked that this example only illustrates the approach and a focus on more complex examples will be put in subsequent papers.

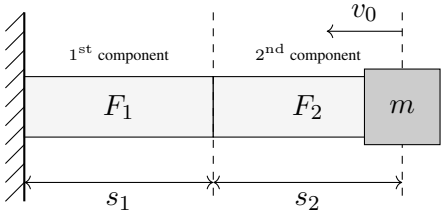


Figure 1: Simple crash problem for a vehicle front structure with two components, compare [5]

In every component, the force-deformation characteristics are modeled as constant. Hence, both components have one degree of freedom and the design variables are F_1 and F_2 with $F = (F_1, F_2)$. The lower bounds of the design variables are given by $F^{\mathrm{l}}_{\mathrm{ds},i} = 0\,\mathrm{kN}$ and the upper bounds by $F^{\mathrm{u}}_{\mathrm{ds},i} = 500\,\mathrm{kN}$, $i = 1, 2$.
Furthermore, the nominal values of the system responses and their thresholds are

$$\check{f}_1(F,p) - \check{f}_{\mathrm{c},1}(p) = F_1 - ma_{\mathrm{c}}, \tag{7}$$
$$\check{f}_2(F,p) - \check{f}_{\mathrm{c},2}(p) = F_2 - ma_{\mathrm{c}}, \tag{8}$$
$$\check{f}_3(F,p) - \check{f}_{\mathrm{c},3}(p) = -s_1F_1 - s_2F_2 + \frac{1}{2}m(v_0)^2, \tag{9}$$
$$\check{f}_4(F,p) - \check{f}_{\mathrm{c},4}(p) = F_1 - F_2, \tag{10}$$

compare [5]. The equations (7)-(8) relate to the maximal acceleration, equation (9) to the energy absorption and equation (10) to the order of deformation of the two components. The section lengths s_1, s_2, the mass m, the initial velocity of the vehicle v_0, and the critical acceleration a_{c} are uncontrollable parameters and are collected in the vector $p = (s_1, s_2, m, v_0, a_{\mathrm{c}}) \in \mathbb{R}^5$. Here, the given nominal values are $\check{s}_1 = 0.30\,\mathrm{m}$, $\check{s}_2 = 0.30\,\mathrm{m}$, $\check{m} = 1500\,\mathrm{kg}$, $\check{v}_0 = 15.6\,\frac{\mathrm{m}}{\mathrm{s}}$, and $\check{a}_{\mathrm{c}} = 300\,\frac{\mathrm{m}}{\mathrm{s}^2}$.
To get the nominal values of a robust design, the tolerances that are considered must be maximized. In order to account for the applicability of problem (6) to this specific system, the tolerances are transformed into relative tolerances with

$$\delta = \frac{F^{\mathrm{u}}_{\mathrm{ds},i} - F^{\mathrm{l}}_{\mathrm{ds},i}}{2}\bar{\delta},\ i = 1, \ldots, m \tag{11}$$
$$\gamma = \check{p}_l\bar{\gamma},\ l = 1, \ldots, q \tag{12}$$
$$\varepsilon = \max\{\check{f}_{\mathrm{c},j}(\check{p}) - \check{f}_j(F,\check{p}) :\ F \in \Omega_{\mathrm{ds}}\}\bar{\varepsilon},\ j = 1, \ldots, m \tag{13}$$

and $0 \leq \bar{\delta}, \bar{\gamma}, \bar{\varepsilon} \leq 1$.

3.2 Results for robust target design

As the constraint corresponding to equation (7) is redundant as well as the constraints on the design space, the optimization constraints for the simple crash design problem reduce to

$$\check{F}_2 + 250\mathrm{kN}\bar{\delta} + 450\mathrm{kN}\bar{\varepsilon} \leq 450\mathrm{kN}(1-\bar{\gamma})^2, \tag{14}$$
$$-0.3\mathrm{m}\,(1-\bar{\gamma})(\check{F}_1 + \check{F}_2) + 150\mathrm{kJ}(1-\bar{\gamma})\bar{\delta} + 117.48\mathrm{kJ}\bar{\varepsilon} \leq -182.52\mathrm{kJ}(1+\bar{\gamma})^3, \tag{15}$$
$$\check{F}_1 - \check{F}_2 + 500\mathrm{kN}\bar{\delta} + 500\mathrm{kN}\bar{\varepsilon} \leq 0, \tag{16}$$

and $-\bar{\delta}, -\bar{\gamma}, -\bar{\varepsilon} \leq 0$. This can be obtained as the maxima of $\check{f}_j(F,p) - \check{f}_{\mathrm{c},j}(p)$, $j = 1, \ldots, m$, are always adopted at the border of the intervals for x and p. In Figure 2, it is shown how increasing $\bar{\delta}$, $\bar{\gamma}$, or $\bar{\varepsilon}$ affect the set of permissible nominal values for $\check{F}_1$ and $\check{F}_2$.

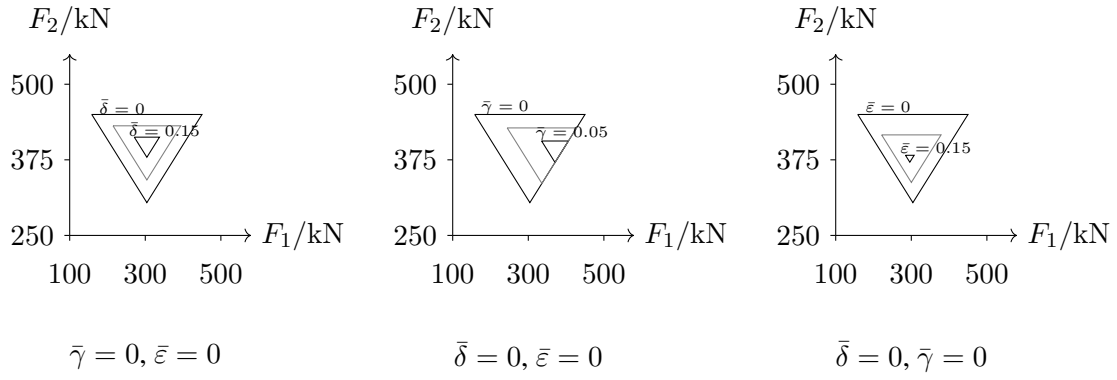


Figure 2: Set of permissible nominal values for $\check{F}_1$ and $\check{F}_2$, depending on $\bar{\delta}$, $\bar{\gamma}$, and $\bar{\varepsilon}$

The location of the set varies, depending on which one of $\bar{\delta}$, $\bar{\gamma}$, and $\bar{\varepsilon}$ is increased. This already gives an idea of the Pareto optimal solutions of the simple crash design problem and their corresponding robust target designs. Some of them are visualized in Figure 3.

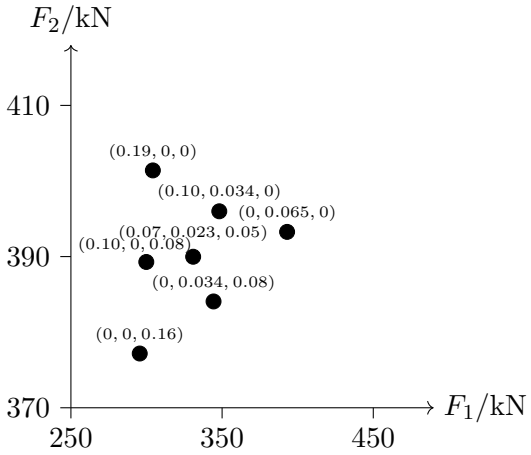


Figure 3: Selected robust target designs for the simple crash design problem together with their tolerances stated in $(\bar{\delta}, \bar{\gamma}, \bar{\varepsilon})$

Here, the dependency of the robust target design values on $\bar{\delta}$, $\bar{\gamma}$, and $\bar{\varepsilon}$ is emphasized. This does not mean that there is no other possible combination of $(\bar{\delta}, \bar{\gamma}, \bar{\varepsilon})$ for any robust target design, but changing this combination leads to a solution which is not Pareto optimal. Given the Pareto optimal solutions, it is the choice of the decision maker to balance the different objectives in order to select the most suitable nominal values for the design variables $\check{F}_1$ and $\check{F}_2$.

4 CONCLUSIONS

In this work, it was introduced how a robust target design for complex systems design that considers various uncertainties can be found by maximizing tolerances (intervals) for the uncertainties. This helps to handle the lack-of-knowledge situation in early development phase. Uncertainties in controllable design variables, uncontrollable parameters, the system responses and their threshold values are considered separately by using multi-objective optimization. If the real values of these uncertainties can be found within the optimized intervals, the complex system always satisfies the given requirements. For a simple crash design problem, Pareto optimal solutions could be calculated and the dependency of the robust target designs on the maximal tolerances for the different uncertainties could be shown. For further research, a general algorithm to solve the proposed problem statement is recommended.

ACKNOWLEDGMENTS

This work was supported by the SPP 1886 "Polymorphic uncertainty modelling for the numerical design of structures" of the German Research Foundation, DFG.

REFERENCES

[1] BEYER, H.-G., AND SENDHOFF, B. Robust optimization – A comprehensive survey. *Computer Methods in Applied Mechanics and Engineering 196*, 33-34 (2007), 3190–3218.

[2] HARWOOD, S. M., AND BARTON, P. I. How to solve a design centering problem. *Mathematical Methods of Operations Research 86*, 1 (2017), 215–254.

[3] HENDRIX, E. M., MECKING, C. J., AND HENDRIKS, T. H. Finding robust solutions for product design problems. *European Journal of Operational Research 92*, 1 (1996), 28–36.

[4] ROCCO, C. M., MORENO, J. A., AND CARRASQUERO, N. Robust design using a hybrid-cellular-evolutionary and interval-arithmetic approach: A reliability application. *Reliability Engineering & System Safety 79*, 2 (2003), 149–159.

[5] ZIMMERMANN, M., AND VON HOESSLE, J. E. Computing solution spaces for robust design. *International Journal for Numerical Methods in Engineering 94*, 3 (2013), 290–307.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Forecasting and Predictive Simulation for Coastal Ocean Processes

Clint Dawson*

*University of Texas at Austin

ABSTRACT

Coastal ocean models are used for many different applications, including environmental studies, modeling of tsunamis and hurricane storm surge modeling. Recent extreme events have pointed to the need to extend current modeling capabilities by including additional physics at multiple spatial and tempral scales, improving algorithms and concurrently enhancing computational speed through high performance computing. In this talk, we will describe recent advances in multi-physics couplings, new algorithmic advances in modeling using discontinuous Galerkin methods, and improvements in high performance computing through the use of High Performance ParalleX (HPX). We will discuss applications to recent hurricanes, and outline needs for future research.

13th World Congress on Computational Mechanics (WCCM XIII) and 2nd Pan American Congress on Computational Mechanics (PANACM II), July 22-27, 2018, New York City, NY, USA

ALGORITHM FOR EXTRACTION OF LOCAL PANELS FROM SURFACE FINITE ELEMENT MODEL AND APPLICATION IN WING DESIGN

SHUVODEEP DE[*], RAKESH K. KAPANIA[±]

[*]Postdoctoral Research Associate
Kevin T. Crofton Department of Aerospace and Ocean Engineering
Virginia Polytechnic Institute and State University, Blacksburg, VA, 24061-0203
Email: shuvode@vt.edu

[±] Norris and Wendy Mitchell Endowed Professor
Kevin T. Crofton Department of Aerospace and Ocean Engineering
Virginia Polytechnic Institute and State University, Blacksburg, VA, 24061-0203
Email: rkapania@vt.edu

Keywords: Finite-element Model, Mesh, Local-panels, Algorithm,

Abstract. Multi-disciplinary optimization (MDO) of structures is gaining popularity due to exponential increase in computational power. It is a common practice to solve problems involving highly complex systems where the system is decomposed into multiple smaller components to make it feasible to use parallel computation to reduce the overall time of optimization. In this work a new algorithm is developed to create local panels from two dimensional (surface) finite element models comprising of triangular element. The algorithm is based on applying set algebra on the connectivity data of the finite element model and is independent of nodal coordinates. The first step is to determine the nodes and the elements on the outer edge of the panel, the second to find the elements except the elements on the boundary that share one of the internal nodes. The elements ids are stored in a vector. Now the elements which share at least one node with the elements listed are found and their ids are stored in the same vector. This step is repeated till the vector do not change and it would contain the elements defining the local panel. The main advantage of this algorithm is that it can be used to create local panels of any shape and size and can be applied used for a wide range of structures including the aero-foil skin of aircraft wing, the cylindrical fuselage of the aircraft or the hull of a submarine. The study also includes creation of stiffeners on the local panels and finding the proper elements for the stiffeners. Once the local panels are determined, the structure is ready for global-local optimization. The algorithm is first demonstrated by dividing a rectangular surface using a family of curves of different orientations. Then it is used to divide the upper and lower skin of the NASA CRM Wing using intersection of curvilinear spars and ribs (*SpaRibs*) of different curvatures and orientation. This algorithm has been integrated to the EBF3GLWingOpt framework which is being developed by Kapania et al. at Virginia Tech to perform global local optimization of wide range of aircraft wing having *SpaRibs*.

1 INTRODUCTION

One of the most important concern while designing vehicles is to reduce structural weight, which can directly lead to reduction in fuel consumption. During the era when computers were expensive and not so powerful, structural design was mostly done by hand calculation on simplified mathematical models. However, since the seventies, due to rapid increase in computational power numerical solution techniques like Finite Element Analysis (FEA) have gained immense popularity. Not only the details and the complexity of the system can be included in the analysis, but multiple disciplines can now be considered while setting up a structural optimization problem. This avenue of research where several disciplines are incorporated into the optimization problem is known as Multidisciplinary Design Optimization (MDO). The major advantage of solving such a problem arise when relevant disciplines are not independent of each other, in other words, the disciplines interact with each other. Application of MDO for structural design can be traced back to work of Schmit [1] [2] [3]. In his work, finite element methods and algorithms for numerical optimization are used. In subsequent years, Haftka [4] [5] [6], Fulton [7] designed aircraft wings considering constraints on strength, stability and flutter velocity. MDO rapidly gained popularity in aerospace engineering and soon problems were solved involving complete model of aircraft [8] [9] [10] [11] [12]. The processes followed in MDO have either monolithic or distributed architectures [13]. In any MDO, the first step is almost always to describe the system using a set of design variables. The goal is to find the best values for the design variables that minimizes (or maximizes) the objective function while satisfying constraints in several disciplines. For example, in problems involving structural design, the size, shape or topology of the structure are described by a set of design variables. By applying appropriate numerical optimization algorithms, the problem is solved for a set of design variables that gives minimum weight or maximum compliance while satisfying constraint like maximum von Mises stress, minimum buckling factor, maximum displacement etc. In a monolithic architecture, all the design variables and constraints are considered in a single optimization process. This process, commonly known as All-at-Once optimization [14], although simple to implement is computationally expensive when the number of design variables is large. Such problems involving large number of design variables are often solved using the other process of MDO i.e. distributed architecture. The distributed MDO architectures involves the decomposition of a complex systems into multiple smaller components which are then described by a lower number of design variables and optimized independently. The process is usually implemented using parallel computation which can reduce wall clock time by several times. This process of decomposition of a system into simple sub-system is often known as global/local design optimization.

The aircraft wing is a complex structure consisting of the outer aerofoil shell known as the wing-skin, and internal stiffening elements: the ribs and spars. The global/local optimization process as described above has been used by several research groups including Cimpa *et al.* [15]. Even though the availability of computational power makes the exploration of large design space feasible, there has always been concern in the industry about manufacturing limitations. It is often very expensive to produce unconventional designs using conventional manufacturing processed. However, with invention of 3D printing techniques, the manufacturing industry is likely to be revolutionized over the next few decades. A new additive manufacturing technique known as Electron Beam Free Form Fabrication or EBF3 in short has recently been developed by Taminger and Hafley [16] at

NASA Langley Research Center to fabricate metallic structures of complex shapes, which now can be printed with significant precision. This technology inspired Kapania et al. at Virginia Tech [17] [18] [19] to propose the use of curvilinear stiffening elements to reduce structural weight and achieve desirable aeroelastic properties for aircrafts. The EBF3GLWingOpt is one of the several optimization frameworks that is being developed at Virginia Tech to optimize aircraft structures using curvilinear spars and ribs (*SpaRibs*). It performs global/local optimization of high aspect ratio cantilever transport aircraft wing for multiple constraints including stress, buckling and crippling. The wing geometry and mesh are generated using commercial software, MSC.PATRAN and MSC.NASTRAN is used for static and buckling analysis. The framework is written in Python environment and it enables use of parallel processing.

In the original version of **EBF3GLWingOpt**, written by Liu et al., the Linked-shape method proposed by Locatelli et al. [18] is used to create *SpaRibs* in each of the wing-boxes using limited number of design variables (which specified the shape of the *SpaRibs*). The upper and the lower skin of the wing are divided into local panels using the intersection of the *SpaRibs* and the stiffeners are attached to on each of the panels. The thickness of each of the local panels, the stiffener height and thickness are considered as design variables. The optimization framework could only explore limited design space where *SpaRibs* could start at the leading-edge spar and end at the trailing-edge spar. In order to overcome this limitation, De et. al. [20] proposed the *Extended-space method* to create *SpaRibs*. By this method not only the constraint on the starting and ending point of the *SpaRibs* was removed but also *SpaRibs* crossing the junction of the inner and outer wing-box can be created. In addition, the algorithm to extract local panel from the finite element model as used the original version of **EBF3GLWingOpt** framework was dependent on nodal coordinate coordinates of the nodes and could extract only panels with four edges from the finite element model. Moreover, the idea of dividing a surface into local panels and assigning a thickness design variable to each of the panels is very generalized and can be applied not only to aircraft wings but different other structures including automobile, ships, buildings etc. Thus, the need was felt to develop a generalized algorithm to break a finite element model into local panels. In the following work, such an algorithm to divide a surface mesh (consisting of triangular elements) has been discussed. The process can be implemented on the CRM wing for any *SpaRibs* configuration as well as other shell-structures like the fuselage or automobile frame with minor modifications. This algorithm is not dependent on nodal coordinates and is purely based on set operations performed on the element connectivity matrix.

The article is organized into seven sections. Section 2 mention the Mesh-continuity algorithm by which element and nodes interior to the local panel can be found. Section 3 mention the order in which the panels are numbered. To make the Mesh-continuity algorithm work, the elements interior to the local panel and along the outer edge need to be determined at first. Section 4 discuss the process of determining these elements. Section 5 demonstrate the algorithm on a simple problem. Section 6 and Section 7 discuss the integration of the algorithm with **EBF3GLWingOpt** framework and demonstrates its effectiveness for range of SpaRibs profiles with example.

2 MESH CONTINUITY ALGORITHM

The goal is to come up with an algorithm to extract local panels from the finite element mesh of a larger structure given its boundary nodes. To do so, the elements interior to the local panel along its outer edge i.e., which share the boundary nodes need to be determined. Once these boundary nodes are determined it is a straightforward process to determine all nodes and elements interior to the local panel using the connectivity matrix information, following the steps given in Figure 1.

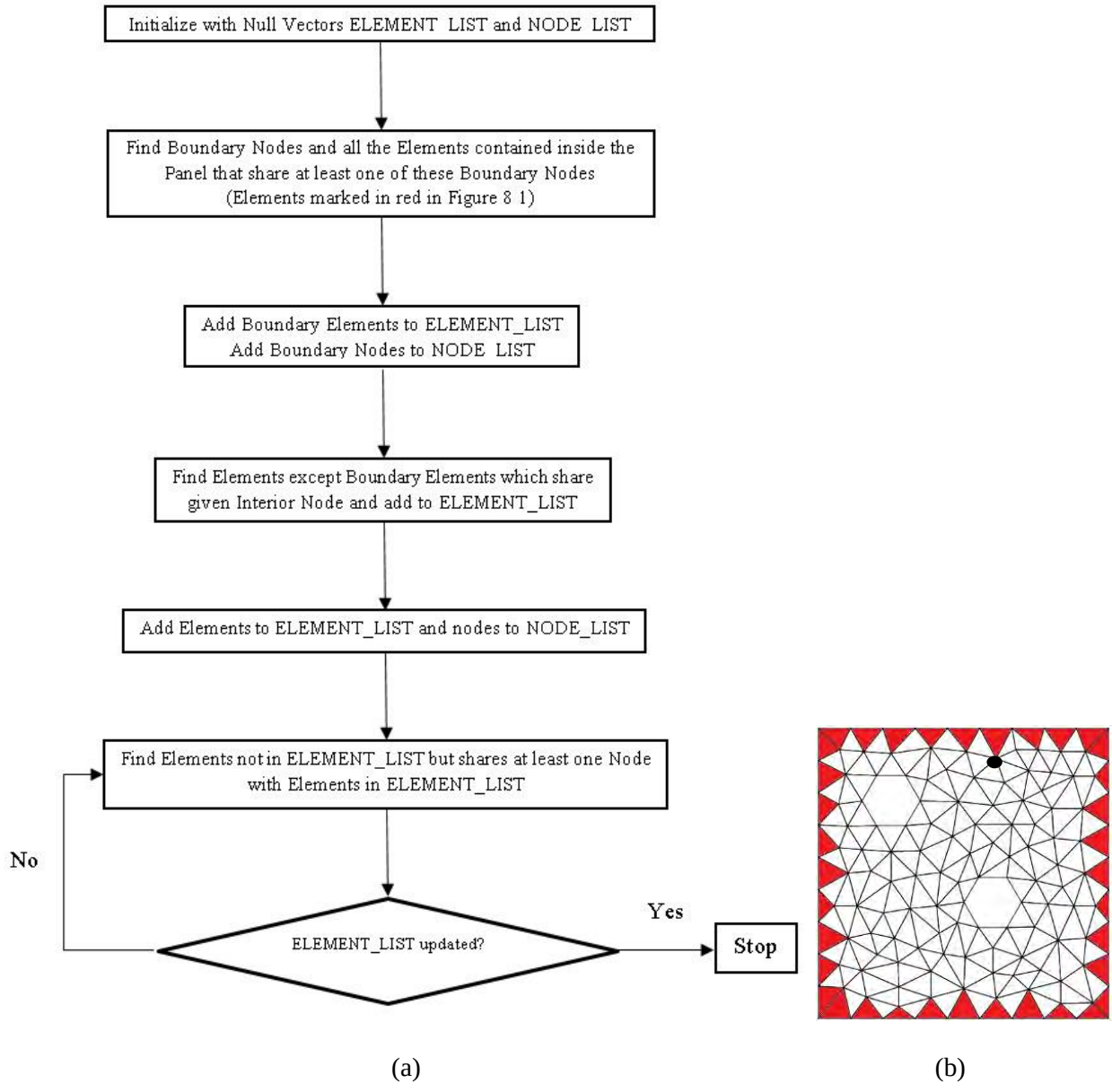


Figure 1: (a) Mesh Continuity Algorithm to find Elements inside Local Panel (b) Determining Panel Elements by Boundary Elements (red) and an Interior Node (black)

3 NUMBERING OF THE LOCAL PANEL

In this method, the finite element model of the wing skin is first sliced using the set of curvilinear ribs and then each slice is again divided using the curvilinear spar. The numbering process of the local panels is shown in Figure 2.

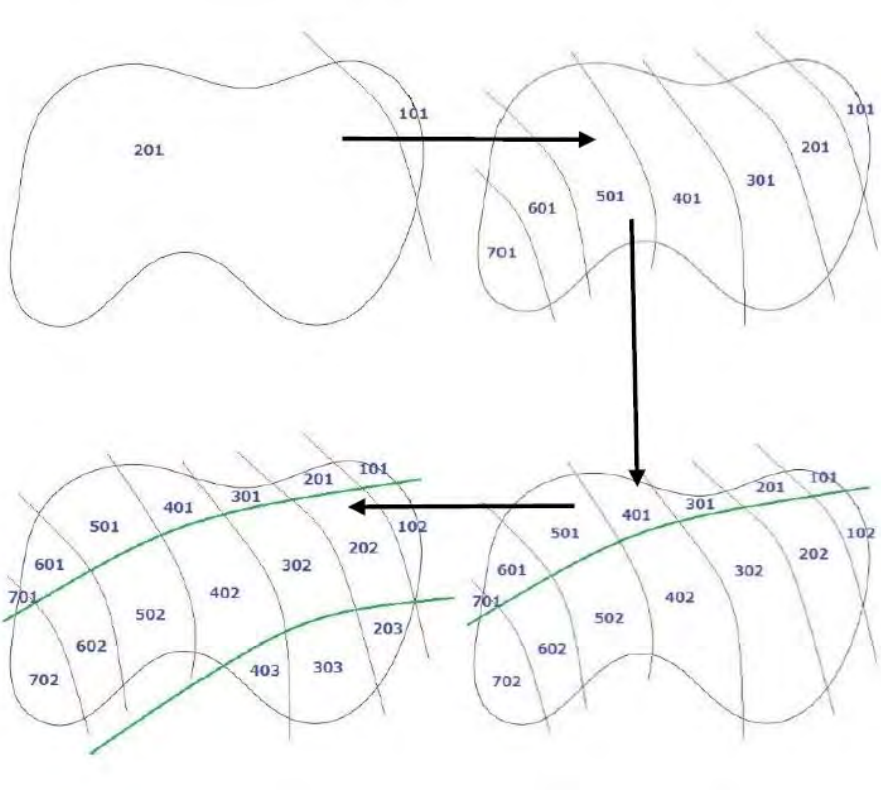


Figure 2: Numbering the Local Panels

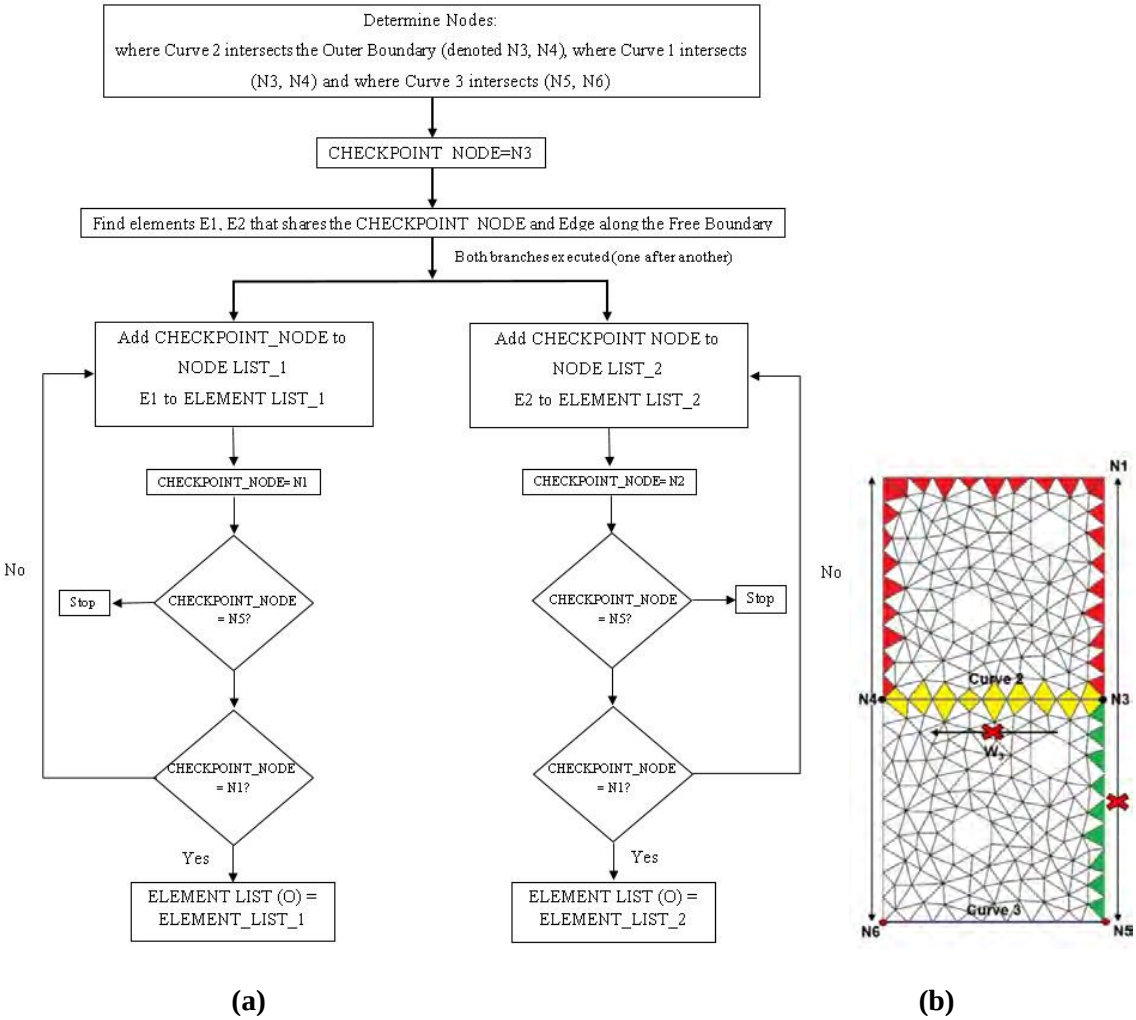
4 ALGORITHM TO DETERMINE THE BOUNDARY ELEMENTS

The Mesh-continuity algorithm is easy to apply once the elements along the outer boundary of the panel is determined. The general process to find this boundary elements is a bit complicated and will be discussed in detail this section with a simple example where the objective is to split a rectangular plate (with holes) meshed with triangular elements into two panels. The process consists of two steps. The first step is to determine all elements along the free boundary that is part of one of the panels. The second step is to determine the elements with edges along the dividing curve which are interior to the panel.

4.1 To determine elements along free boundary:

The plate shown in Figure 3 (b) is needed to be split along Curve 2 (Curve 3 is the next curve in the family, Curve 1 is the previous one). First elements along the free edge of the panels will be

found. In the algorithms described in this section, CHECKPOINT_NODE refers to the node with respect to which the positions of other nodes are determined. ELMENT_LIST_1 and ELMENT_LIST_2 are vector containing [Element ID, Connectivity Nodes] while NODE_LIST_1 and NODE_LIST_2 are list of Nodes. All of them are initialized as null sets.



(a) **(b)**

Figure 3: (a) Plate are Split by Three Non-Intersecting Curves (b) Algorithm to determine Elements along the Outer (free) Boundary

The nodes along Curve_1 is already known. Thus, finding the elements along this curve is very simple. All it need is to find the elements that has at least two nodes along Curve_1. The elements in ELEMENT_LIST (O) and those along Curve_1 are marked in red.

The algorithm described in Figure 3 is not applicable to find the elements interior to the local panel with edges along Curve_2, as will include elements outside the local panel as well (elements shown in Yellow in Figure 4 b). This is because all those elements have edges along the curve. To find the elements only interior to the panels another algorithm has been developed. To do this, another algorithm has been developed, which is named Middle Element Algorithm (MEA).

4.2 Middle Element Algorithm (MEA):

Here the objective is to determine elements on the left/right side of a curve C (red) in Figure 4 (a).

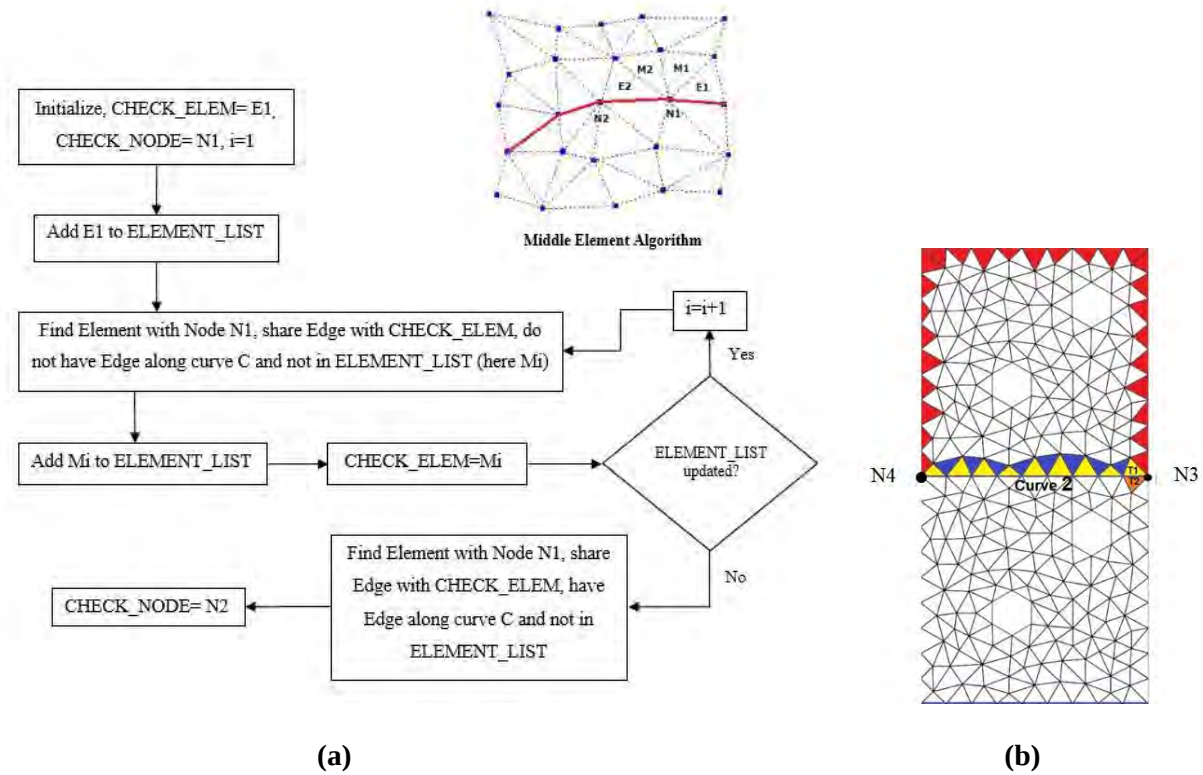


Figure 4: (a) Middle Element Algorithm (b) Using Middle Element Algorithm to find Elements in Local Panel

The elements contained in the vector ELEMENT_LIST consists of elements only above Curve 2 (marked by yellow and blue in

Figure 4. The elements contained in ELEMENT_LIST (O) and ELEMENT_LIST forms the outer boundary of the panel above the Curve 2. Once these elements along the outer boundary are determined, the mesh Continuity Algorithm can be used to find all the elements belonging to the panel.

5 EXAMPLE WITH SIMPLE PROBLEM

The algorithm is demonstrated first on a simple example. The rear wing-box of Boeing HSCT N+2 Wing containing 7 *SpaRibs* in the span-wise direction and 8 *SpaRibs* in the chord-wise direction is constructed in MSC.PATRAN as shown in Figure 5.

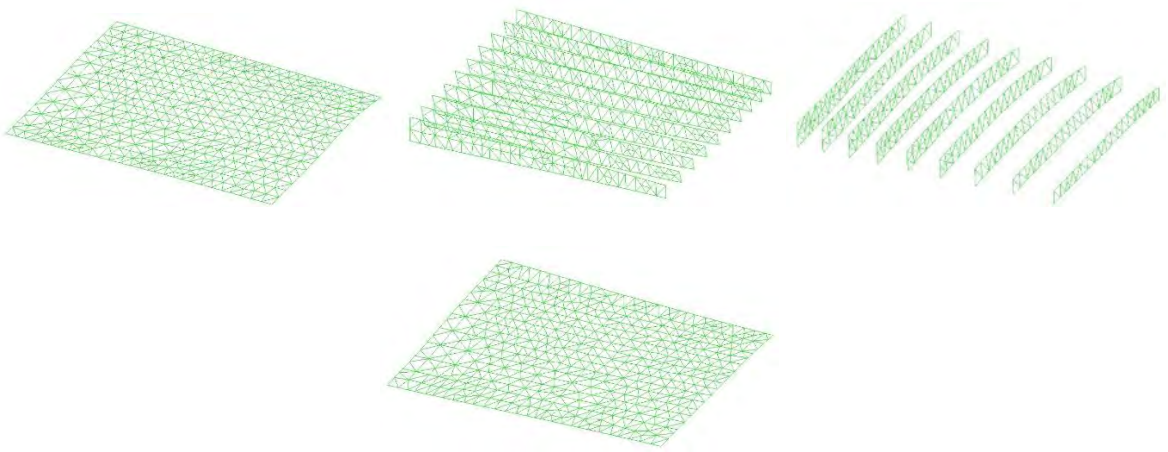


Figure 5: (a) Geometry of Rear Wing-box of Boeing HSCT N+2 Wing using Linked-shape Method (b) Mesh using Triangular Elements

Figure 6 shows a local panel from the top skin from the wing-box using *SpaRibs* intersection created using the algorithm.

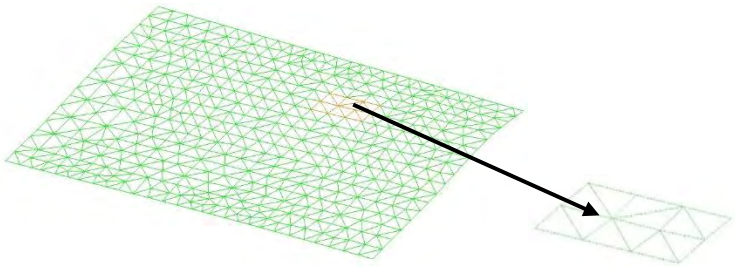


Figure 6: Local Panel from Upper Skin of Boeing N+2 HSCT Wing-box

6 INTEGRATION OF ALGORITHM WITH EBF3GLWINGOPT

The algorithm as discussed is integrated with **EBF3GLWingOpt** framework to create local panel on the upper and lower skin of the NASA CRM Wing (high-aspect ratio transport aircraft wing) for a range of *SpaRibs* configurations possible using the *Extended-space Method*. The wing-skin is first divided by the set of *SpaRibs* which replace the ribs. Each of the sections is then divided by the family of *SpaRibs* that replace the spars. The boundary nodes are the nodes common to the wing-skin and the *SpaRibs,* thus bounding the local panel. Since the algorithm is completely based on set operations performed on the connectivity matrix and independent of nodal coordinates, the algorithm can be used in a variety of problems requiring generation of local panels. The process is

also independent of the element ids and it works no matter in whatever order the elements are distributed. Depending on the shape of the bounding *SpaRibs* the panel can have any number of edges starting from three and up. Another advantage of this method is that the boundary nodes of each of the local panels is already determined and the information is stored to be used to impose boundary conditions during the optimization process.

In case of irregular panels, it is more difficult to determine the order in which the edges are numbered in MSC.PATRAN. Further a panel can have any number of edges. This makes it a challenging to develop a generalized parameterization method to create stiffener on panels. An alternative approach is developed where stiffeners are laid down on the global model and are meshed with the quad elements. The element size is chosen to be larger than the height of the stiffeners to ensure that the stiffeners are represented by a chain of quad elements with each elements sharing two common nodes with the skin. The nodes belonging to each of the local panels is already known by the method of creating local panels using the Mesh Continuity Algorithm. The MSC.NASTRAN .bdf file for the stiffeners are generated and read to find the quad elements with nodes common with the nodes of each of the local panels. These elements form the stiffeners for respective local panels. An example of such a stiffened panel is shown in Figure 7.

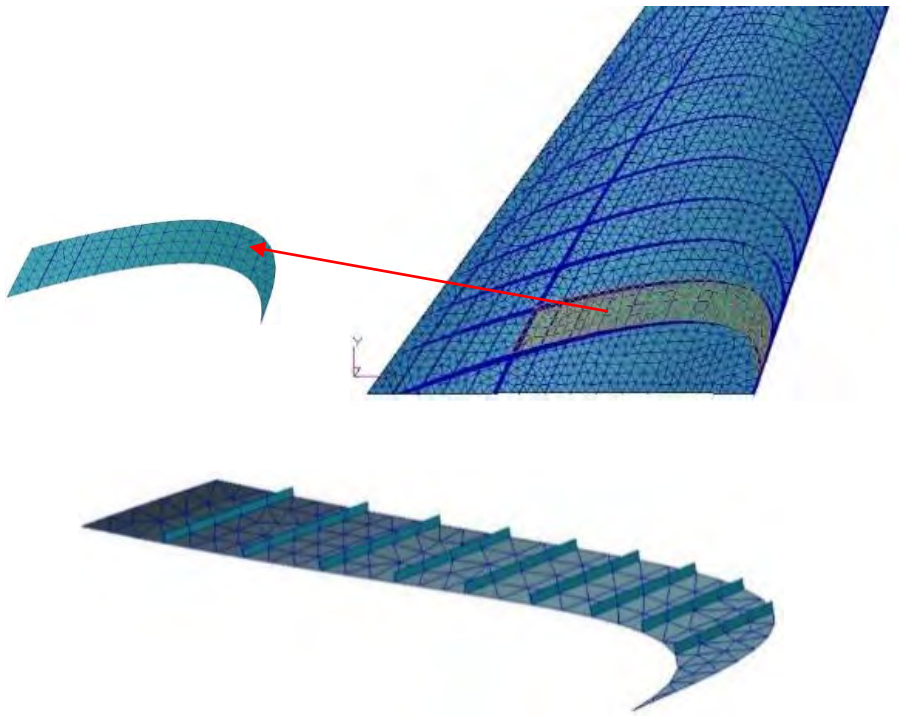
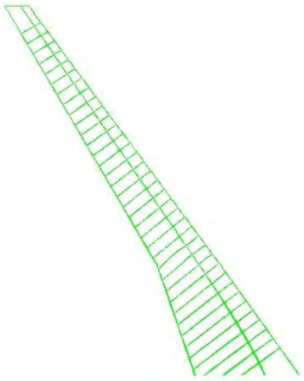
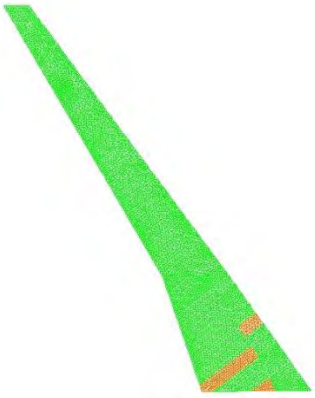
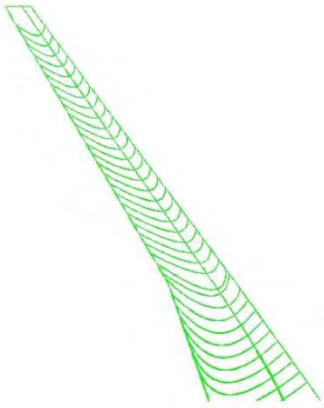
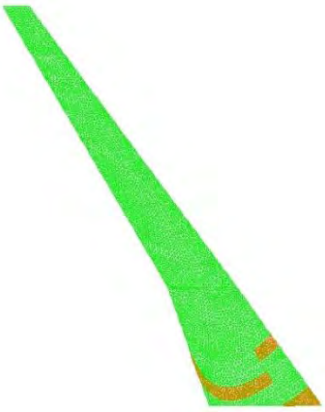
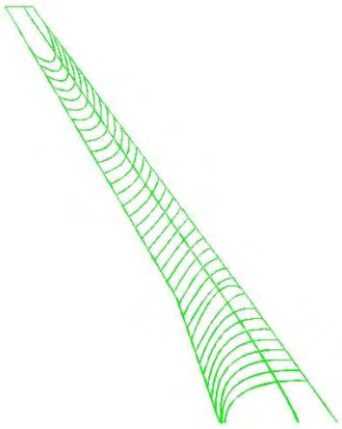
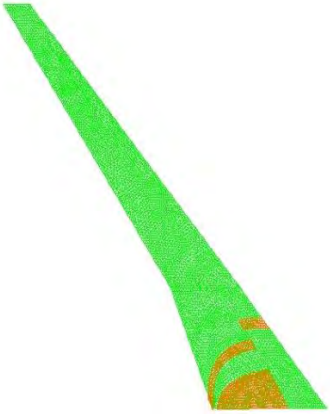


Figure 7: Local Panel with Stiffeners (formed by Quad Elements)

7 EXAMPLES OF APPLICATION

The proposed algorithm has been implemented on wings with different *SpaRibs* profile and is found to be effective for *SpaRibs* of different orientation and curvature. Table 1 shows some of the examples.

Table 1: Creation of Local Panels from NASA CRM Wing using SpaRibs intersection

SpaRibs Profile	Example of Local Panels
	
	
	

8 CONCLUSIONS

This paper gives a detailed description of a new algorithm to create stiffened local panels from the finite element model of the wing. The algorithm used in the original **EBF3GLWingOpt** framework to create local panels fails for many of the *SpaRibs* configurations possible to be created using the new method of parameterization as it was limited to the creation of four-edged panels only with two edges along adjacent spars. The new algorithm and is based on performing set operations on the connectivity data of the wing finite element model and is independent of nodal coordinate. It can be used to create local panels of any shape and size and can be used for structures other than the NASA CRM wing. Elements of the stiffeners attached with each of the local panels are found and stiffened panels are created. Once the local panels are determined, the structure is ready for global-local optimization.

REFERENCES

[1] L. A. Schmit and R. K. Ramanathan. Multilevel Approach to Minimum Weight Design Including Buckling Constraints. AIAA Journal (1978) 16:97–104

[2] L. A. Schmit. Structural Synthesis: Its Genesis and Development. AIAA Journal (1981) p. 1249–1263,

[3] L. A. Schmit. Structural Design by Systematic Synthesis. Pittsburg (1960)

[4] R. T. Haftka. Optimization of Flexible Wing Structures Subject to Strength and Induced Drag Constraints. (1977) 15:1101-1106

[5] J. H. Starnes Jr. and R. T. Haftka. Preliminary Design of Composite Wings for Buckling, Strength, and Displacement Constraints. Journal of Aircraft (1979) 16:564–570

[6] R. T. Haftka, J. H. Starnes Jr., F. W. Barton and S. C. Dixon. Comparison of Two Types of Optimization Procedures for Flutter Requirements. AIAA Journal. (1975) 13:1333–1339

[7] R. E. Fulton, J. Sobieszczanski, O. Storaasli, E. J. Landrum and D. Loendor. Application of Computer-Aided Aircraft Design in a Multidisciplinary Environment. Journal of Aircraft, (1974) 11:369–370

[8] I. Kroo, S. Altus, R. Braun, P. Gage and I. Sobieski. Multidisciplinary Optimization Methods for Aircraft Preliminary Design. 5th AIAA Symposium on Multidisciplinary Analysis and Optimization (1994)

[9] V. M. Manning. Large-scale design of supersonic aircraft via collaborative Optimization, PhD Thesis, Stanford University. (1999)

[10] N. E. Antoine and I. M. Kroo. Framework for aircraft conceptual design and environmental performance studies. AIAA Journal. (2005) 43:2100-2109

[11] R. P. Henderson, J. Martins and R. E. Perez. Aircraft Conceptual Design for Optimal Environmental Performance. Aeronautical Journal (2012) 116:1

[12] J. J. Alonso and M. R. Colonno. Multidisciplinary optimization with applications to sonic-boom minimization. Annual Review of Fluid Mechanics. (2012) 44:505-526

[13] J. R. R. A. Martins and A. B. Lambe. Multidisciplinary Design Optimization: A Survey of Architectures. AIAA Journal. (2013) 51:2049-2075

[14] J. Sobieszczanski-Sobieski and R. T. Haftka. Multidisciplinary Aerospace Design Optimization: Survey of Recent Developments. Structural Optimization. (1997) 14:1-23

[15] P. D. Ciampa and B. Nagel. Global Local Structural Optimization of Transportation Aircraft Wings. 51st AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference, Orlando, Florida. (2010)

[16] K. M. Taminger and R. A. Hafley. Electron Beam Freeform Fabrication for Cost Effective Near-Net Shape Manufacturing," in , VA: NATO/RTOAVT-139 specialists' meeting on cost effective manufacture via net shape processing. Amsterdam (The Netherlands): NATO (2006) Hampton (2006)

[17] D. Locatelli, S. B. Mulani and R. K. Kapania. Wing-Box Weight Optimization Using Curvilinear Spars and Ribs (SpaRibs). Journal of Aircraft. (2011) 48:1671-1684

[18] D. Locatelli, A. Y. Tamijani, S. B. Mulani and R. K. Kapania. Multidisciplinary Optimization of Supersonic Wing Structures Using Curvilinear Spars and Ribs (SpaRibs). 54th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference, Structures, Structural Dynamics, and Materials and Co-located Conferences, Boston, Massachusetts. (2013) AIAA 2013-1931.

[19] M. Jrad, S. De and R. K. Kapania. Global-Local Aeroelastic Optimization of Internal Structure of Transport Aircraft Wing. 18th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference, Denver,Colarado. (2017)

[20] S. De, M. Jrad, D. Locatelli, R. K. Kapania and M. Baker. SpaRibs Geometry Parameterization for Wings with Multiple Sections using Single Design Space. 58th AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials, Dallas. (2017)

[21] K. Singh, W. Zhao and R. K. Kapania. Optimal Design of Curvilinearly Stiffened Shells. 58th AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference, Washington DC. (2017)

[22] I. Sobieski and I. Kroo. Aircraft Design Using Collaborative Optimization. 34th Aerospace Sciences Meeting and Exhibit. (1996) AIAA-96-0715

[23] R. Braun, P. Cage, I. Kroo and I. Sobieski. Implementation and Performance issues in Collaborative Optimization. 6th AIAA/NASA/ISSMO Symposium on Multidisciplinary. (1996). AIAA-96-4017

[24] J. Sobieszczanski-Sobieski, B. B. James and A. R. Dovi. Structural Optimization by Multilevel Decomposition. AIAA Journal. (1985) 23: 1775–1782

[25] J. Sobieszczanski–Sobieski. Optimization by Decomposition: A Step from Hierarchic to Non-Hierarchic Systems. NASA Langley Research Center TR-CP-3031, Hampton, VA (1988)

[26] Q. Liu, M. Jrad, S. B. Mulani and R. K. Kapania. Global/Local Optimization of Aircraft Wing Using Parallel Processing. AIAA Journal. (2016) 54: 3338-3348

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

An Efficient Solution Approach for Multiphysics Modeling of Electrosurgery

Suvranu De*, Rahul .,**, Zhongqing Han***

*Rensselaer Polytechnic Institute, **Rensselaer Polytechnic Institute, ***Rensselaer Polytechnic Institute

ABSTRACT

Instruments that utilize radiofrequency (RF) alternating current are increasingly being utilized to perform a variety of surgical and other therapeutic procedures. Modeling of such procedures considering coupled electro-thermo-mechanical multiphysics and multiscale interactions with high degree of realism is challenging. Current best practices for the efficient solution of such multiphysics problems are based almost exclusively on multigrid methods and preconditioned Krylov subspace methods [1]. However, design of efficient application specific monolithic multiphysics multigrid solvers or preconditioners for the Krylov solvers is challenging [2]. We have developed a multi-physics model to investigate the effects of cellular level mechanisms on the electro-thermo-mechanical response of hydrated soft tissues with radiofrequency (RF) activation. A level set method is used to capture the interfacial evolution of tissue damage with the level set evolution equation derived from the second law of thermodynamics. We propose a coupled scheme to solve the resulting algebraic set of equations for the electric charge conservation, linear momentum balance, and temperature evolution equation. The coupled systems of equations are solved simultaneously using a Krylov subspace based iterative solver (e.g. GMRES) with an efficient block preconditioner. The block preconditioning technique effectively deflates the spectrum of the system matrix by clustering eigenvalues of system matrix around suitably chosen parameters [3]. This results in exponential convergence of the Arnoldi iterations with linear increase in the computational cost with increasing number of degrees of freedom when compared to the well-known block Jacobi and an algebraic multigrid (AMG) based preconditioners. Example problems illustrate the computational accuracy and efficiency of the technique. References [1] Keyes, D.E., McInnes, L.C., Woodward, C., et al., 2013. Multiphysics simulations: Challenges and opportunities. Int. J. High Perform. Comput. Appl. 27, 4-83. [2] Verdugo, F., Wall, W.A., 2016. Unified computational framework for the efficient solution of n-field coupled problems with monolithic schemes. Comput. Methods Appl. Mech. Eng., 310, 335-366. [3] Rahul, De, S., 2011. An efficient block preconditioner for Jacobian-free global-local multiscale methods. Int. J. Numer. Methods Eng., 87, 639-663.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Micropolar Asymptotic Homogenization for Periodic Cauchy Materials

Maria Laura De Bellis*, Andrea Bacigalupo**, Giorgio Zavarise***

*University of Salento, **IMT Lucca, ***Polytechnic University of Turin

ABSTRACT

We present a micropolar-based asymptotic homogenization approach [1,2] for the analysis of composite materials with periodic microstructure. The up-scaling relations are inspired by those originally proposed by [3] in the framework of the computational homogenization, expressing the local displacement field as a function of a cubic polynomial kinematic map depending on first, second and third order homogeneous tensors directly related to the classical and micropolar 2D deformation modes [4,5,6]. The local displacement field is described as superposition of the macroscopic driven kinematic map and local periodic perturbation fields. These perturbation functions are inherently related to the heterogeneous nature of the composite medium and are derived from the solution of recursive cell problems. The down-scaling relations are derived from a newly proposed third order asymptotic expansion of the local displacement field in terms of the macroscopic displacement and its first, second and third order gradients. The overall micropolar elastic tensors derive from a properly conceived energy equivalence between the macroscopic point and a representative portion of the heterogeneous material at the microscopic scale. Different applications to bi-phase orthotropic layered material to are proposed in order to exploit the capabilities of the proposed approach. [1] Smyshlyaev V. and Cherednichenko K. On rigorous derivation of strain gradient effects in the overall behaviour of periodic heterogeneous media. Journal of the Mechanics and Physics of Solids, 48(6):1325 1357, (2000). [2] Bacigalupo, A., Second-order homogenization of periodic materials based on asymptotic approximation of the strain energy: formulation and validity limits Meccanica, (49), 1407-1425 (2014). [3] Forest, S., Sab, K., Cosserat overall modelling of heterogeneous materials. Mech. Res. Commun. 25, 449454 (1998). [4] Addessi, D., De Bellis, M. L. and Sacco, E. Micromechanical analysis of heterogeneous materials subjected to overall Cosserat strains.Mechanics Research Communications, 54:27-34, (2013). [5] Addessi, D., De Bellis, M. L. and Sacco, E. A micromechanical approach for the Cosserat modeling of composites. Meccanica, 51(3):569–592, (2016). [6] Bacigalupo, A. and Gambarotta, L.Computational two-scale homogenization of periodic masonry: Characteristic lengths and dispersive waves. Computer Methods in Applied Mechanics and Engineering 213:16-28, (2012).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Mechanical and Structural Multi-scale Modelling of Bone Material

Paolino De Falco*, Li Xi**, Wolfgang Wagermaier***, Richard Weinkamer****, Peter Fratzl*****, Himadri Shikhar Gupta******

*(1) School of Engineering and Material Sciences, Queen Mary University of London, (2) Max Planck Institute of Colloids and Interfaces, Department of Biomaterials, **(1) School of Engineering and Material Sciences, Queen Mary University of London, (3) Department of Nuclear Engineering, North Carolina State University, ***(2) Max Planck Institute of Colloids and Interfaces, Department of Biomaterials, ****(2) Max Planck Institute of Colloids and Interfaces, Department of Biomaterials, *****(2) Max Planck Institute of Colloids and Interfaces, Department of Biomaterials, ******(1) School of Engineering and Material Sciences, Queen Mary University of London

ABSTRACT

To enhance the predictive power of mechanical models of bone, not only do the models have to be improved, but also new experimental data matched to model predictions at multiple hierarchical levels. At the level of the mineralized bone matrix, relatively few computational studies exist linking the structural parameters and mechanical properties at different length scales. Here, we propose a two dimensional and two-level hierarchical model of the bone matrix (mineralized fibril and lamella) to predict fibrillar mechanical response as a function of architectural parameters of the mineralized matrix. Specifically, we built a modified version of the laminate theory to predict the Young's modulus of bone as a function of the aspect ratio of mineral platelets [1] and degree of orientation. Our model shows that lowered mineralization combined with altered mineral nanostructure leads to lowered mechanical competence in bone. Our approach was also applied to fit experimental data obtained by small angle X-ray scattering (SAXS) on models of healthy and glucocorticoid induced osteoporotic bone showing how the reduced mineral volume fraction, reduced degree of alignment and aspect ratio are responsible for reduced mechanical properties in osteoporotic bone. In an attempt to expand scattering experiments for structural investigations of the bone mineral nanostructure to three dimensions, we also present first results on a new approach based on 3D SAXS experiments and Computed Tomography algorithms. These investigations can be used as tool for the diagnosis of bone diseases and the prediction of mechanical consequences of structural changes.

13th World Congress on Computational Mechanics (WCCM XIII) and 2nd Pan American Congress on Computational Mechanics (PANACM II), July 22-27, 2018, New York City, NY, USA

A COMPUTATIONAL GEOMETRY BASED ALGORITHM FOR SOLVING THE YIELD-LINE PROBLEM

M. DE FILIPPO*, J. S. KUANG†

*The Hong Kong University of Science and Technology
Clear Water Bay, Kowloon, Hong Kong
mdefilippo@connect.ust.hk

† The Hong Kong University of Science and Technology
Clear Water Bay, Kowloon, Hong Kong
cejkuang@ust.hk

Keywords: Collapse Mechanism, Computational Geometry, Computational Mechanics, Reinforced Concrete Slabs, Yield-line.

Abstract. Horizontal Reinforced Concrete (RC) slabs are commonly used in civil engineering industry for the construction of floors, ceilings, and more importantly bridges. The adoption of Finite Element Method (FEM) in industry has become massive to an extent to which engineers are starting to blindly rely on such analyses. However, the usage of FEM is not proper for every structural problem or purpose. For the case of structural assessment of flat RC slabs due to transverse load, plastic methods represent a more valid alternative and suitable approach. The plastic analysis involving the problem of assessing their strength and researching the most critical collapse mechanism due to flexure is well-known in literature as yield-line problem. Throughout the last century, many researchers have attempted to solve such problem. For simple geometries and boundary conditions, exact solutions were found, but they have showed lack of general applicability. Several techniques of approximated upper and lower bound methods have then been proposed, however nowadays the problem yet remains only partially solved. This paper aims at targeting the problem of collapse mechanism detection, and proposes an algorithm based on the solution of a set of computational geometry problems. The input is given by a plastically admissible moment field, which can be obtained through whatever method, and a fully automated technique is built according to the location of each yielded and next-to-yield moment triad in the physical domain. The results are shown along with the method of solution for the typical case of square simply supported slab under transverse distributed load.

1 INTRODUCTION

The yield-line method of analysis is a long-established hand method for evaluating the maximum carrying capacity of a slab, and its linked collapse mechanism. In the early ages of last century, the first version of such method has been proposed. In 1923, Ingerslev[1] was the first to coin the term 'yield-line', which describes subsequent locations along which yielding conditions are fulfilled. The estimation of such yield-line patterns gives an approximate evaluation of the collapse mechanism of the slab. As introduced, an analysis of the assessment of a slab is then subdivided into two parts, namely, estimation of maximum sustainable load, and detection of collapse mechanism. This paper will focus on this last aspect of the problem. In the past decades, this field of research has attracted the interest of many researchers. Middleton[2] developed a computer program for the assessment of RC slabs, famous nowadays in the UK, called COBRAS[3]. The software is based on a library of potential crack patterns. He has observed several recurrent collapse mechanisms that may occur when analyzing square slabs under different boundary and load conditions. He has then implemented them in an experience-based software. Chan[4], Munro et al.[5], and Balasubramanyam[6] also proposed several techniques for the identification of the most critical layout of yield-lines. Many of the proposed methods of solution involve the implementation of optimization techniques through either Linear Programming (LP) or Conic Programming (CP), according to the degree of the imposed constraints. Given the complex fractural behavior of RC slabs, the problem is mathematically and geometrically hard to solve. Many attempts turned to be successful, but only on specific cases. Nowadays, there is still lack of fully automated yield-line analysis tools able to properly detect the collapse mechanism of RC slabs due to bending. This paper aims at presenting an easy-to-compute technique for the detection of a layout of yield-lines linked to the collapse of slabs, implemented through the usage of simple computational geometry algorithms. The simple case of a square simply supported slab under uniform transverse load has been taken as sample, and the overall procedure along with obtained results are shown throughout this paper.

2 ASSUMPTIONS

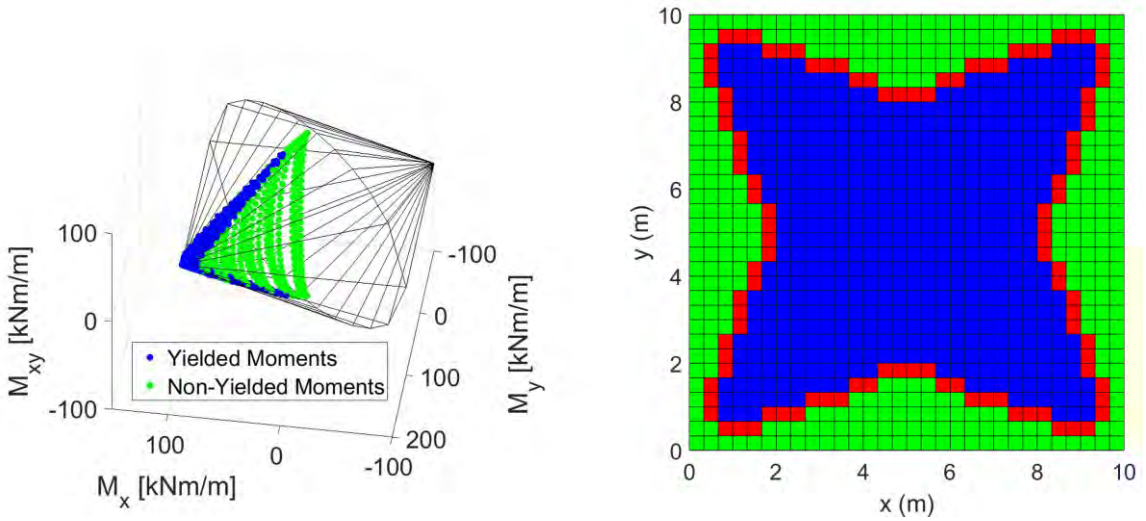
The method of detection of collapse mechanisms for RC slabs to be introduced in the next section is based on the following assumptions:

- The problem is restricted to static plate bending due to transverse loading conditions.
- Collapse mechanisms are solely associated with bending. The effects of shear are not taken into account by any mean. Shear failure is also disregarded.
- It is assumed that ductility of the slab is adequate enough for brittle failure to not occur.
- A plastically admissible field of moments has to be provided as input. Bending moments in the two directions of the slab, twisting moment, and principal moments are required. They can have been evaluated through different tools, such as a Non-linear FE analysis including the effects of plasticity in both concrete and steel.

In the case to be shown, the field of moments has been computed through the so-called Pseudo-Lower Bound Method for RC Slabs [7].

3 YIELD-CHECK

Given the definition of Yield-line, it is imperative to perform a check on whether yielding conditions are fulfilled by triads of moments, $\mathbf{m}^{e(i,j)} := \left\{M_x^{e(i,j)}, M_y^{e(i,j)}, M_{xy}^{e(i,j)}\right\}$, individually associated to a certain element e at the *i*-th row and *j*-th column in the mesh. The detection of physical locations in the slab where yielding is reached is of critical importance for the identification of a collapse mechanism. A bi-conical linearized version of Nielsen's criterion[8,9], as shown in a 3-dimensional $M_x - M_y - M_{xy}$ space in Fig. 1(a), is used as reference yield criterion, and it is referred to as f. Such figure also shows a sample configuration of moment triads with reference to the mentioned criterion. Yielded moments and non-yielded moments are marked accordingly. Fig. 1(b) illustrates the location of such yielded moments in the physical domain of the slab.



(a) (b)

Figure 1: Moments Configuration: (a) Location of yielded and non-yielded moment triads in the moments space. (b) Location of yielded and non-yielded moments on the slab, respectively, in blue and green elements. Non-yielded neighbors of yielded elements (next-to-yield) are depicted in red.

A yield-check is performed according to the yielding condition given in the following Eq.

$$\mathbf{m}^{e(i,j)} := \left\{M_x^{e(i,j)}, M_y^{e(i,j)}, M_{xy}^{e(i,j)}\right\} \mid f\left(\mathbf{m}^{e(i,j)}\right) = 0 \qquad (1)$$

4 METHODOLOGY

4.1 Mechanism triggering criterion

The moment triads have been located, respectively, in the slab, and in the moment space. Given the configurations shown in Fig. 1, it has to be defined whether yielding in the slab is triggering a collapse mechanism or not. In order to do so, a criterion has to be established for automatically evaluate the eventual occurrence of a collapse. Such criterion is formulated as it follows:

"Collapse of an RC slab under transverse load, due to flexure, is occurring if and only if at least a set of yield lines can be tracked from the center of load to all constrained edges, creating a convex closed polygon composed by triangular facets."

Hence, the problem of detection of the collapse mechanism can mathematically be expressed as it follows.

Given the physical domain of the slab, composed by the set $\mathbf{\Lambda}$ of all elements $\mathrm{e(i,j)}$ constituting the mesh, the subset $\mathbf{\Psi}$ of yielded elements is defined by the elements satisfying the condition given in Eq. (1), hence it follows that

$$\mathbf{m}^{\mathrm{e(i,j)}} := \left\{ \mathrm{M}_{\mathrm{x}}^{\mathrm{e(i,j)}}, \mathrm{M}_{\mathrm{y}}^{\mathrm{e(i,j)}}, \mathrm{M}_{\mathrm{xy}}^{\mathrm{e(i,j)}} \right\} \mid f\left(\mathbf{m}^{\mathrm{e(i,j)}}\right) = 0 \vdash \mathrm{e(i,j)} \in \mathbf{\Psi} \tag{2}$$

The subset $\mathbf{\Omega}$ of non-yielded elements $\mathrm{e(i,j)}$ having $\mathrm{e(i \pm 1, j)}$, left- or right-neighbor, or $\mathrm{e(i, j \pm 1)}$, bottom- or top-neighbor, as yielded element, hence satisfying at least one of Eq. (3) and (4), are classified as non-yielded neighbors of yielded elements, or more simply as next-to-yield elements.

$$\left\{ \mathbf{m}^{\mathrm{e(i,j)}} \mid f\left(\mathbf{m}^{\mathrm{e(i,j)}}\right) < 0, f\left(\mathbf{m}^{\mathrm{e(i\pm1,j)}}\right) = 0 \right\} \vdash \mathrm{e(i,j)} \in \mathbf{\Omega} \tag{3}$$

$$\left\{ \mathbf{m}^{\mathrm{e(i,j)}} \mid f\left(\mathbf{m}^{\mathrm{e(i,j)}}\right) < 0, f\left(\mathbf{m}^{\mathrm{e(i,j\pm1)}}\right) = 0 \right\} \vdash \mathrm{e(i,j)} \in \mathbf{\Omega} \tag{4}$$

A representation of their location in the slab is given in Fig. 1(b). Yield line patterns have to be searched within the subset $\mathbf{\Upsilon} := \mathbf{\Psi} \cup \mathbf{\Omega} \subseteq \mathbf{\Lambda}$ of yielded and next-to-yield elements. The subset of elements in $\mathbf{\Omega}$ are hence conservatively considered to have the same residual capacity of a yielded element. Their exclusion from $\mathbf{\Upsilon}$ would provide an additive reserve of bearing capacity.

Given the set of all vertices in the slab, $\mathbf{V} = \{v_1, v_2, \dots\}$, the subset of yielded and next-to-yield vertices is then defined as given in the following

$$\forall\, \mathrm{e(i,j)} \subseteq \mathbf{\Upsilon}\,, \mathbf{Y} \coloneqq \{v_1, v_2, \dots\} \in \mathrm{e(i,j)} \subseteq \mathbf{\Upsilon} \tag{5}$$

By defining edges as connections of geographically subsequent vertices in $\mathbf{Y}$, and their weights d, as the distances from one vertex to another, an undirected graph is created. A representation of such graph, according to the location of yielded and next-to-yield elements is given in Fig. 2.

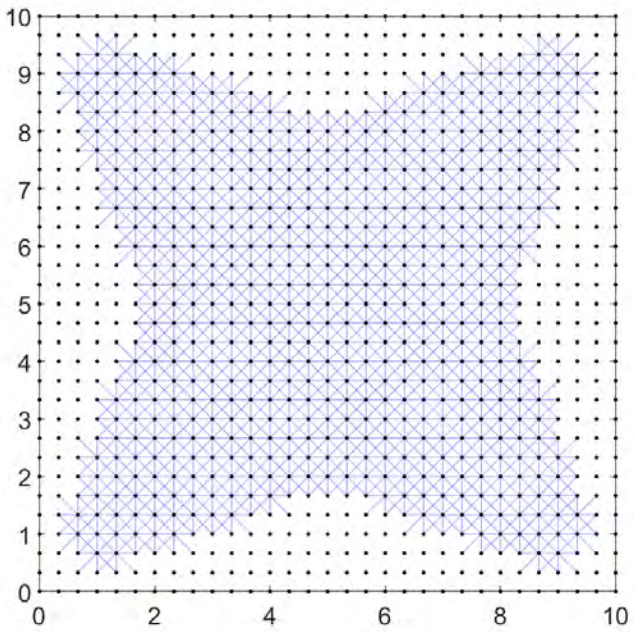


Figure 2: Undirected graph obtained through vertices $\mathbf{Y}$*, according to the configuration given in Fig. 1.*

Let $\mathbf{B} \coloneqq \{b_1, b_2, \dots, \}$ be the set of vertices along the constrained boundaries, as displayed in Eq. (6), $\mathbf{\Phi}$ is defined as the subset of yielded vertices at the boundaries, and as consequence it follows that $\mathbf{\Phi} \subseteq \mathbf{B}$, $\mathbf{\Phi} \subseteq \mathbf{Y}$.

$$\forall\, b \in \mathbf{B} \mid b \in \mathbf{Y} \therefore b \in \mathbf{\Phi} \tag{6}$$

If the boundary conditions at the vertex b do not constrain the bending moments, $\mathrm{M_x}$ and $\mathrm{M_y}$, hence in case at least one of Eq. (7) or Eq. (8) is satisfied, then such vertices will also be included in $\mathbf{Y}$, and hence in $\mathbf{\Phi}$.

$$\forall\, b \in \mathbf{B} \mid \mathrm{M}_{\mathrm{x}}^{b} = 0 \vdash b \in \mathbf{Y} \therefore b \in \mathbf{\Phi} \tag{7}$$

$$\forall\, b \in \mathbf{B} \mid \mathrm{M}_{y}^{b} = 0 \vdash b \in \mathbf{Y} \therefore b \in \mathbf{\Phi} \tag{8}$$

As consequence of the aforementioned definition of mechanism triggering criterion, a set of paths has to be found from the center of load c to at least two yielded vertices at each constrained boundary $b \in \mathbf{\Phi}$.

4.2 Yield-line tree

A set of feasible yield-lines can be found by solving a set of Shortest Path Problems (SPP) from the center of load to the subset of yielded and next-to-yield vertices in $\mathbf{\Phi}$ at each constrained boundary. As shown in the above figure, no path exists connecting the vertex

located at the center of load c (corresponding to the center of the slab in the current case of uniformly distributed load) and any vertex $b \in \mathbf{\Phi}$, because $\mathbf{\Phi} := \emptyset$ **,** hence a collapse mechanism cannot be triggered. An example in which, instead, a feasible solution to the SPP problem exists, is illustrated in Fig. 3.

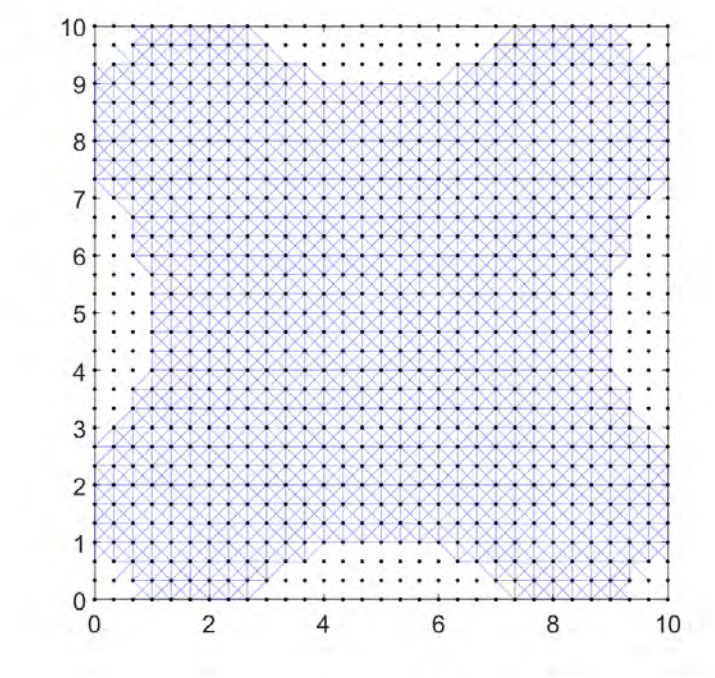


Figure 3: Undirected graph obtained through vertices ***Y****, according to a moment configuration corresponding to a higher load intensity that the one shown in Fig. 1.*

The SPP returns m sets of paths **P**, composed by vertices $v \in \mathbf{Y}$, ending in each reachable vertex $b \in \mathbf{\Phi}$ at each constrained boundary, with different weights $d(\mathbf{P})$. They are all feasible solutions for triggering a collapse mechanism. In accordance with the mechanism criterion, the set of non-coincident paths **S** with minimum $d(\mathbf{P})$, hence the shortest (two per each boundary), are chosen to be the most critical. Eq. (9) summarizes the above-mentioned concept, and Fig. 4 displays a sample yield-line tree found for the undirected graph of yielded and next-to-yield vertices and edges illustrated in Fig. 3.

$$\mathbf{S} := \{c, \dots, v, \dots, b\} \mid \min_{v \in \mathbf{Y}, b \in \mathbf{\Phi}} d(\mathbf{P_k}) \tag{9}$$

with	$\mathbf{P}_k := \{c, \dots, v, \dots, b\}$	sample k-th shortest paths from c to b
	$b \in \mathbf{\Phi} \subseteq \mathbf{B}$	a yielded or next-to-yield vertex at the boundary
	$k = \{1, \dots, m\}$	index of found path

m	amount of feasible paths from c to each reachable vertex $b \in \mathbf{\Phi}$ for a single constrained edge

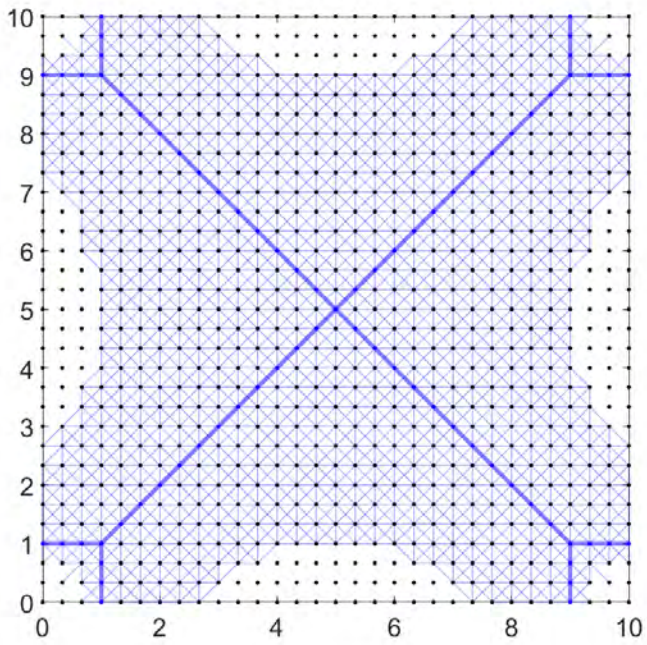


Figure 4: Undirected graph obtained through vertices $\mathbf{Y}$ *for a moment configuration for which a yield-line tree, representing the cracking patterns, can be detected. Such set of yield-lines is highlighted with blue lines.*

4.3 Axes of rotation

The last requirement enounced in the mechanism triggering criterion for the occurrence of collapse, is the creation of a convex closed path connecting the end points of the set of paths **S** such that triangular facets can be created. The yield-lines constituting such paths are commonly referred in literature as axes of rotation or hogging yield-lines. A collapse mechanism is expected to occur within the closed path, with the triangular facets rotating with respect to each other around yield-lines, and rotating around the axes of rotation. The parts of the slab falling outside the closed path constituted by axes of rotation are expected to remain intact, hence they do not participate in the collapse mechanism. The rotation around the axes of rotation requires yielding to occur due to a hogging moment, therefore the solution is contained within a subset $\mathbf{\Upsilon}^- = \mathbf{\Psi}^- \cup \mathbf{\Omega}^- \subseteq \mathbf{\Lambda}$. The subset $\mathbf{\Psi}^-$ defines yielded hogging elements, so that Eq. (10) is satisfied. The subset $\mathbf{\Omega}^-$ of non-yielded elements $\mathrm{e(i,j)}$ for which at least one of Eq. (11) and (12) is satisfied, are classified as non-yielded neighbors of yielded hogging elements, or more simply as next-to-yield hogging elements.

$$\left\{\mathbf{m}^{\mathrm{e(i,j)}} \mid \mathrm{M}_1^{\mathrm{e(i,j)}} < 0, f\left(\mathbf{m}^{\mathrm{e(i,j)}}\right) = 0\right\} \vdash \mathrm{e(i,j)} \in \mathbf{\Psi}^- \tag{10}$$

$$\left\{\mathbf{m}^{e(i,j)} \middle| \, M_1^{e(i,j)} < 0, f\left(\mathbf{m}^{e(i,j)}\right) < 0, f\left(\mathbf{m}^{e(i\pm1,j)}\right) = 0\right\} \vdash e(i,j) \in \boldsymbol{\Omega}^- \quad (11)$$

$$\left\{\mathbf{m}^{e(i,j)} \middle| \, M_1^{e(i,j)} < 0, f\left(\mathbf{m}^{e(i,j)}\right) < 0 \, f\left(\mathbf{m}^{e(i,j\pm1)}\right) = 0\right\} \vdash e(i,j) \in \boldsymbol{\Omega}^- \quad (12)$$

with $\left|M_1^{e(i,j)}\right| > \left|M_2^{e(i,j)}\right|$ hogging principal moments greater in absolute value than other principal moments at the same location

The subset of yielded and next-to-yield hogging vertices is then defined as

$$\forall \, e(i,j) \subseteq \boldsymbol{\Upsilon}^-, \mathbf{Y}^- \coloneqq \{v_1, v_2, \dots\} \in e(i,j) \subseteq \boldsymbol{\Upsilon}^- \quad (13)$$

Similarly as previously done for **Y**, again edges are defined as connections of geographically subsequent vertices in $\mathbf{Y}^-$, and their weights d, as the distances from one vertex to another. An undirected graph composed of such edges and vertices is created. A representation of such graph, according to the locations of yielded hogging elements, is illustrated in Fig. 5.

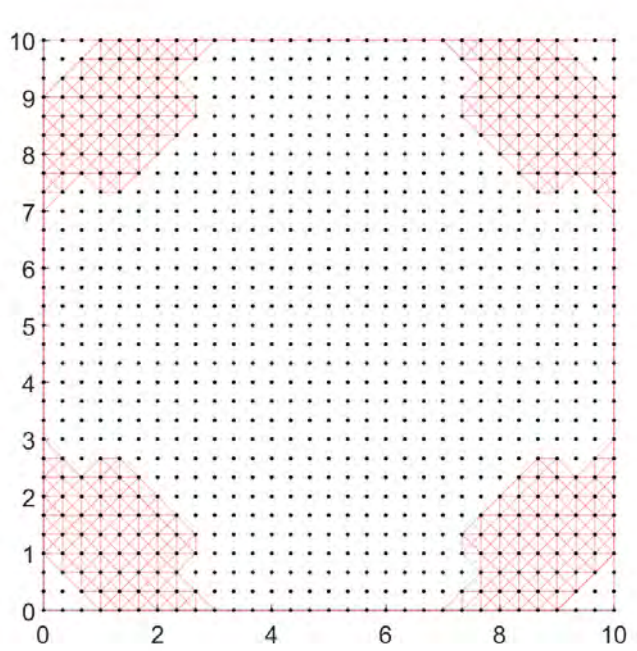


Figure 5: Undirected graph obtained through vertices $\boldsymbol{Y}^-$.

The path **R** is obtained through the junction of all the n shortest paths **P**, composed by vertices $v \in \mathbf{Y}^-$, passing through all the end vertices $b \in \mathbf{S}$. Such path is found by the individual assessment of SPPs between subsequent end vertices in the paths **S**. The above-mentioned concept is summarized in Eq. (14). The paths can be evaluated according to subsequent vertices either clockwise or counterclockwise.

$$\mathbf{R} := \{b_1, \dots, v, \dots, b_2\} \cup \dots \cup \{b_n, \dots, v, \dots, b_1\} \mid \min_{v \in \mathbf{Y}^-, b \in \mathbf{S}} \mathrm{d}(\mathbf{P}_r) \qquad (14)$$

with	$\mathbf{P}_r := \{b_l, \dots, b_{l+1}\}$	sample r-th shortest path from b_l to b_{l+1}
	l	generic index
	$r = \{1, \dots, n\}$	index of found path
	n	amount of paths necessary to connect all the geographically subsequent vertices $b \in \mathbf{S}$

The path **R** defines the axes of rotation, to and is superposed the yield-line tree, shown in Fig. 4, obtaining as result the collapse mechanism displayed in Fig. 6. Axes of rotation and yield-line tree are respectively depicted in red and blue lines.

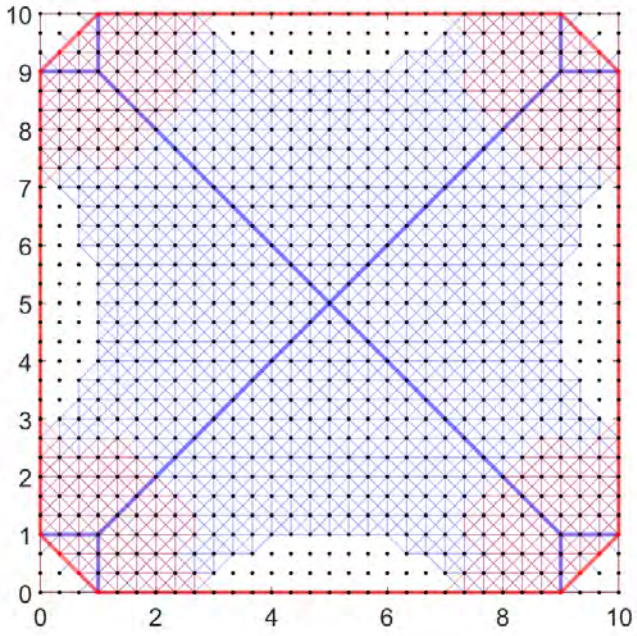


Figure 6: Collapse Mechanism composed by Yield-line tree (blue line) and axes of rotation (red line), respectively lying in the undirected graphs defined by vertices in $\boldsymbol{Y}$ *and* $\boldsymbol{Y}^-$.

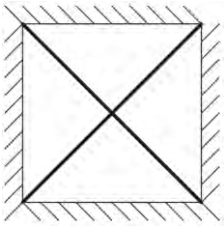


Figure 7: Exact analytical solution of the case of simply supported slab under uniform transverse load.

A close match between the results obtained through the above-shown methodology and the collapse mechanism of RC slabs is found. The exact analytical solution of the analyzed case of simply supported slab under uniform transverse load is given in Fig. 7.

5 DISCUSSION

From the comparison of Fig. 6 and 7, it can be noticed that the obtained solution fits well the collapse mechanism of the slab. It can immediately be observed that the crack patterns differ at the corners. When approaching the corners, the yield-line tree tends to split into two ends at the two boundaries. Among the assumptions at the basis of this study, failure in the slab is solely associated with bending, hence the effect of shear is not considered. The input of the proposed method is provided by a plastically admissible moment field. At a free or a simply supported boundary, both bending moments are theoretically null. Hence, it is obvious that, in the results of the algorithm, cracks tend to turn to region of the slab where yielding is already reached or is next to be reached, and moments are higher. In Fig. 4, it is clearly illustrated that the undirected graph created from $\mathbf{Y}$ does not include the vertices close to the corners, therefore it is impossible for the algorithm to detect a yield-line ending at the corner. Moreover, as shown in Fig. 5, regions approaching the corners are not included in $\mathbf{Y}^{-}$ neither. A test carried out by Nilson et al.[10], displayed in Fig. 8, shows experimental evidence of such phenomenon for a simply supported slab under uniform transverse load.

Figure 8: Corner crack of a simply supported beam under uniform transverse load.[10]

6 CONCLUSIONS

A simple algorithm based on computational geometry problems has been presented as attempt of solving the yield-line problem for RC slabs. The evaluation of ultimate load capacity has not been carried out. The focus of the present study is the identification of the most critical collapse mechanism. It has been demonstrated that the problem of identifying critical yield-line patterns leading to collapse of a slab can be formulated through a junction of well-known simple computational geometry problems. The development of a fully reliable method for the automated obtention of crack patterns leading to the collapse mechanism of slabs has not been achieved yet. For many decades several researchers have proposed hand- and automated-based techniques of upper and lower bound limit analyses, with the intention of returning the yield-lines configuration as output. Automated methods mainly involve the usage of non-linear mathematical optimization procedures with either linear or quadratic constraints. The hardness of implementation of such optimization procedures, its computational cost, and the lack of evidence of full reliability, leave the problem yet unsolved. Through the proposed technique, the complexity of the problem has been considerably reduced. The shown analogy gives evidence of a pragmatic match with the desired collapse mechanism obtained with a very low computational cost. The main aim is to overturn the hard belief that recourse to complex mathematical optimization procedures is always necessary when facing this type of problems. SPP is a computational geometry problem for which its solution is largely validated since decades. The analogy of obtained results with collapse mechanisms shows a base of foundation for a more global adaptability. Given the mathematical reliability of the results obtained through SPP, the mentioned analogy is hence founded on a solid basis of geometrical trustworthiness. The method of solution has been tested for the shown simple case, hence its application to more cases remains yet to be investigated. However, the methodology has been thought observing the behavior of RC slabs for several load and boundary condition cases. General applicability and adoption is the biggest challenge in this field of research. The development of a fully reliable technique may potentially be achieved through the involvement of several case-based machine learning algorithms. The ongoing research is focused on the development of a lower bounded solution for the assessment of RC slabs, including both evaluation of load-carrying capacity and detection of collapse mechanism.

REFERENCES

[1] Ingerslev Å. The strength of rectangular slabs. *Journal of the Institution of Structural Engineers*. 1923;1(1):3-14.

[2] Middleton CR. Concrete bridge assessment. *Bridge Surveyor Conference*. Mar 24, 1998.

[3] Middleton CR, Cambridge Enterprise Limited University of Cambridge. Cobras. 2014.

[4] Chan H. The collapse load of reinforced concrete plate. *Int J Numer Methods Eng*. 1972;5(1):57-64.

[5] Munro J, Da Fonseca A. Yield line method by finite elements and linear programming. *Struct. Eng.* 1978;56B:37-44.

[6] Balasubramanyam KV, Kalyanaraman V. Yield-Line analysis by linear programming. *J Struct Eng*., ASCE, 1988;114(6):1431-1437.

[7] De Filippo M, Kuang JS. Concept of a pseudo-lower bound solution for reinforced concrete slabs. *International Journal of Civil and Environmental Engineering*. 2018;12(3):349-353.

[8] Nielsen MP, Hoang LC. Limit analysis and concrete plasticity. CRC press; 2016.

[9] Nielsen MP. Yield criteria for reinforced concrete slabs. *flydebetingelser for jernbetonplader. (translated from) nordisk betong, 1963, 7(1), 61-82.* 1963.

[10] Nilson AH, Darwin D, Dolan CW. *Design of concrete structures.* 15th ed. McGraw-Hill Education (India) Pvt Limited; 2012.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Optimization of Piezoelectric Actuator Polarization and Topology: A Simultaneous Approach Based on the Controllability Gramian

Daniel De Leon*, Juliano Gonçalves**, Eduardo Perondi***

*Federal University of Rio Grande do Sul (UFRGS), **Federal University of Rio Grande do Sul (UFRGS), ***Federal University of Rio Grande do Sul (UFRGS)

ABSTRACT

This article addresses the problem of piezoelectric actuator design for active structural vibration control using the topology optimization method and a simultaneous approach for the optimization problem with respect to piezoelectric actuator topology and polarization profile is investigated. The optimization problem is written in terms of the controllability Gramian which is a measure that describes the ability of the actuator input to move the system states from an initial condition to a desired final state, at rest for instance, in a finite time interval. A coupled finite element model of the structure with embedded in-plane actuators is derived assuming a two-phase material, and this structural model is written into the state-space representation considering modal displacements and velocities as state variables. Then, the optimization procedure aims to determine the distribution of piezoelectric material and polarization which maximizes the controllability for a given vibration mode. In order to achieve this goal, the material interpolation scheme is carried out by means of the Piezoelectric Material with Penalization and Polarization (PEMAP-P) model [1] and both the optimum actuator layout and polarization profile are obtained simultaneously. The derivatives with respect to the polarization and design variables are calculated analytically. Numerical examples are presented considering the control of bending vibration modes in beams for a couple of boundary conditions and different target vibration modes are taken into account in the optimization problem to show the efficiency of the proposed formulation. A Linear-Quadratic Regulator (LQR) is synthesized for each case of controlled structure in order to compare the influence of the polarization profile on the displacement responses with active damping and we can observe that the simultaneous optimization approach presents an improvement in the control performance for all analyzed cases. The results are also compared to a formulation that does not take into account the electrode polarity in the optimization problem, i.e., the polarization profile is stated a priori and positive and negative regions are insulated of each other by means of null-polarity areas. Moreover, this approach allows the synthesis of a simple control system with only one input channel which is more suitable for practical applications. Therefore, the formulation presented in this work is an initial study towards a single formulation considering several aspects of the actuator topology design problem based on controllability. [1]~Silva ECN, Kikuchi N (1999) Design of piezoelectric transducers using topology optimization. Smart Materials and Structures 8(3):350-364.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Recent Progress on Isogeometric Reduced Quadrature Techniques

Laura De Lorenzis*, Frederik Fahrendorf**, Hector Gomez***

*TU Braunschweig, **TU Braunschweig, ***Purdue University

ABSTRACT

An efficient implementation of isogeometric analysis (IGA) requires non-standard quadrature techniques. Standard Gaussian rules are not well-suited for IGA, since they do not take advantage of the higher continuity of the shape functions. Therefore different quadrature strategies have been investigated. Bringing the concept of reduced quadrature to the extreme, collocation methods have been proposed and have recently gained increasing attention for linear as well as non-linear problems. A recent important development in isogeometric collocation and, more generally, reduced quadrature techniques has emerged in the context of the so-called variational collocation method. The idea is that for isogeometric basis functions there exists a set of points, termed Cauchy-Galerkin points, such that collocation at these points reproduces the Galerkin solution exactly. Good estimates of these points have been found by means of superconvergence theory. In this talk, we report on recent advancements made possible by the concept of variational collocation both in isogeometric collocation methods and in reduced quadrature rules for Galerkin schemes. In the former, significant advantages are obtained over classical collocation schemes in terms of spatial convergence rates. In the latter, new schemes can be proposed which can be seen as intermediate between the Galerkin variational formulation and the direct evaluation of the strong form in collocation approaches. The potential of the new methods in several research directions is also outlined.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Modelling Thermo-osmosis within Elastic-plastic Porous Media Undergoing Finite Strains

Nico De Marchi*, Valentina Salomoni**

*University of Padova, **University of Padova

ABSTRACT

Thermo-osmotic processes have been observed in clay-rich materials. Thermal and even chemical osmotic flows are in fact two of the main coupled flows caused by heat and ion transport in clay-rich media (Roshan and Rahman, 2011); the overall direction of water flow by thermo-osmosis depends on the entropy difference between water in the clay pores and that of water trapped in the diffuse interface layer or clay interlayers. Particularly, by assembling the most exhaustive data including the parameters necessary for the analysis on thermo-osmosis available in literature, Gonçalvès et al. (2012) confirmed that thermo-osmosis may prevail over the classical Darcy flow driven by pressure gradients, in clay-rich formations under natural or artificial thermal gradients. A coupled three-dimensional THM model in finite strains within the framework of the modified mixture theory is here presented, developed from a previous HM version (Spiezia et al., 2016) for saturated porous media. The upgraded model accounts for a permeability tensor dependent on deformation of the solid skeleton and thermo-osmosis, as well as a mixed three-dimensional finite element is implemented for ensuring stability requirements of the adopted formulation. References: 1. Roshan, H., Rahman, S.S., 2011. A fully coupled chemo-poroelastic analysis of pore pressure and stress distribution around a wellbore in water active rocks. Rock Mech. Roch Eng. 44(2): 199-210. 2. Gonçalvès, J., de Marsily G., Tremosa, J., 2012. Importance of thermo-osmosis for fluid flow and transport in clay formations hosting a nuclear waste repository. Earth Planet. Sci. Lett. 339-340: 1-10. 3. Spiezia, N., Salomoni, V.A., Majorana, C.E., 2016. Plasticity and strain localization around a horizontal wellbore drilled through a porous rock formation. Int. J. Plasticity 78: 114-144.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Strengthening Optimization in Curved Masonry Structures by Tensegrity Modelling

Mariella De Piano*, Valentino Paolo Berardi**, Rosa Penna***, Luciano Feo****, Raffaele Miranda*****

*University of Salerno, Italy, **University of Salerno, Italy, ***University of Salerno, Italy, ****University of Salerno, Italy, *****University of Salerno, Italy

ABSTRACT

A tensegrity procedure is used to design to the minimal mass of tensile reinforcements of masonry structures with arbitrary shapes [1]-[2]. The proposed strengthening methodology allows for the design of minimal mass resisting mechanisms of systems formed by a network of masonry rods, mainly working in compression, and grids of tensile reinforcements. It creates a minimal mass output of the strengthened model, which can be observed as lumped stress network and connect model of the exanimated structures [3]-[4]. Assuming a perfectly plastic response by each member, the existence of such resisting mechanisms ensures that the reinforced structure is stable under the examined loading conditions, due to the safe theorem of the limit analysis of elastic-plastic bodies. The approach includes an explicit determination of the state of pre-stress to be applied to tensile reinforcements, in order that they are effective under pre-existing loading conditions. Different numerical examples show the potential of the proposed approach in designing minimal mass FRP/FRCM reinforcements of masonry vaults and domes, which are aimed at preserving sufficient 'cracking-adaptation' capacity of the reinforced structure. References [1] Fraternali, F., Carpentieri, G., Modano, M., Fabbrocino, F., Skelton R.E., "A tensegrity approach to the optimal reinforcement of masonry domes and vaults through fiber-reinforced composite materials", Composite Structures; 134, 247–254 (2015). [2] Fabbrocino, F., Farina, I., Berardi, V.P., Ferreira, A.J.M., Fraternali, F., "On the thrust surface of unreinforced and FRP-/FRCM-reinforced masonry domes". Composites. Part B, Engineering, 83, 297-305, (2015). [3] Fraternali, F, "A Thrust Network Approach to the Equilibrium Problem of Unreinforced Masonry Vaults via Polyhedral Stress Functions". Mechanics Research Communications; 37, 198-204, (2010). [4] Berardi, V.P., Chiozzi, A., Fraternali, F., Grillanda, N., De Piano, M., Milani, G., Tralli A., "A numerical approach to the evaluation of collapse load multiplier of masonry curved structures" Proc. XXIII Aimeta Congress, 1515-1525 (2017).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

FE Investigation of Bond Behaviour of PBO-FRCM Composite for the Strengthening of Masonry Structures

Mario De Stefano*, Valerio Alecci**, Luisa Rovero***, Giulia Misseri****, Gianfranco Stipo*****

*Università di Firenze, **Università di Firenze, ***Università di Firenze, ****Università di Firenze, *****Università di Firenze

ABSTRACT

Protection and safeguarding of existing masonry structures, especially those classified as cultural heritage, require to define sustainable and compatible intervention technologies, material acceptance standards and, more importantly, adequate design tools. Innovative intervention strategies pivoting on the use of fibre-reinforced composites have increasingly proliferated in the last years, and have enabled the development of specific applications for existing masonry, using organic-modified cement-based matrixes associated to either organic or inorganic fibre nets characterised by loose weft-warp layouts. In particular, from an engineer-conservationist angle, Fibre Reinforced Cementitious Matrix (FRCM) solutions have overcome major drawbacks of FRPs, such as deterioration of the substrate layer (i.e. ancient masonry to be preserved) due to the well-known debonding phenomena, capacity cutback for high operating temperatures and low breathability, [1-2]. However, results already available in the literature need further investigation especially devoted to the development of reliable safety assessment and design tools, [3]. In this investigation, the response of a poly-benzoxazole (PBO) FRCM system experimentally tested on both its standalone constituents and on composite layout adhered to bricks, i.e. double-shear test (DST), is FE modelled. The mechanical properties of materials were refined on experimental evidences of the composite constituents to fit the response of the composite system FEM model to the experimented DST equilibrium path. In particular, assuming a plane strain model, the substrate, i.e. a clay brick, and the PBO fibre are considered as linear elastic, with elastic stiffness retrieved from experimental tests. Then, the cement-based matrix is discretised in 2D-quadratic elements with total strain smeared-crack failure criterion, assuming a multilinear tension softening law, calibrated on dedicated three-point bending tests. Furthermore, fibre-matrix interface is lumped at 0D elements on which normal and shear elastic stiffness as well as non-linear bond-slip law have been refined to fit outcomes of the experimental DST global behaviour. FEM outcomes agree well with the DST experimental behaviour, which revealed an undisturbed substrate and a failure mechanism at fibre matrix interface. Moreover, FEM non-linear analyses adequately represents the phenomenology of the DST response, i.e. a first linear branch, loss of stiffness due to crack increase, and final softening branch with matrix-fibre slippage. In conclusion, experimental results confirmed the efficacy of FRCM systems for repair and strengthening historical buildings, given the increase in ductility and load carrying capacity that they can provide. Besides, FEM outcomes showed that, in this framework, further investigation is necessary for other constituent materials, systems and test layouts. [1] Alecci, V., De Stefano, M., Luciano, R., Rovero, L., Stipo, G., 2015. Journal of Composites for Construction 04015041. [2] Alecci, V., Focacci, F., Rovero, L., Stipo, G., De Stefano, M., 2016. Composite Structures 149, 184–196. [3] D'Ambrisi, A., Feo, L., Focacci, F., 2013. Composites Part B: Engineering 46, 15–20.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Extended Numerical Modelling of Structural Adhesive Joints

Stijn Debruyne*, Mathias Creyf**, Korneel Van Massenhove***

*KU Leuven, Mechanical Engineering @ Bruges campus, **KU Leuven, Mechanical Engineering @ Bruges campus, ***KU Leuven, Mechanical Engineering @ Bruges campus

ABSTRACT

Abstract: This work presents a novel approach of modelling structural adhesive joints in a finite element context. On the one hand it focuses on modelling time-evolving mechanical characteristics of adhesive joints. In adhesive bonding, ageing phenomena affect the adhesive bulk material and the adhesive-adherent interface characteristics differently. Both zones of an adhesive joint are thus to be modelled adequately to capture structural ageing effects. In this work, the adhesive bulk material is represented by a 3D mesh applying a nonlinear material model which allows element rupture. This is based on unidirectional tensile, compressive and shear curves. The adhesive-adherent interface is modelled by cohesive zone elements and seeded with mode I & II interface fracture toughness data. This approach allows for the simulation of cohesive, adhesive and mixed cohesive-adhesive failure of the adhesive joint. Through-thickness effects (e.g. due to moisture diffusion into the adhesive bulk material) are taken into account by dynamically updating the element material properties corresponding to the applied ageing conditions and duration. On the other hand, the presence of defects and voids makes the mechanical behavior of adhesive joints even more complex to analyse and predict. Therefore, this work presents the results of an extensive uncertainty quantification which analyses the effects of heterogeneities in adhesive joints on their static and dynamic stiffness. The work concludes with a summary of ongoing research work and prospects to further related challenges in structural adhesive joining. References: Banea M, da Silva L.F.M, Campilho R. Mode I fracture toughness of adhesively bonded joints as a function of temperature: Experimental and numerical study. International Journal of Adhesion and Adhesives, 2011, 31, p. 273-279. Chaves F.J.P, da Silva L.F.M, de Moura M.F.S.F, Dillard D.A, Esteves V.H.C. Fracture Mechanics Tests in Adhesively Bonded Joints: A Literature Review. The Journal of Adhesion, 2014, 90, p. 955-992. Datla N.V, Ulicny J, Carlson B, Papini M, Spelt J.K. Mixed-mode fatigue behavior of degraded toughened epoxy adhesive joints. International Journal of Adhesion and Adhesives, 2011, 31, p. 88-96.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Computational Methods for the Dynamic Analysis of Conventional and Innovative Railway Tracks

Kris Decroos*, Patrick Vanhonacker**

*D2S International, **APT

ABSTRACT

In this paper a computational method for the efficiency determination of different source related mitigation measures for railway induced vibrations is presented. Comparison between the dynamic behaviour of railway vehicles (passenger/freight) on ladder tracks (a proposed mitigation system) is compared to the behaviour on a conventional ballasted concrete sleeper (tie) track using a combined finite element and multibody model. A numerical method for the comparison between ground-borne vibrations propagation on ladder track and concrete sleeper (tie) track under quasi static and dynamic loads is presented. Besides the impact of vehicle speed and suspension stiffness, several types of excitation and their impact on the dynamic behaviour are investigated: rail roughness, geometric track deviation, corrugation, wheel flats …

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

The Effect of Imperfectly Known Local Subsoil Conditions on The Response of Buildings to Ground Vibration

Geert Degrande*, Manthos Papadopoulos**, Stijn Fran?ois***, Geert Lombaert****

*KU Leuven, **KU Leuven, ***KU Leuven, ****KU Leuven

ABSTRACT

Dynamic soil-structure interaction plays a crucial role in the response of buildings to ground vibration. Ground vibration in the built environment are produced by earthquakes or environmental sources like road and railway traffic or construction and industrial activities. Geotechnical investigations suggest that the soil properties exhibit considerable spatial variability even within apparently homogeneous soil deposits. As the soil immediately below a building may have a dominant role in the structural response, the aim of this paper is to assess the influence of imperfectly known local subsoil conditions on the response of buildings to ground vibration in the frequency range between 1 Hz and 80 Hz which is of interest for environmental induced vibration. A probabilistic finite element-perfectly matched layers model is developed for the analysis of the stochastic dynamic soil-structure interaction problem where the shear modulus of the soil in the vicinity of a building is modeled as a conditional random field. A subdomain formulation is employed to impose loading by an external incident wave field in the model. The uncertainty on the subsoil properties is propagated to the response of the building by means of Monte Carlo simulation. A case study is considered to investigate the influence of the spatial correlation length of the random field representing the shear modulus of the subsoil, and the foundation type of the building. A building with raft foundation and a building with individual foundation footings are studied. The buildings are excited by the wave field generated by a remote vertical point load at the soil's surface. The uncertainty on the response of the buildings varies over frequency bands but as a general trend increases with frequency. The foundation type is a crucial parameter determining the structural response and the associated uncertainty bounds.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Calculation of a Steady Water Surface Using Deforming Grids and Fluid-structure Interaction Techniques

Joris Degroote*, Toon Demeester**, Harald van Brummelen***, Jan Vierendeels****

*Ghent University, Flanders Make, **Ghent University, ***Eindhoven University of Technology, ****Ghent University, Flanders Make

ABSTRACT

Steady water surfaces are present around ships moving at a constant speed in open waters or in straight canals, but also in confluences of rivers or canals. Numerical simulation of these steady free surfaces can be performed with a fitting or a capturing method. While capturing methods use a stationary grid and some marker to indicate the presence of water, fitting methods deform the grid such that the water surface corresponds with the top of the grid. Several fitting methods involve a (pseudo) time stepping process with limited step size for stability and are consequently not efficient in cases where steady state is only reached after a long physical time. By contrast, the technique developed by van Brummelen et al. (JCP, 2001) is truly steady, but requires a coupled solver where the pressure gradient and vertical velocity can be combined implicitly in a boundary condition. The goal of this research is to develop a new fitting method for steady free surface flow using a general-purpose steady CFD solver. To support this development, an analysis of a simplified test case has been performed, namely two-dimensional, incompressible and inviscid flow over a flat bottom, with a specified mean flow velocity and water depth. The relation between a sinusoidal perturbation of the free surface and the resulting perturbation of the pressure in the flow at the top of the domain has been calculated for different ratios of the water depth to wave number and water depth to flow velocity (Froude number). With the insight from this stability analysis, different iterative schemes are investigated. Quasi-Newton techniques can deal with unstable modes and modes which converge slowly, but the latter increase in number as the mesh is refined, requiring multi-grid or other techniques.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Emerging Applications of Earthquake Simulations for Performance-Based Risk Assessment and Decision Making

Gregory Deierlein*, Nenad Bijelic**, Ting Lin***, Frank McKenna****

*Stanford University, **Stanford University, ***Marquette University, ****University of California

ABSTRACT

Technologies to computationally simulate earthquakes and their effects on the built environment are advancing to the stage of providing meaningful data for engineering applications for design and policy development. This presentation will review developments in a number of areas, including validation of earthquake simulations and development of computational workflows to facilitate their practical applications. Physics-based earthquake simulations, conducted by researchers associated with the Southern California Earthquake Center (SCEC) and other organizations, are providing data to more realistically characterize the effects of local and regional geology (basin effects, etc.) on earthquake ground motions. Data from SCEC's Cybershake simulations are now being used to improve regional hazard maps for the Los Angeles Basin and undertake risk assessments of buildings and other infrastructure (https://scec.usc.edu/scecpedia/CyberShake). Studies of building collapse risk with simulated seismograms offer new opportunities to apply machine learning techniques to deaggregate risk to identify causal earthquake faults and features. The Natural Hazards Engineering Research Infrastructure (NHERI) SimCenter is developing computational workflow tools to integrate a broad array of simulation software with high-performance computing platforms and data repositories to facilitate these applications. For example, a recent testbed application by the SimCenter involves simulating the response of 1.8 million buildings to a simulated M7.0 Scenario earthquake in the San Francisco Bay Area (https://simcenter.designsafe-ci.org/framework/). By integrating earthquake simulation and urban planning tools, these computational workflows offer important opportunities to incorporate earthquake risk into decision making for public policies and planning. However, in as much as these applications offer tremendous promise, they also raise many research challenges, ranging from needs to (1) streamline workflows to optimize computational resources and data management, (2) devise scalable approaches to characterizing uncertainties in input data and models, and (3) plan simulations and organize the resulting data in ways that can effectively inform decision making.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

An Immersed Interface Approach for Fluid Structure Interaction Using Discontinuous Shape Functions

Facundo Del Pin*, Iñaki Çaldichoury**, Rodrigo Paz***, Chien-Jung Huang****

*Livermore Software Technology Corporation, **Livermore Software Technology Corporation, ***Livermore Software Technology Corporation, ****Livermore Software Technology Corporation

ABSTRACT

It is of general knowledge that the pre-processing of complex geometries used in engineering applications is a major burden in Finite Element analysis of fluid problems. There are many situations where a detailed high quality mesh is preferred and possible mandatory. Such is the case for problems where shear stresses are an important component of the total force, i.e. ground vehicle aerodynamics, aircraft drag prediction and some bio-mechanics applications where the stresses in the endothelium are need to predict the development of some diseases. There are many other applications though where pressure forces are enough in terms of accuracy or where rapid prototyping of engineering parts do not need the accuracy required in the final stages of engineering design. In these cases the geometry could be simplified by approximating the domain walls immersing them inside a much simpler domain. This simplification becomes even more appealing in the presence of an internal structure that interacts with the fluid. In the current work the sub-element interfaces of the geometry will be approximated by level set distance functions. The walls could be part of a flexible structure or they could be rigid. The pressure discontinuity across the wall (in the case of shell structural elements) will be approximated by discontinuous shape functions as described in [1]. One of the main advantages of this approach is that it is easily adapted to an existing solver since no additional degrees of freedom need to be added. The presentation will include details of the additions that the existing solver needed such as: 1) boundary recognition; 2) level set representation; 3) sub-element splitting; 4) computation of the new interpolation functions and integration; 5) assembly and solution.
[1] R.F. Ausas, F.S. Sousa, G.C. Buscaglia, An improved finite element space for discontinuous pressures, Comput. Methods Appl. Mech. Engrg. (2009), doi: 10.1016/j.cma.2009.11.011

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Error-driven Reduction and Optimization of Chemical Kinetic Mechanisms

Aurelie Delaroque*, Patrick da Costa**, Alexis Matynia***

*Sorbonne Université, **Sorbonne Université, ***Sorbonne Université

ABSTRACT

With the stiffening of environmental regulations, pollutants emission calculations are crucial in the conception and optimization of engine combustion chambers. To ensure precision of the computed species profiles, a detailed chemical kinetic mechanism must be used. For complex fuels, such model can contain up to a thousand species, each of them adding a new equation to the system describing the reactive flow. Therefore, an efficient way to reduce computational cost is to reduce the number of species. Reduction methods for kinetic mechanisms are based upon chemical and/or mathematical properties of the system. In this work, the Directed Relation Graph [1] and Sensitivity Analysis reduction methods were used for an automatic reduction in perfectly stirred reactors (0D configuration) and freely propagating flames (1D configuration). An optimization using genetic algorithm [2] can then be performed to compensate the reduction induced error. This error was evaluated in two ways: comparison of the profiles integrals and through quantities of interest inspired by the work of Selim et al.[3]. The algorithm enables the user to choose several species of interest with different error tolerances. An iterative reduction is performed, each of the targets having an adaptive cut-off threshold scaled on the error of the reduced model. Independent thresholds allows the reduction procedure to carry on separate branches of the directed graph or different parts of the sensitivities matrices when one target reaches the maximal error allowed. The ability of the algorithm to reduce combustion kinetic mechanisms is assessed for different configurations and operating conditions (equivalence ratio, pressure, etc.). The importance of the error evaluation criteria is assessed and the tool performances are presented. Summary of the presentation : • Numerical combustion: origin of the computational cost and how to reduce it • Reduction with error-driven adaptive threshold • Post reduction model optimization References : [1] T. Lu, C. K. Law : A directed relation graph method for mechanism reduction. Proceedings of the Combustion Institute, 2005. [2] L. Elliott , D.B. Ingham, A.G. Kyne, N.S. Mera, M. Pourkashanian, C.W. Wilson : Genetic algorithms for optimization of chemical kinetics reaction mechanisms. Progress in Energy and Combustion Science, 2004 [3] H. Selim, S.Y. Mohamed, A.E. Dawood, S. Mani Sarahy : Understanding premixed flame chemistry of gasoline fuels by comparing quantities of interest. Proccedings of the Combustion Institute, 2016

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A DPG Approach to Raman Gain in Optical Fiber Amplifiers

Leszek Demkowicz*, Sriram Nagaraj**, Jacob Grosek***, Socratis Petrides****

*ICES, UT Austin, **ICES, UT Austin, ***AFRL, ****ICES, UT Austin

ABSTRACT

This talk will focus on the use of the DPG methodology in the modelling and simulation of optical fiber laser amplifiers with nonlinear Raman gain. Specifically, we study the operation of an optical fiber as an amplifier, i.e., a mechanism to convert pump light into signal light. The signal and pump fields are governed by two weakly coupled nonlinear time harmonic Maxwell equations to be solved using curvilinear 3 dimensional elements. Our model for the Raman gain is novel, and reflects the third order nature of the non linearity. We consider an ultra weak DPG formulation for the discretization of two systems of equations and the non linearity is handled by using fixed point (simple) iterations between the two systems. We use a DPG implementation of perfectly matched layer (PML) at the exit end of the fiber. Our results verify the Raman gain model and indeed show that the signal field gains power along the fiber with an expected efficiency. In addition, our results pave the way for the study of additional thermal effects modelled by coupling the electromagnetic phenomena with the heat equation. These thermal effects lead to detrimental modal instabilities in the fiber called transverse mode instability (TMI). Along the way, we show how the desirable properties of DPG, namely, mesh-independent uniform stability, and a computable error indicator leading to automatic adaptivity are useful in this application. To the authors' best knowledge, this is the first comprehensive fully vectorial 3-dimensional DPG model of this problem.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Topology Optimization of Hyperelastic Lattice Structures that Exhibit Negative Stiffness Behavior

Hao Deng*, Lin Cheng**, Albert C To***, Devlin Hayduke****

*University of Pittsburgh, **University of Pittsburgh, ***University of Pittsburgh, ****Materials Sciences Corporation

ABSTRACT

Lattice materials that exhibit negative stiffness, also known as phase transformation, is characterized by a long serrated loading and unloading plateaus, making these materials suitable for energy absorption and damping applications. Instead of exploiting plastic deformation, these materials are designed to be hyperelastic in the negative stiffness regime and hence their deformation is fully recoverable. Topology optimization, such as material distribution-based methods, has become a popular approach to design high-performance structures and is employed in this work to design negative stiffness lattices. Design of hyperelastic materials incorporates both geometric and material nonlinearity due to large deformations. An appropriate method is adopted here to avoid mesh excessive distortion in low density area to stabilize numerical simulations. The topology optimization of lattice structures that exhibit negative stiffness contains nonlinear stability optimization and material failure constraints. The lattice structure, which shows snap-through behavior, usually presents damping properties, which is closely related to multiple stable configurations and the transformations between these phases. Therefore, to some extent, if stable phase can be optimized through topology optimization, this will open the door to optimize energy dissipation of lattice structure. Meanwhile, hyperelastic material failure constraint should be taken into consideration to make our structures fully recoverable, which is a distinct difference with other energy absorption material such as metal. Thus, our goal in this paper is to optimize lattice structures stable phase with material failure constraints so that our objective of energy dissipation ability will greatly increase, which will make this lattice structure be an ideal material for damping and energy absorption application.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Computational Modeling of Bronchial Airway Narrowing Mechanics for Elucidation of Respiratory Airflow Limitation in Health and Disease

Linhong Deng*, Xiaohao Shi**, Linlin Zhu***, Che Zhao****, Shengye Zhou*****

*Institute of Biomedical Engineering and Health Sciences, Changzhou University, Changzhou, Jiangsu, China,
**Institute of Biomedical Engineering and Health Sciences, Changzhou University, Changzhou, Jiangsu, China,
***Institute of Biomedical Engineering and Health Sciences, Changzhou University, Changzhou, Jiangsu, China,
****Institute of Biomedical Engineering and Health Sciences, Changzhou University, Changzhou, Jiangsu, China,
*****Institute of Biomedical Engineering and Health Sciences, Changzhou University, Changzhou, Jiangsu, China

ABSTRACT

Introduction: Although it is important to explore potential treatment of chronic obstructive airway diseases such as asthma, as well as to discover interesting biophysical phenomena in airway system, the research of biomechanical models of airway narrowing remains a both appealing and challenging field. Here we report some of the most recent work, in particular, that emphasize on asthmatic airway narrowing behavior. More specifically, we focus on the modeling of individual airway behaviors as well as interactions due to coupling between airways and their surrounding structures. This includes interesting phenomena involving the airways and the airway smooth muscle (ASM) layer embedded within the airway wall. The airway wall was modeled as a composite tubular structure embedded with ASM layer that was characterized by the volume, Young's modulus and orientation of ASM in either healthy or diseased state (e.g. asthma). Methods and Materials: CT scan images of airway tree from an adult male was obtained, from which a digital geometrical model of human airway tree from 0 to 5/6 level was reconstructed. Subsequently, a finite element model (FEM) of the airway tree was established, which incorporated ASM hyperplasia and hypertrophy by changing the volume of ASM layer, and ASM orientation by changing the effective modulus on the relevant direction. Using FEM analysis, the airflow-ASM interactions under different ventilation patterns were simulated via computational fluid dynamics (CFD) methods. The characteristic volume, Young's modulus of the ASM were measured using fresh airway tissues from pig lungs cut at 0°, 15°, 30°, 45°, 60°, and 75° to the longitudinal and transverse direction and stained Results: ASM layer thickness and mechanical properties in the airway wall were highly nonlinear, and hyperelastic. The experimental results of the airway wall mechanical properties was able to be fitted by the Holzapfel strain-energy density function. We found that as ASM layer became thicker under the same ventilation condition, the shear stress on the airway wall and airflow velocity increased; whereas increase of the angle between ASM and horizontal plane would reduce the stress on the circumferential direction, but the shear stress was greater for the same breath pattern and airway thickness. Conclusions: With computational modeling method, we were able to simulate in situ airflow-ASM interactions during ASM contraction, in the absence or presence of pathological condition relevant to asthma including hyperplasia and hypertrophy, structural reorganization, and hopefully elucidate the connection between airway hyperresponsiveness (AHR) and abnormal ASM contraction patterns.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Rapid Computation of Inversion Heat Conduction Problems with Reduced Order Models

Brian Dennis*, Ashkan Akbariyeh**

*University of Texas at Arlington, **University of Texas at Arlington

ABSTRACT

Many inverse problems in heat conduction, such as determination of unknown boundary conditions or unknown shapes, require the solution of a parametric optimization problem. Typically this involves the coupling of a numerical optimization routine with a thermal analysis model based on a numerical method such as the finite element method. Since many of these problems are ill-conditioned, many calls to the analysis routine may be required by the optimizer to find an accurate minimum of the objective function. If the analysis model is large due to complex geometry, the computational time may be on the order of hours using a computer cluster. Many researchers make use of meta models to reduce the computing cost of optimization problems with expensive analysis calls. This involves making a predictive regression model to accelerate the objective function evaluation. Response surface modeling is the most common statistical tool used for meta modeling but artificial neural networks and kriging have also been used. However, if the analysis model is based on a finite element discretization of a partial differential equations, then a Galerkin method utilizing a reduced order basis could produce a rapidly computable meta-model based on the original differential equation. The basis functions are determined using proper orthogonal decomposition (POD) based on training data generated by the finite element model. Typically POD is applied to time vary data, but we show that is can also be successfully applied to data varying in parametric space as well. In our case the POD is applied to data generated by the finite element models that are evaluated over a range of parameter values. In this work we compared the performance of reduced order modeling (ROM) to response surface methods (RSM) and demonstrated that ROMs are more accurate and require a smaller set of training data. In addition, the resulting computational model, once trained, is so rapidly computed that it can be used in real time systems, such as model predictive control applications. We present applications to the inverse determination of unknown boundary conditions and the inverse determination of unknown shapes in steady and unsteady heat conduction. These examples involve finite element models with hundreds of thousands of degrees of freedom but the resulting ROM-based inverse problem can be solved in real time on a modest notebook computer.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Long-Duration Blast Response of Steel Columns: The Influence of Section Orientation

Jack Denny*, Simon Clubley**

*University of Southampton, **University of Southampton

ABSTRACT

Explosive blast loading has potential to exert forces on structural columns far higher than their capacity, causing permanent deformation. Recent large-scale industrial accidents such as the 2005 Buncefield disaster, the 2013 West Texas fertiliser factory explosion and the 2015 Tianjin disaster have highlighted a growing need to understand the response of structures to long-duration blasts. Typically defined by positive pressure durations over 100ms, long-duration blasts develop in the later stages of propagation i.e. in the 'far field' from the source of detonation. Such blasts are extremely powerful, generating substantial impulse and dynamic pressures (blast winds) capable of exerting damaging drag loads on columns. In reality, structures and their constituent column elements may be subjected to blast loads from various angles of incidence (section orientation) depending on the detonation location. Characterising such blast loading on columns can be complex, typically requiring approximation using drag coefficients for which there is limited availability or understanding, particularly when concerning different section orientations. Blast resistant design manuals and simplified predictive methods are generally limited to considering orthogonal axes, with no prior studies or guidance pertaining to the structural response of columns at different section orientations. Representing part of a broader experimental programme, six full-scale long-duration blast trials were conducted to investigate and quantify the influence of column section orientation on loading, transient dynamic response and final damage state. Nine steel square hollow section (SHS) columns were tested at orientations of 0, 30 or 45 degrees to the direction of blast propagation. Specimens were instrumented with surface pressure transducers, permitting calculation of column blast loading as a function of section orientation. High-speed video and high-fidelity laser topology quantified column transient dynamic response and permanent deformation respectively. Columns at oblique section orientations measured higher loading than orthogonal or symmetric orientations, resulting in larger permanent deflections. Analysis showed that column orientation greatly influenced loading and structural response due to varying projected area, aerodynamics and section mechanical properties. Importantly, results demonstrate that section orientation is non-trivial and has potential to cause considerably different final damage states. Results of this study provide new understanding of direct relevance to both engineering design practitioners and researchers.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Non Parametric Probabilistic Modeling for the Problem of Scattering Waves by a Solid with a Random Geometry into an External Acoustics Fluids

Christophe Desceliers*

*Université Paris-Est

ABSTRACT

A random computational model for the scattering of acoustical waves by a solid with an uncertain geometry into an acoustic external fluid is presented. The construction of a parametric probabilistic model for such a random geometry involves an important number of random variables. Since the stochastic dimension of such probabilistic model can be important, then the solving of the inverse statistical problem of random geometry can be very computationally tricky. This is the reason why a new nonparametric probabilistic model is developped. Nevertheless, It should be noted that the random acoustic impedance matrix which is a frequency-dependent random matrix is such that its real and imaginary parts must verify the Kramer-Kronig relations which implies its analyticity in the complex upper half-plane in order to get the causality of the random physical system [1, 2]. Consequently, it is necessary to take into account the Kramer-Kronig relations for the construction of the probabilistic model of the random impedance matrix. The strategy for constructing of the probabilistic model of the random impedance matrix consists in constructing the probabilistic model of its frequency-dependent real part and then to obtain the probabilistic model of the frequency-dependent imaginary part in using a Hilbert transform such that the Kramer-Kronig relations are verified. The theory of information is used to construct the probabilistic model of the real part of the random impedance acoustic matrix by taking into account the available information that is the positivity of the real part, its mean values and that the random frequency-response of the random computational model is a second-order random vector. A numerical example is presented which corresponds to the scattering of an incident wave by a solid for which the geometry is random. A parametric probabilistic model of the geometry is constructed and compared with the proposed nonparametric probabilistic model. [1] Christian Soize, Igor E. Poloskov. Time-domain formulation in computational dynamics for linear viscoelastic media with model uncertainties and stochastic excitation. Computers and Mathematics with Applications, Elsevier, 2012, 64 (11), pp.3594-3612. [2] Rémi Capillon, Christophe Desceliers, Christian Soize. Uncertainty quantification in computational linear structural dynamics for viscoelastic composite structures. Computer Methods in Applied Mechanics and Engineering, Elsevier, 2016, 305, pp.154-172.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Towards Predicting Instabilities of Lipid Monolayers: A Benchmark Problem

Luca Deseri*, Massimiliano Fraldi**, Giuseppe Mensitieri***, Stefania Palumbo****, Valentina Piccolo*****, Luka Pocivavsek******

*University of Trento (Italy), University of Pittsburgh (USA), **University of Napoli-Federico II (Italy), ***University of Napoli-Federico II (Italy), ****University of Trento (Italy), *****University of Trento (Italy), ******University of Pittsburgh Medical Center

ABSTRACT

Surfactants at air/water interfaces in lungs are subject to cyclic dynamical straining during breathing. Often time, in-plane and out-of-plane rearrangements of the lipid structures coating lungs alveoli are exhibited in pathological situations, eventually leading to their collapse. Similar, although more controllable, situations are observed in planar lipid monolayers set up in the laboratory, where uniaxial squeezing is induced to test the response of such systems. Preliminary studies towards an understanding of the collapse mechanisms exhibited by such structures are presented through the analysis of a benchmark problem. There, the stress relaxation in the out-of-plane mode turns out to be characterized by a scaling law between the wavelength at the onset of instability and the geometrical and constitutive parameters. Given the findings on the wavelength mentioned above, the current predictions based on Molecular Dynamics do not relate collapse through bending at the observed experimental scales. Henceforth, a predictive strategy that can provide the right scaling and modes is still missing. A platform owing to the first insights on the length scales involved in such phenomena is envisioned based on the preliminary results of the analytical and experimental of thin films mimicking the lipid monolayer on a viscous substrate.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Applying the Multiscale Hybrid Mixed Method to the Numerical Simulation of Discrete Fracture Networks

Philippe Devloo*, Chen-Song Zhang**, Wenchao Teng***

*FEC/UNICAMP, **NCMIS & LSEC, Academy of Mathematics and System Sciences, ***School of Engineering, Peking University

ABSTRACT

The multiscale hybrid mixed method (MHM) is applied to the numerical approximation of two-dimensional fluid flow in porous media with fractures. The two-dimensional fluid flow in the reservoir and the one-dimensional flow in the discrete fractures are approximated using mixed finite elements. The coupling of the two-dimensional flow with the one-dimensional fracture flow is enforced using the pressure of the one-dimensional flow as a Lagrange multiplier to express the conservation of fluid transfer between the fracture flow and the divergence of the one-dimensional fracture flux. A zero-dimensional pressure (point element) is used to express conservation of mass where fractures intersect. The issuing simulation is then reduced using the MHM method leading to surprisingly accurate results with a very reduced number of global equations. A general system was developed where fracture geometries and conductivities are specified in an input file and meshes are generated using the public domain GMsh software. Several test cases illustrate the effectiveness of the proposed approach comparing the multiscale results with direct simulations.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

On Geometry-based High-order Unstructured Methods for Structural-acoustics

Saikat Dey*

*US NRL

ABSTRACT

We discuss recent developments in high-order finite and infinite element based approaches for accurate solution of problems in structural acoustics. We present several applications related to vibratory and scattering response of elastic structures excited by mechanical and/or acoustic sources. We identify and highlight the importance of high-order discretizations and the role of geometry for accurate solution of such wave-dominated problems.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Quasi-Static and Dynamic Finite Element Analysis of Hydroelastic Problems Considering Structural Geometric Nonlinearities

Jean-François Deü*, Christophe Hoareau**, Roger Ohayon***

*Conservatoire national des arts et métiers, Paris, France, **Conservatoire national des arts et métiers, Paris, France, ***Conservatoire national des arts et métiers, Paris, France

ABSTRACT

This work concerns the nonlinear modeling of elastic structures containing internal liquids with free surface. This kind of hydroelastic problem is still the subject of active researches, e.g. for the design of flexible tanks in aeronautical or space industry, in which linearized approaches can be questioned [1, 2]. The objective of this work is therefore to take into account geometrical nonlinearities in the structural part of fluid-structure interaction problems for quasi-static solution and vibration prediction. Firstly, we propose to address the quasi-static equilibrium state of the nonlinear coupled system by using the finite element method. The effect of the incompressible internal fluid on the structure is modeled by hydrostatic follower forces without meshing the internal fluid domain. In order to take into account the evolution of the wetted surface during the non-linear deformation of the structure (by considering the fluid volume conservation) a level-set approach is adapted to the fluid-structure interface elements, thus avoiding any remeshing [3]. In a second part, we study the linearized vibrations of the fluid-structure coupled problem around this prestressed state. We show that the structural vibrations are not only influenced by the presence of the liquid (added mass effect) but also by the initial stress state of the structure, both effects can play in an opposite direction. Reduced order models, based on both Modal Superposition and Proper Orthogonal Decomposition approaches will be finally proposed to perform parametric studies on the influence of structural nonlinearities on the vibrations of the coupled system. Several numerical examples will be also presented to illustrate the effectiveness of the developed approaches. [1] J.-S. Schotté, R. Ohayon, Linearized formulation for fluid-structure interaction: Application to the linear dynamic response of a pressurized elastic structure containing a fluid with a free surface, Journal of Sound and Vibration, 332 (10), 2396-2414, 2013. [2] R. Ohayon, C. Soize, Nonlinear model reduction for computational vibration analysis of structures with weak geometrical nonlinearity coupled with linear acoustic liquids in the presence of linear sloshing and capillarity, Computers & Fluids, 141, 82-89, 2016. [3] C. Hoareau, J.-F. Deü. Non-linear finite element analysis of an elastic structure loaded by hydrostatic following forces, Proceedings of EURODYN 2017, Procedia Engineering, 199, 1302-1307, 2017.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Computational Method for Moving Particles on Thin Deformable Shells: Application to Surface Tessellation

Sanjay Dharmavaram*, Robijn Bruinsma**, Luigi Perotti***

*Department of Physics and Astronomy, UCLA, **Department of Physics and Astronomy and Department of Chemistry, ***Department of Radiological Sciences and Department of Bioengineering

ABSTRACT

Many problems in softmatter and membrane biophysics, such as finding equilibrium configurations of protein clusters on cell-membranes, highly defect ridden structure of Gag polyproteins in immature HIV capsids, and the unusual fluid-like state of Archaeal viruses [1] can all be understood as systems of interacting particles (typically representing proteins or protein capsomers) on deformable surfaces. The coupled interactions between the particles and the underlying elastic medium to which they are constrained pose significant computational challenges. For example, finite element methods typically: 1) impose expensive constraints to anchor particles to the surface; 2) use multi-step minimizations by sequentially moving particles on a rigid surface and subsequently updating the surface to accommodate the new particle configuration; or 3) restrict particles to the nodes of the underlying mesh (of the surface) giving a coarse approximation of the equilibrium state. In this study, we propose a new variational formulation to circumvent these challenges. Our method is based on a Lagrangian description of particle positions where instead of treating the particle positions on the current surface as the degrees-of-freedom, we treat the particle positions on the reference configuration (the ``pull-back '') as the degrees-of-freedom. The advantage of this method is that particles automatically lie on the surface and no multi-step minimizations or additional constraints are necessary, and since the particles are not restricted to lie at the nodes of the mesh, they are free to explore all possible equilibrium configurations. We demonstrate the efficacy of this method by applying it to three benchmark problems in different dimensions and show that the theoretical convergence rates in energy and displacement norms are realized. We also apply this method to particles moving on deformable unduloid surfaces as model for Archaeal viruses. In this application, we show how the proposed method can be applied to compute the tessellation of a deformable surface with positive and negative Gauss curvature and therefore its optimal tiling in terms of basic pentamers, hexamers, and heptamers. [1] Useful scars: Physics of the capsids of archaeal viruses, L.E. Perotti et. al, Phys Rev E 94 (2016).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A New Joint Element for the Modeling of Contact Interaction and Damage in SFR Fuel Assemblies

François Di Paola*, Bertrand Leturcq**, Jean-Baptiste Minne***

*Atomic Energy Commission (CEA), **Atomic Energy Commission (CEA), ***Communication et Systèmes (CS-SI)

ABSTRACT

The fuel assembly of a sodium fast nuclear reactor (SFR) is a hexagonal tube containing around 200 fuel pins made of steel. In order to avoid overheating and damage on the assembly, a helical steel wire is wound around each pin. This wire maintains a suitable distance between pins and ensures a proper mixing of the sodium. Nevertheless, the intense fast neutron irradiation induces a significant isotropic swelling and creeping of the pins. This progressively leads to contact closure, helical bowing of the pins, and a strong ovalisation of the cladding sections. At such an interaction level, there is a possibility of cladding damage due to thermal creep accumulation. Modeling such a structure is a numerical challenge: around 10 000 contact areas, highly nonlinear material behavior laws, high mesh density needed for damage location. Thus, a simplified approach is developed: the two components are modeled by classical finite elements with a low mesh density: the hexagonal tube by shell elements, the fuel pins by beam elements. In addition, we have developed a new joint element dedicated to the contact interaction between components and the radial crushing of the pins. This element, with only two nodes, connects the neutral fiber of neighboring beams (or the mid-surface of shells). It takes into account: - the gap and the contact between two pins (or a pin and the tube), - the thermal expansion and the irradiation swelling of the pin cross sections (including heterogeneity of temperature), - the radius increase by creeping under internal pressure loading, - the elastic rigidity of the pin crushing (locally pinching a short section of a tube), - the contact force, altered by the two creeping behaviors, when pinching this 3D tube section, - the counter ovalisation force due to internal pressure on the deformed shape of the pins, - the hot point stress and strain tensors on the internal skin (strain concentration), - the hot point damage accumulation due to thermal creeping only. This connecting element has been implemented in the Cast3M finite element code (http://www-cast3m.cea.fr). Eventually, the model validation is made: - on the joint element, and compared to detailed 3D solid calculations, - on the global fuel assembly model, and compared to a few relevant assembly experiments, which were conducted in the PHENIX French SFR. It shows good agreement to the measurements and a very significant CPU performance gain compared to 3D solid models.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Aftershock Fragility and Residual Capacity Assessment of Infilled Frames Using an IDA Based Framework

Fabio Di Trapani*, Gabriele Bertagnoli**, Marzia Malavisi***

*Politecnico di Torino (Italy), **Politecnico di Torino (Italy), ***Politecnico di Torino (Italy)

ABSTRACT

Seismic sequences frequently occurred in many regions of the world. The initial event (mainshock) is followed by a number of secondary shakings (aftershocks) which may lead structures to collapse because of progressive damage accumulation [1]. Reinforced concrete frame structures are generally infilled with masonry walls, and it is well known that these strongly interact with primary structures during seismic events. Infills significantly increase overall strength and stiffness, and also modify collapse modalities. The paper investigates seismic response of bare and infilled frames subject to mainshock/aftershock sequences. Aftershock fragility curves are obtained making use of a new specific assessment framework, based on a double Incremental Dynamic Analysis (IDA) [2]. Ground motions are in fact obtained combining mainshocks at fixed intensities with increasing intensity aftershocks. OpenSees [3] software platform is used to perform analyses of a reference prototype structure. The adopted double-IDA procedure, allows defining residual capacity diagrams, showing reduction of average collapse PGA as a function of mainshock intensity. Results show that masonry infills provide noticeable additional capacity seismic to resist aftershock shakings in comparison with bare frame structures, but only if local shear failure of reinforced concrete members is avoided. References [1] Hosseinpour F, Abdelnaby AE. Effect of different aspects of multiple earthquakes on the nonlinear behavior of RC structures. Soil Dyn Earthq Eng 2017;92:706–25. [2] Vamvatsikos, D., Cornell, A.C., 2002, Incremental dynamic analysis, Earthquake Engineering and Structural Dynamics, 31(3), 491–514. [3] McKenna, F., Fenves, G.L., Scott, M.H., 2000. Open system for earthquake engineering simulation, University of California, Berkeley, CA.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Probability Density Function for Polycrystalline Two-dimensional Materials

Christopher S. DiMarco*, James Hone**, Jeffrey W. Kysar***

*Columbia University, **Columbia University, ***Columbia University

ABSTRACT

We examine the intergranular failure of polycrystalline two-dimensional materials by calculating a probability density function (PDF) based on a multiscale model and validated against nanoindentation experiments. Two-dimensional materials are of particular research interest due to their low defect density, which results in fracture strengths approaching their theoretical limits. Since scalable synthesis methods results in a polycrystalline structure, an understanding of the mechanics of their grain boundaries is necessary. Nanoindentation experiments on free-standing circular membranes reveal these materials have a non-Gaussian distribution in their critical failure load. First, we consider the transition in failure mechanisms through simulations of the nanoindentation experiments using the finite element method (FEM). The model admits two modes of failure: (1) within the grain boundary due to void nucleation and (2) within the grain due to a structural instability. A membrane-based cohesive zone model (CZM) is formulated based on molecular dynamic simulations to model the grain boundary behavior and a 5th order nonlinear anisotropic elastic constitutive relation describes the material behavior within each grain. The material properties of graphene are applied for these initial investigations. A simplified domain containing a single straight grain boundary is considered to develop a force-distance relationship between the critical failure load and the grain boundary distance from the indenter tip. Second, the force-distance relationship is fit with a piecewise continuous function and utilized to calculate a PDF. Initially, a periodic, hexagonal grain structure is considered as motivation. Then, a more realistic grain structure is considered by using a randomly generated Voronoi Tessellation. Finally, the resulting PDF is compared against the nanoindentation experiments in an effort to validate the material properties of the grain boundary.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Critical Analysis of the Drucker-Prager/Cap (DPC) Model When Modeling Pharmaceutical Die Compaction Process

Harona Diarra*, Vincent Mazel**, Pierre Tchoreloff***

*Université de Bordeaux/ Université Paris Sud, **Université de Bordeaux, ***Université de Bordeaux

ABSTRACT

The numerical simulation with DPC model requires the characterization of the model parameters. Depending on the method used, the instrumentation of the devices or the accuracy of the measures, the data obtained from experiments for the characterization of the model parameters may vary from a study to another. In this work, the influence of the elastic and plastic parameters on the numerical results during the compression cycle is discussed. Variations of ±20% on the values of Young's modulus E and Poisson's ratio obtained from the literature were applied. The variation of E has no influence on the final tablet thickness and the radial transmission curve. The distributions of the density, the axial and radial stresses do not change when E varies. A small Poisson's ratio gives high residual die wall pressures and low tablet thickness and vice versa. The stress distribution is completely dependent on Poisson's ratio. For numerical study with DPC model, a better characterization of Poisson's ratio is capital. The failure surface of the DPC model consists of two principal parts: the failure line and the cap surface. The failure line parameters are the cohesion d and the friction angle b. The cap parameters (hydrostatic pressure pa, eccentricity R and hydrostatic yield pressures pb) are calculated from d and b. Thus the variation of R, pa and pb is due to the variation of d and b. The parameters d and b are obtained from failure strengths sd and su. In this work, variations of ±53% were applied to sd and su and the corresponding values of b and d were calculated. The numerical representation of the compression curves shows that the curves obtained from the variation of d and b are superimposed. Thus, the variations of the failure line have no consequence on the compression and decompression results. An alternative model without failure line (modified Cam-Clay (MC-C) model) is introduced to simulate the powder behavior during die compaction process. This model is simple to use and requires less experimental tests for the parameter characterization. The axial stress-tablet thickness curves obtained from the two models are superimposed. The radial transmission curve obtained from MC-C model is identical to that obtained from DPC model. The stress and the density distributions are the same for the two models. This shows that the MC-C model is able to predict the powder behavior during the compression as well as the DPC model.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Overview of Brazilian Scientific Production in Engineering Areas

Patricia Dias*, Tales Moreira**, Thiago Dias***, Gray Moita****

*CEFET-MG, **CEFET-MG, ***CEFET-MG, ****CEFET-MG

ABSTRACT

From the access and extraction of data sources of large-scale scientific publications, several studies are possible to obtain information about the published works, besides the possibility of categorization and visualization of them. In this study, data are used for the scientific production of the Brazilian researchers who work in the area of Engineering. Therefore, the data are obtained through a data extraction and processing framework responsible for obtaining the Lattes Platform curricula. With the extraction of all the curricula of the selected set it is possible to characterize the individuals as well as describe a panorama of their scientific production using bibliometric analyzes to quantify how these individuals have divulged their researches.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Temporary Analysis of the Main Topics of Engineering Research in Brazil

Thiago Dias*, Jether Oliveira**, Gray Moita***

*CEFET-MG, **CEFET-MG, ***CEFET-MG

ABSTRACT

The Internet and its services are fundamental factors that have boosted the significant growth in the dissemination of scientific articles in recent decades. Consequently, there is an overall increase in researchers from all areas of knowledge interested in understanding scientific development. Since this understanding can provide important inputs to assist different types of decision making, such as assisting researchers in choosing new research themes, making researchers more productive, and also serving as a basis for research. scientific policies aiming at new advances in science. Thus, this paper aims to identify and analyze the main topics investigated between 1962 and 2016 by Brazilian doctors who work in the areas of engineering. For this, bibliometric studies are carried out on the whole set of keywords of the scientific articles referring to the great area of ??engineering, published in proceedings of congresses and in journals by the Brazilian doctors.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

DAMASK - The Düsseldorf Advanced Material Simulation Kit for Modeling Multi-Physics Crystal Plasticity, Thermal, and Damage Phenomena

Martin Diehl*, Pratheek Shanthraj**, Philip Eisenlohr***, Franz Roters****, Dierk Raabe*****

*Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany,
**Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany, ***Chemical Engineering and Materials Science, Michigan State University, East Lansing, MI 48824, USA,
****Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany,
*****Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

ABSTRACT

Crystal plasticity modeling is a powerful computational materials science approach for the investigation of mechanical structure-property relations in metals and has been successfully applied to study diverse micromechanical phenomena ranging from strain hardening in single crystals to texture evolution in polycrystals. However, when considering the increasingly complex microstructural composition of modern alloys and their exposure to - often harsh - environmental conditions, the focus in materials design has shifted towards incorporating more constitutive and internal variable details of the process history and environmental factors into these structure-property relations. A number of niche tools, containing multi-physics extensions of the crystal plasticity method, have been developed to address such topics. Such implementations, while being very useful from a scientific standpoint, are, however, designed for specific applications and substantial efforts are required to extend them into flexible multi-purpose tools that enable a general end-user community to implement custom-made constitutive solutions for particular applications. With DAMASK we, therefore, undertake the effort to provide an open, flexible, and easy to use implementation to the scientific community that is highly modular and allows the use and straightforward implementation of different types of constitutive laws and numerical solvers. The internal modular structure of DAMASK follows directly from the hierarchy inherent to the employed continuum description. The highest level handles the partitioning of the prescribed field values on a material point between its underlying microstructural constituents and the subsequent homogenization of the constitutive response of each constituent. The response of each microstructural constituent is determined, at the intermediate level, from the time integration of the underlying constitutive laws for elasticity, plasticity, damage, phase transformation, and heat generation. A number of selected examples are shown to demonstrate the capabilities of DAMASK to predict structure-property relations in different material classes.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A PGD Arithmetic Toolbox: Explicit Solution of the Discrete Version of Parametric Problems

Pedro Diez*, Antonio Huerta**, Sergio Zlotnik***

*Universitat Politècnica de Catalunya, BarcelonaTech, **Universitat Politècnica de Catalunya, BarcelonaTech, ***Universitat Politècnica de Catalunya, BarcelonaTech

ABSTRACT

Separable approximations efficiently deal with high-dimensional data. In particular, the Proper Generalized Decomposition (PGD) provides separable functions as solutions of boundary value problems. The general PGD framework contains a large family of methodologies, all of them providing solutions in for of separable objects, that is a sum of terms, being each term a product of 1D functions (or arrays). Some of the PGD methodologies have been conceived to tackle nonlinear problems. We present a general methodology to perform basic operations (sum, product, division, exponentiation…) for this type of objects. The idea is based on the principle of the PGD compression, that is a separable least squares approximation of any multidimensional function. The PGD compression is extensively used in practice to compact the separable solution in less terms without loss of accuracy. Here, this concept is applied to both algebraic tensor structures and functions in multidimensional Cartesian domains. Moreover, a straightforward extension of this concept is devised to operate with multidimensional objects stored in the separable format. That allows creating a toolbox of PGD arithmetic operators. Thus, the toolbox is used to perform elemental operations with PGD type objects. This is of particular interest to solve nonlinear problems with PGD techniques by simply replicating the iterative algebraic solvers that are used in the standard Finite Element framework.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Spherical Indentation on Biological Films with Surface Energy

Yue Ding*, Wei-Ke Yuan**, Gang-Feng Wang***

*Department of Engineering Mechanics, Xi'an Jiaotong University, **Department of Engineering Mechanics, Xi'an Jiaotong University, ***Department of Engineering Mechanics, Xi'an Jiaotong University

ABSTRACT

Micro-/nano-indentations have been widely used to measure the mechanical properties of biological cells and tissues, but the direct application of classical Hertzian contact model would lead to overestimation of elastic modulus due to the influence of finite thickness and surface energy. In this work, we analyze spherical indentation of biological films considering both large deformation and surface energy. The hyperelastic behavior of biological films is characterized by neo-Hookean model, and the influence of surface energy is addressed through finite element simulation. Based on dimensional analysis, the explicit expressions of load-depth relation accounting for film thickness, large deformation and surface energy are achieved for bonded or non-bonded films. Under a specific load, the consideration of large deformation increases the indent depth, while the finite thickness of films tends to decrease the indent depth, compared to the linear elastic Hertzian solution. More importantly, surface energy evidently alters the load-depth relation for micro-/nano-indentations, which reduces the indent depth and makes the films seemingly stiffer. These results provide a fundamental relationship to accurately extract the mechanical properties of biological films from indentation tests.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Dislocation Dynamics Based Continuum Model for FCC and BCC Metals under Shock Loading

Nenad Djordjevic*, Rade Vignjevic**, Lewis Kely***, Simon Case****

*Brunel University London, UK, **Brunel University London, UK, ***Brunel University London, UK, ****Atomic Weapon Establishment, UK

ABSTRACT

Recent experimental data has reviled that, over a short time (nanoseconds scale) at the beginning of the shock loading of metals, the precursor amplitude greatly exceed Hugoniot Elastic Limit (HEL), before decaying to the level of the HEL. To capture this aspect of material behaviour at the continuum scale, physical effects related to high rate dislocation mechanics have to be taken into consideration [1,2]. The dislocation mechanics approach used here is described by three microscale state variables: density of mobile dislocations, density of immobile dislocations and velocity of dislocations (each calculated per slip system). Mobile dislocation density and dislocation velocity are incorporated at the continuum level by using the generalised Orowan relation, whilst the immobile dislocation density controls the yield strength of the material. The density evolutions of mobile and immobile dislocations are controlled by dislocation kinetic equations, which account for the generation of new dislocations, immobilisation of mobile dislocations at the barriers and annihilation of mobile dislocations with other mobile dislocations and of mobile dislocations and immobile dislocations. Dislocation velocity is determined by integration of the equations of motion for the dislocations. The dislocation mechanics model combined with the continuum scale material model [3] was implemented in the LLNL Dyna3d, together with the vector shock equation of state, which was developed for modelling the response of orthotropic metals to high strain rate loading including the shock loading. Model validation was done by comparison of numerical results with experimental data for plate impact tests (1D strain state) for FCC (aluminium and copper) and BCC (tantalum) single crystal structures. The difference between the experimental and numerical values of the compared parameters (longitudinal stress, pulse length, elastic precursor relaxation time) was within 10%. Notably the plate impact tests show that over the first 50ns after impact the pre-cursor wave has an amplitude similar to the stress levels behind the shock wave, relaxing to HEL with time (wave propagation). 1. A.E. Mayer, K.V. Khishchenko, P.R. Levashov, P.N. Mayer, Modelling of plasticity and fracture of metals at shock loading, Journal of Applied Physics, 113(19), 2013. 2. V. Krasnokov, A. Mayer and A. Yalovets, Dislocation based high-rate plasticity model and its application to plate-impact and ultra short electron irradiation simulation, International Juornal of Plasticity, 27, 1294-1308, 2011. 3. R. Vignjevic, N. Djordjevic, V. Panov, Modelling of Dynamic Behaviour of Orthotropic Metals Including Damage and Failure, International Journal of Plasticity, 38, 47-85, 2012.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Finite Element Analysis of Abdominal Aortic Aneurysm - Benefits of EVAR Procedure and Predictions of Post-operative Complications

Smiljana Djorovic*, Igor Koncar**, Lazar Davidovic***, Nenad Filipovic****

*Faculty of Engineering, University of Kragujevac, Kragujevac, Serbia; Bioengineering Research and Development Center (BioIRC), Kragujevac, Serbia, **Clinic for Vascular and Endovascular Surgery, Serbian Clinical Center, Belgrade, Serbia, ***Clinic for Vascular and Endovascular Surgery, Serbian Clinical Center, Belgrade, Serbia, ****Faculty of Engineering, University of Kragujevac, Kragujevac, Serbia; Bioengineering Research and Development Center (BioIRC), Kragujevac, Serbia

ABSTRACT

Abdominal aortic aneurysm (AAA) requires endovascular aneurysm repair (EVAR) procedure in case of high-risk patients. Last years, computational modeling and analysis of AAA and implanted stent grafts (SGs) have become useful methods to define the present state of the patient and predict risk of post-operative complications [1, 2]. With that aim, this study analyzed the patient-specific AAA after EVAR procedure and SG implantation and determined biomechanical parameters which cannot be measured in vivo, such as the Von Mises stress and displacements of SG and aortic wall, as well as the velocity field of blood. The study included computational simulation of blood flow through implanted SG and interaction between SG, intraluminal thrombus (ILT) and aortic wall. The fluid-solid interaction was solved using the finite element (FE) method. Every domain of the patient-specific geometrical model was created on the basis of computed tomography (CT) scan images and consisted of a 3D finite element mesh. The computational simulation of cardiac cycle was performed for an average blood properties and parabolic blood flow, which was considered incompressible, viscous and laminar. Solid domains (aortic wall, SG and ILT) were modeled under the assumption of linearly-elastic isotropic material, whereby aortic wall and SG had constant thickness. Considering the difficulties in SG reconstruction, simplified SG was modeled, with material characteristics of equivalent composite material. As result, at the peak systolic moment aortic wall displacements and Von Mises stress in the aortic wall were decreased and in normal range, which indicated that EVAR procedure reduced risk of AAA growth and rupture. On the other hand, SG was under the high Von Mises stress, especially at the SG bifurcation where jet of blood, created during systole provided high velocity, which may cause SG migration and endoleaks. In summary, the results showed that EVAR procedure was beneficial for AAA, but in needs the follow-up, by means of biomechanical parameters determination, in order to predict post-operative complications.
[1] Z. Li, C. Kleinstreuer, “Blood flow and structure interactions in a stented abdominal aortic aneurysm model”, Medical Engineering & Physics, 27(5), pp. 369-382, June 2005. [2] D.S. Molony, A. Callanan, E.G. Kavanagh, M.T. Walsh, T.?. McGloughlin, “Fluid-structure interaction of a patient-specific abdominal aortic aneurysm treated with an endovascular stent-graft,“ BioMed Eng OnLine, vol. 8, October 2009.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Multi-scale Topological Optimization of Innovative Materials Using Computational Vadamecum

Tristan Djourackovitch*, Nawfal Blal**, Nahiene Hamila***, Anthony Gravouil****

*Univ Lyon, INSA-Lyon, CNRS UMR5259, LaMCoS, F-69621, France, **Univ Lyon, INSA-Lyon, CNRS UMR5259, LaMCoS, F-69621, France, ***Univ Lyon, INSA-Lyon, CNRS UMR5259, LaMCoS, F-69621, France, ****Univ Lyon, INSA-Lyon, CNRS UMR5259, LaMCoS, F-69621, France

ABSTRACT

Topological optimization is a key issue to reduce structure weight while preserving suitable mechanical properties. The latest developments of 3D printing techniques make it possible nowadays to design more innovative materials with suitable optimized micro-architectures. This needs connect the topological optimization of both the structure (under given boundary conditions and external loadings) and the micro-architecture. In order to go through the different scales of the design process (from the micro-designed material to the optimal macro-structure), computational homogenization approaches [1] provide a suitable framework to achieve multi-scale topological optimization. However, the prohibitive memory and computational costs of such methods still remain an open issue for engineering applications. In order to highly decrease the expensive costs, we propose a reduced order strategy based on an offline/online approach. At the offline stage, the effective behavior at the scale of the microstructure is optimized taking into account the viabilities of the underlying parameters. This step is done once for all using a multi-scale topological optimization solver. Two methods are then compared: 1) the SIMP (Solid Isotropic Material with Penalization) method [2] based on the introduction of a density parameter as the design variable, and 2) the level set method which consists in moving interfaces between material and voids using shape derivative. The offline step allows the constructions of parametric computational vadamecums of optimized microarchitectures. These latter can be used at the online phase to perform the optimization of the structure [3]. [1] M. Geers, V. Kouznetsova, W. Brekelmans, Multi-scale computational homogenization: trends and challenges, J. Comput. Appl. Math. 234 (7) (2010) 2175–2182. [2] O.Sigmund. Materials with Prescribed Constitutive Parameters: an inverse Homogenization Problem. Int. J. Solids Structures, 1994.? [3] Ferrer, A., Oliver, J., Cante, J. C., Lloberas-Valls, O., 2016. Vademecum-based approach to multi-scale topological material design. Adv. Model. and Simul. in Eng. Sci. , 3 – 23

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Energy-based Modeling of the Non-local Damage Behavior in the Adhesive Interface of FRP-Metal Hybid Material Systems

Michael Dlugosch*, Jens Fritsch**, Stefan Hiermaier***

*Fraunhofer-Institute for High-Speed Dynamics, Ernst-Mach-Institut, EMI, **Fraunhofer-Institute for High-Speed Dynamics, Ernst-Mach-Institut, EMI, ***Fraunhofer-Institute for High-Speed Dynamics, Ernst-Mach-Institut, EMI

ABSTRACT

Motivated by efficiency goals and upcoming strict EU-regulations for CO2-emissions, lightweight design plays an increasingly important role in automotive engineering. Novel hybrid material systems combining advanced composite materials (such as CFRP and GFRP) with conventional body-in-white steels are one way to reduce the vehicle weight while simultaneously meeting the growingly stringent crash safety requirements. While various previous studies were able to document the general potentials of such hybrid material systems for crash structural applications [1, 2], defining efficient modeling techniques for numerical crash simulations in the early vehicle concept development phase poses a great challenge to engineers and researchers alike [3]. Next to the development of material models and model complexity issues (such as the number of shell elements used to model a laminate), finding a technique to efficiently model the adhesive interface's binary behavior under crash conditions is critical. The exploration of strongly simplified rigid tie connections – with respect to cohesive zone modeling approaches - on a structural subsystem level leads to the identification of a very particular damage phenomenon and to the revelation of a significant drawback of existing techniques. This study introduces the experimental investigation of this phenomenon, which comprises the non-local damage behavior of the adhesive interface within a hybrid material system upon FRP-fracture under tension. A new energy-based analytical model including a hybrid specific modification of the BK cohesive zone fracture model is able to accurately predict the damaged interface area upon FRP-fracture and may thus be used to enhance strongly simplified and efficient interface modeling techniques for vehicle subsystem concept structures under crash loading. The presentation will include the results of the experimental procedures to analyze the special damage phenomenon as well as the stepwise derivation of the energy-based model and a discussion of results and further implementation strategies References [1] Bambach, M. R. 2013. Fibre composite strengthening of thin-walled steel vehicle crush tubes for frontal collision energy absorption. Thin-Walled Structures 66, 15–22. [2] Dlugosch, M., Lukaszewicz, D., Fritsch, J., and Hiermaier, S. 2016. Experimental investigation of hybrid material systems consisting of advanced composites and sheet metal. Composite Structures, 152, 840–849. [3] Mildner, C. 2013. Numerische und experimentelle Untersuchungen des Crashverhaltens von FVK-verstärkten Metallstrukturbauteilen. Dissertation, Technische Universität München.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

An XFEM Enriched Computational Model Generation Library for Multi-material and Multi-physics Applications

Keenan Doble*, Kurt Maute**, David Noble***, Miguel Aguilo****

*University of Colorado Boulder, **University of Colorado Boulder, ***Sandia National Laboratories, ****Sandia National Laboratories

ABSTRACT

In this work, an eXtended Finite Element Method (XFEM) model generation library is presented. The library's core functionality will be discussed and its numerical performance analyzed. The library's interface with a geometry engine is abstracted to accommodate many types of geometry descriptions including analytic, discrete distance fields and surface meshes. The geometry model is then immersed in the computational domain and the library computes an XFEM discretization. The result is a geometry conforming pseudo-mesh. This pseudo-mesh separates the computational domain by material which enables integration of the weak form of the governing equations for each material phase individually. This is useful for multi-physics and multi-material applications. To support phase change problems and shape optimization, the pseudo-mesh contains interface node and side sets that store information about how their positions change as the interface geometry is perturbed. The interface side sets are double sided which allows for weak enforcement of interface conditions. Additionally, the conformal pseudo-mesh stores enrichment information which is crucial for consistent interpolation of the solution fields. A discussion of this enrichment strategy is provided. Since the library is aimed to be used on exa/petascale problems, the method of generating a conformal and parallel consistent XFEM model has been developed with minimizing parallel communication in mind. The decomposition method and a study of the library's scalability in the number of CPU's will be provided. The library recursively handles geometry models allowing for an arbitrary number of materials in the computational domain. The scalability regarding the number of materials will be demonstrated. Two examples are to be shown. The first example is the XFEM model generation of a femur using CT scan data to show the robustness of the library in handling complex geometry configurations. The second is a composite fiber example where each fiber is a different material to show the library's ability to handle multiple materials.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Experimental and Numerical Analysis of the Surface Properties of the PC/ABS

T. Doca*, F.M. Andrade Pires**

*University of Brasília, **University of Porto

ABSTRACT

The constant improvement of additive manufacture [1] creates several interesting opportunities for the enhancement of mechanical components. For instance, the engineering of new materials from the combination of others while keeping the best properties of each one of them. In this work, we present the experimental and numerical analysis of an effective combination of two polymers [2]: Polycarbonate (PC) and Acrylonitrile Butadiene Styrene (ABS). This combined material has high impact strength, high stiffness, heat resistance and is very easy to process. It is employed in the manufacture of car parts, portable hand-held devices, gas tanks and structural components in general. The study aims the investigation of surface properties [3], such as coefficient of friction, roughness, hardness, wear resistance and wear morphology. Moreover, an analysis of these parameters is used to verify the potential of the PC/ABS as protective coatings. Simulations of the wear process [4] are also conducted in order to evaluate the challenges of modelling such complex material. References [1] I. Gibson, D. Rosen, B. Stucker. Additive Manufacturing Technologies. Second edition, Springer, New York, (2015). [2] B. S. Lombardo, H. Keskkula, D. R. Paul. Influence of ABS type on morphology and mechanical properties of PC/ABS blends. Journal of Applied Polymer Science, 54, 1697–1720 (1994). [3] B. Bhusan. Modern tribology handbook. CRC Press, ?Boca Raton, Florida, (1949). [4] T. Doca, F.M. Andrade Pires. Finite element modeling of wear using the dissipated energy method coupled with a dual mortar contact formulation. Computers and Structures 191, 62–79 (2017).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

An Interface-based Approach for Segmentation of Multiphase Microstructure Images

Gunay Dogan*

*Theiss Research, NIST

ABSTRACT

Image segmentation is the problem of identifying homogeneous regions or phases and their interfaces/boundaries in given images. It is a fundamental step for quantitative analysis of microstructure images. It is also a necessary step for finite element (FE) simulations of microstructure physics using of OOF, because the FE simulations require a mesh that conforms to the phases and interfaces encoded in the microstructure image. Unfortunately, the multiphase image segmentation problem is NP-hard, namely, a globally optimal algorithm to find an unknown number of phases to delineate them in a given image is computationally impractical. However, effective heuristic algorithms exist, and in this talk, we present one that focuses on the interfaces between the phases. Identifying the interfaces in a given microstructure image effectively segments the image partitioning the image domain into the distinct regions or phases. In this approach, instead of categorizing or labeling each pixel, we start with an initial set of candidate interfaces (or boundary curves in 2d images), and evolve them gradually to find and fit the real interfaces in the given image. The initial interfaces can be provided by the users or an automated initialization routine. The interfaces are usually represented very compactly with a much smaller number of unknowns than the number of pixels in the image, reducing the memory requirements and running times dramatically. The interface evolution itself is guided by a segmentation energy that is minimized when the interfaces partition the image into phases, each of which can be approximated by an average value (of image intensity, orientation, or other image characteristic). The interface evolution is essentially a gradient descent process. To improve convergence of the algorithm and to further reduce running times, we incorporate second order sensitivity of the segmentation energy, and realize an accelerated descent in the form of a shape-Newton algorithm. This improved descent procedure increases the robustness of the segmentation with respect to imaging conditions as well. We demonstrate the effectiveness of our algorithm with several examples.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Nonlinear Multiscale Modeling of Porous and Composite Materials Under Small and Large Deformations

Issam Doghri*, Marieme El Ghezal**, Ludovic Noels***, Ling Wu****

*Université catholique de Louvain, **Université catholique de Louvain, ***Université de Liège, ****Université de Liège

ABSTRACT

Multiscale models are proposed for plastic matrix materials in which multiple cavities or solid inclusions are embedded. Semi-analytical micromechanical models are proposed based on mean-field homogenization (MFH) and verified against full-field finite element (FE) analyses on representative volume elements (RVEs). For composites, two finite strain MFH formulations are proposed. For both, local constitutive equations of each solid phase are based on a multiplicative decomposition of the deformation gradient onto elastic and inelastic parts and hyperelastic-plastic stress-strain relations. The first MFH formulation is an incremental-tangent one [1] based on relating the macroscopic rate values of the nominal stress (transpose of first Piola-Kirchhoff) and the deformation gradient. The second MFH formulation is an incremental-secant one [2]. It is based on unloading the composite material to zero macroscopic stress and taking into account per-phase residual strains and stresses in each phase. The formulation uses Cauchy and Kirchhoff stresses and logarithmic strains in each phase. Finally, we propose an original micromechanical formulation for a rigid plastic matrix containing multiple spherical inclusions [3]. It is based on coupling Gurson's single cavity solution with a generalized self-consistent (GSC) model at the RVE level. A secant formulation of GSC using second statistical moments in each phase is proposed. For all three contributions, numerical algorithms were developed and implemented. The MFH predictions were extensively tested against direct FE simulations of RVEs or unit cells, for several heterogeneous microstructures under various loadings. [1] Doghri, I., M.I. El Ghezal, L. Adam, 2016. « Finite strain mean-field homogenization of composite materials with hyperelastic-plastic constituents », International Journal of Plasticity, 81, 40-62, 2016. [2] El Ghezal, M.I., L. Wu, L., I. Doghri, L. Noels, 2017. "Finite strain extension of the incremental-secant homogenization formulation for elasto-plastic composites", submitted. [3] El Ghezal, M.I., I. Doghri, 2017. "Porous plasticity: predictive second moment homogenization models coupled with Gurson's solution", submitted.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Design of System to Control the Fall of a Suborbital Payload

Diego Domínguez*, Fernando Velázquez**

*UNAM, **UNAM

ABSTRACT

One of the most important problems in suborbital flights is the recovery of the payload. Avoiding difficult access areas (mountains, forests, lakes, lagoons, rivers, etc.) or dangerous areas (populated areas, vehicle ways, etc.) is very convenient. In this work, a mechatronic system to control the fall of a suborbital payload is proposed, considering the use of a paraglider. The simulation of the paraglider movement controller is shown, considering wing flight techniques. The air disturbances common in this type of missions, dynamic model and the prohibited areas of landing are also considered to design the controller. The results obtained from the simulation will be copared with the results that will be obtained after the implementation of the mechatronic system in suborbital flights of the CSM-UNAM (Mexican Service Load UNAM).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Reduction-Consistent and Thermodynamically-Consistent Formulation and Associated Algorithm for Multiphase Flows of N Immiscible Incompressible Fluids

Suchuan Dong*

*Purdue University

ABSTRACT

In this talk we focus on the dynamics of an isothermal system of N (N >=2) immiscible incompressible fluids with different physical properties (e.g. densities, viscosities, and pair-wise surface tensions). These problems are characterized by multiple types of fluid interfaces and pairwise surface tensions, multiple types of three-phase lines, density contrasts and viscosity contrasts among multiple fluids, and multiple types of moving contact lines and multiple contact angles when solid walls are present. We present a reduction-consistent and thermodynamically consistent formulation and an associated numerical algorithm for simulating such N-phase problems. By reduction consistency we refer to the property that if only a set of M (1 <=M<=N-1) fluids are present in the system (while the other fluid components are absent) then the N-phase governing equations and boundary conditions will exactly reduce to those for the corresponding M-phase system. By thermodynamic consistency we refer to the property that the formulation honors the thermodynamic principles and rigorously satisfies the mass conservation, momentum conservation, second law of thermodynamics, and the Galilean invariance principle. Our N-phase formulation is based on a more general method that allows for the systematic construction of reduction-consistent formulations, and the method suggests the existence of many possible forms of reduction-consistent and thermodynamically consistent N-phase formulations. An efficient numerical algorithm for simulating N-phase problems based on this formulation are developed. Extensive numerical experiments will be presented for several multiphase flow problems involving multiple fluid components and large density ratios and large viscosity ratios, and simulation results are compared with the physical theories or the available physical solutions. These comparisons demonstrate that our method produces physically accurate results for this class of problems. References: 1. S. Dong, " Wall-bounded multiphase flows of N immiscible incompressible fluids: Consistency and contact-angle boundary condition", Journal of Computational Physics, 338, 21-67, 2017. 2. S. Dong, " Physical formulation and numerical algorithm for simulating N immiscible incompressible fluids involving general order parameters ", Journal of Computational Physics, 283, 98-128, 2015. 3. S. Dong, " Multiphase flows of N immiscible incompressible fluids: A reduction-consistent and thermodynamically consistent formulation and associated algorithm ", arXiv:1707.09023, 2017.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Fully Lagrangian SPH-based Method for Simulation of Abrasive Waterjet Impacting on Metallic Surface

Xiangwei Dong*, Zengliang Li**

*College of Mechanical and Electronic Engineering, China University of Petroleum(East China), **College of Mechanical and Electronic Engineering, China University of Petroleum(East China)

ABSTRACT

A lagrangian model for the numerical simulation of the impact of abrasive waterjet on metallic surface is proposed in this paper. In the method both fluid (water) and solid phases (target) are described by smoothing particle hydrodynamics (SPH). Waterjet is modeled as a viscous fluid with weak compressibility, metallic target is modeled as an elastic-plastic material. Abrasive particles, which are explicitly included in the waterjet, are modeled as rigid bodies and are initially surrounded by the water. The interactions between fluid and solid, between abrasive and solid, and between abrasive and fluid, are modeled through suitable terms that are commonly used in the SPH. Simulation tests of impact of abrasive-water-jet are carried out as challenging examples to verify the applicability of the proposed model. The result demonstrates the attractiveness of this new approach in relevant applications such as abrasive waterjet (AWJ) cutting and solid particle erosion (SPE). Advantages of the method are robustness, conceptual simplicity and relative ease of incorporating new physics.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Long Term Integration of Burgers Equation with Rough Noise

Yuchen Dong*, Zhongqiang Zhang**

*WPI, **WPI

ABSTRACT

We propose a restarted stochastic collocation methods for Burgers equation driven by white noise. The standard stochastic collocation methods suffer from the curse of dimensionality. To reduce the dimensionality in random space, we apply independent component analysis to reconstruct the computed solutions every few time steps. After such a reconstruction, we then match in time and compute solutions with appropriate stochastic collocation methods and repeat the aforementioned procedure until desired integration time instant. Numerical results and some basic analysis of the proposed methodology will be presented. Reference: [1] Z. Zhang, M. V. Tretyakov, B. Rozovskii, and G. E. Karniadakis. A recursive sparse grid collocation method for differential equations with white noise. SIAM J. Sci. Comput., 36(4): A1652-A1677, 2014. [2] H. Cagan Ozen, Guillaume Bal. Dynamical polynomial chaos expansions and long time evolution of differential equations with random forcing. SIAM/ASA J. Uncertain. Quantif., 4(1):609-635,2016. [3] A. Hyvärinen, J. Karhunen, E.Oja. Independent Component Analysis. John Wiley & Sons, New York, 2001.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Atomic Scale Modeling of Structural Response of 2D Materials to Mechanical and Chemical Environments

Avinash Dongare*, Jin Wang**

*University of Connecticut, **University of Connecticut

ABSTRACT

Transition metal dichalcogenides (TMDs), such as molybdenum disulfide (MoS2), have attracted attention for applicability in next-generation electronic materials and energy storage technologies. This talk highlights the current understanding of the atomic scale structural response of these layered materials when subjected to strains as well as solid-state reactions during intercalation and de-intercalation. The strain response is investigated for chemical vapor deposition (CVD) grown flakes few layered MoS2 that are either free standing or supported on to a substrate using classical molecular dynamics (MD) simulations. The chemical response is investigated for the structural transformations during solid-state reactions related to intercalation and de-intercalation reactions using density functional theory calculations. The mechanisms of strain relaxation and the energetics of intercalation-induced transformations at the atomic scales will be presented.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Uncertainty Quantification Using Low-fidelity Data

Alireza Doostan*, Jerrad Hampton**, Hillary Fairbanks***, Akil Narayan****

*CU Boulder, **CU Boulder, ***CU Boulder, ****University of Utah

ABSTRACT

The use of model reduction has become widespread as a means to reduce computational cost for uncertainty quantification of PDE systems. In this work, we present a model reduction technique that exploits the low-rank structure of the solution of interest, when exists, for fast propagation of high-dimensional uncertainties. To construct this low-rank approximation, the proposed method utilizes models with lower fidelities (hence cheaper to simulate) than the intended high-fidelity model. After obtaining realizations to the lower fidelity models, a set of reduced basis and an interpolation rule are identified and applied to a small set of high-fidelity realizations to obtain this low-rank, bi-fidelity approximation. In addition to the construction of this bi-fidelity approximation, we present convergence analysis and numerical results. This is a joint work with Hillary Fairbanks (CU Boulder), Jerrad Hampton (CU Boulder), and Akil Narayan (U of Utah).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Isogeometric Dual Mortar Coupling for Complex NURBS Surface Patch Models

Wolfgang Dornisch*, Joachim Stöckler**, Ralf Müller***

*University of Kaiserslautern, **TU Dortmund University, ***University of Kaiserslautern

ABSTRACT

Isogeometric analysis fosters a further integration of design and analysis by using the geometry description of the CAD system also for the numerical analysis. Hereby, the use of Non-Uniform Rational B-splines (NURBS) surfaces is common, but entails the need for a coupling of non-conforming patches in order to avoid unnecessary refinement for complex multi-patch models. The use of mortar methods [1] allows a coupling which requires neither additional variables nor empirical parameters. The use of mortar methods in the style of [1] for the coupling of two NURBS surface patches has been proposed in [2]. A more efficient dual mortar method with local support along the interfaces has been proposed in [3]. An arbitrary number of patches can be coupled, but additional treatment for intersecting interfaces is required. Within this contribution, an improved class of dual basis functions is presented, which allows a complete decoupling of the individual interfaces. This is of high relevance for the sparsity and condition of the global stiffness matrix, as well as for the efficiency of the computations and the accuracy of the solution. Numerical examples show the influence of the chosen concept for the dual basis functions on the aforementioned criteria. A comparison to computations with conforming meshes shows that both accuracy and efficiency of the proposed mortar method are highly competitive to standard conforming computations. [1] C. Bernardi, Y. Maday, A. T. Patera, Domain Decomposition by the Mortar Element Method, in: H. G. Kaper, M. Garbey, G. W. Pieper (Eds.), Asymptotic and Numerical Methods for Partial Differential Equations with Critical Parameters, Springer Netherlands, Dordrecht, pp. 269-286, 1993. [2] W. Dornisch, G. Vitucci, S. Klinkel, The weak substitution method – An application of the mortar method for patch coupling in NURBS-based isogeometric analysis, Int. J. Numer. Meth. Engng. 103, 205-234, 2015. [3] W. Dornisch, J. Stöckler, R. Müller. Dual and approximate dual basis functions for B-splines and NURBS – Comparison and application for an efficient coupling of patches with the isogeometric mortar method. Comput. Methods Appl. Mech. Engrg. 316, 449-496, 2017.

13th World Congress on Computational Mechanics (WCCM XIII) and 2nd Pan American Congress on Computational Mechanics (PANACM II), July 22-27, 2018, New York City, NY, USA

ROTATIONS OF THE PARAMETRIC *N*-PENDULUM WITH A VIEW ON ENERGY HARVESTING FROM OCEAN WAVES

FRANCO E. DOTTI*, FLORENCIA REGUERA†, AND SEBASTIÁN P. MACHADO*

*Grupo de Investigación en Multifísica Aplicada, Facultad Regional Bahía Blanca, Universidad Tecnológica Nacional. Consejo Nacional de Investigaciones Científicas y Técnicas.
11 de Abril 461
B8000LMI Bahía Blanca, Buenos Aires, Argentina
fdotti@frbb.utn.edu.ar; smachado@frbb.utn.edu.ar

†Area Hidráulica, Departamento de Ingeniería, Universidad Nacional del Sur. Grupo de Investigación en Multifísica Aplicada, Facultad Regional Bahía Blanca, Universidad Tecnológica Nacional.
Av. Alem 1253
B8000LMI Bahía Blanca, Buenos Aires, Argentina
florencia.reguera@uns.edu.ar

Key words: Parametric *N*-pendulum, Wave Energy, Nonlinear Dynamics.

Abstract. In this article, we expand the knowledge on the dynamics of the parametric *N*-pendulum, as a universe of non-linear behavior is unveiled. With the final purpose of extracting energy from the ocean waves, we focus on rotational motion which is the most energetic steady state. The existence of rotating attractors is explored, for different configurations of the *N*-pendulum. The nonlinear parametric dynamics is explored by means of numerical simulations in order to comprehend the behavior of the *N*-pendulum and to establish the best conditions for energy harvesting. Results are presented through control spaces, bifurcation diagrams and basins of attraction.

1 INTRODUCTION

Among the large number of designs aimed at wave energy harvesting, pendulum wave energy converters (WECs) are attractive due to the simplicity of the mechanisms involved, in combination with the high kinetic energy available in its rotational motion. The concept is very simple and intuitive: a pendulum on a floating platform, to which the sea waves impose a vertical motion at a certain (predominant) frequency. If stable rotational motion of the pendulum is achieved, part of the kinetic energy of rotations can be converted into electrical energy by a generator attached to the pendulum axis[1]. Now, given the low frequencies of the sea waves, it is impractical to consider a simple pendulum since the length required to achieve parametric

resonance results to be prohibitively large. A pendulum of multiple concentric masses, i.e. a *N*-pendulum, comes to solve this problem as low natural frequencies can be achieved with a relatively small size of the WEC[2].

Rotations are not uncommon in the dynamics of the parametric pendulum, although most of the times they coexist with other responses. Steady rotations are classified in four categories[3]: pure rotations, oscillating rotations, straddling rotations and large amplitude rotations. Pure rotations have a significant attribute in terms of energy harvesting: the angular velocity always maintains the same sign. This ensures that there is no change in the direction of rotation, implying no oscillatory motion of any kind. In other words: being the parametric pendulum a potential well system, pure rotations always ensure a "walk out of the well", thus being the most energetic motion of the pendulum[4]. Given the symmetry of the system, pure rotations exist in conjugate pairs: if a clockwise rotation orbit exists, then an equivalent anticlockwise orbit must also exist[5]. In this article, pure rotations are regarded as synonymous of *rotations*, while the other categories are regarded merely as *oscillations*. Rotations can also be categorized according to their period, *n*. The most energetic are period-1 ($n = 1$), i.e, one rotation per load cycle. Rotations with $n = 2$ (one rotation per two load cycles) or higher are slower and thus less energetic. Period-1 rotations are pursued for energy harvesting purposes. However, rotations of period two or more are not negligible in terms of energy extraction.

By means of numerical simulations, we address in this article the nonlinear dynamics of a parametric *N*-pendulum system with the purpose of establishing the best conditions for energy harvesting. The article is organized as follows. After this introduction, we introduce the mathematical model (Section 2). Then, in Section 3, the nonlinear dynamics of the system is addressed by means of numerical simulations. Finally, the results of the study are presented and discussed (Section 4).

2 MATHEMATICAL MODEL

Figure 1 shows a schematic *N*-pendulum, which is contained in the *xy* plane. Each of the *N* masses are separated by a fixed angular distance $\psi = 2\pi/N$, and arranged concentrically around a pivot axis. Length l_1 is assumed to be greater than or equal to any of the other lengths (l_2, l_3,..., l_N), and the same assumption is made for mass m_1 with respect to m_2, m_3,..., m_N. Both l_1 and m_1 constitute the *main arm*, as pointed. The angle θ is measured with respect to the main arm and denotes the angular position relative to the vertical direction. A time-dependent external motion $Y(t)$ is imposed to the pivot axis. The center of mass of the system is located at the point *C*.

From classic mechanics of systems of particles[6], kinetic, potential and dissipative energy terms can be derived respectively as

$$T = \tfrac{1}{2} M \left\{ \left[Y' + l_C \theta' \sin\left(\theta + \varphi\right) \right]^2 + \left[l_C \theta' \cos\left(\theta + \varphi\right) \right]^2 \right\} + \tfrac{1}{2} K_0 \left(\theta'\right)^2,$$

$$V = gM \left[l_1 - l_C \cos\left(\theta + \varphi\right) \right], \tag{1}$$

$$D = \tfrac{1}{2} b \left(\theta'\right)^2 \sum_{i=1}^{N} l_i^2,$$

where g is the gravity, φ is the phase shift of the center of mass with respect to the main arm and l_C is the distance from C to the origin. These are given by

$$\varphi = \arctan\left[\left(x_C / y_C\right)\Big|_{\theta=0}\right], \qquad l_C = \left(\sqrt{x_C^2 + y_C^2}\right)\Big|_{\theta=0}, \tag{2}$$

where x_C and y_C are the coordinates of the point C, given by

$$\begin{aligned} x_C &= \frac{1}{M}\sum_{i=1}^{N} m_i l_i \sin\left[\theta + (i-1)\psi\right], \\ y_C &= l_1 - \frac{1}{M}\sum_{i=1}^{N} m_i \left\{l_1 - l_i \cos\left[\theta + (i-1)\psi\right]\right\}, \end{aligned} \tag{3}$$

and $M = \sum_{i=1}^{N} m_i$. The factor K_0 in (1) is associated to the kinetic energy relative to the center of mass, and it is given by

$$K_0 = \sum_{i=1}^{N}\left\{m_i\left\{l_i^2 + l_C^2 - 2 l_i l_C \cos\left[(i-1)\psi - \varphi\right]\right\}\right\}. \tag{4}$$

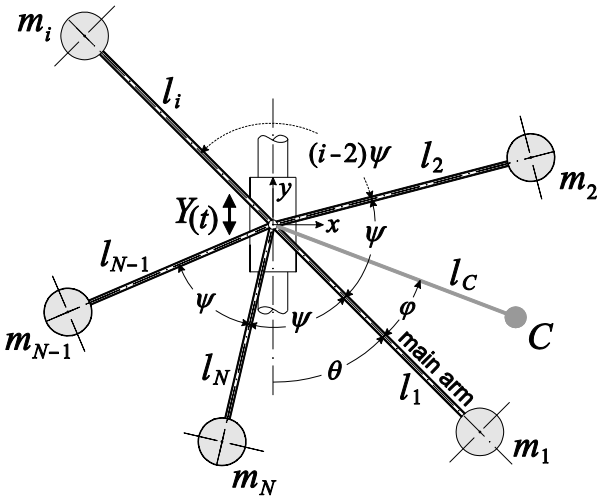


Figure 1. Scheme of the vertical parametric N-pendulum.

The viscous friction coefficient b in (1) is defined as independent of mass shapes, since bobs are very similar one to each other. By introducing (1) into Lagrange equation for one degree of freedom non-conservative systems, the equation of motion for an arbitrary vertical forcing $Y(t)$ is obtained as

$$I\theta'' + b\theta'\sum_{i=1}^{N} l_i^2 + M\, l_C\left(Y'' + g\right)\sin\left(\theta + \varphi\right) = 0, \tag{5}$$

where the inertia of the system is defined as $I = K_0 + M\, l_C^2$. Now, if a sinusoidal motion of the form $Y(t) = -H_S \cos \Omega_S t$ is considered as external forcing, (5) can be written as

$$I\theta'' + b\theta'\sum_{i=1}^{N} l_i^2 + M\, l_C\left(H_S\, \Omega_S^2 \cos\Omega_S t + g\right)\sin\left(\theta + \varphi\right) = 0. \tag{6}$$

Now, in order to gain in generality, (6) can be expressed in its dimensionless form as

$$\ddot{\theta} + \beta\dot{\theta} + \left(R\cos\omega\tau + 1\right)\sin\left(\theta + \varphi\right) = 0, \tag{7}$$

where the superimposed dots over some symbols indicate derivation with respect to the dimensionless time $\tau = \omega_0 t$. The dimensionless forcing parameters ω and R are defined as

$$\omega = \Omega/\omega_0\,, \qquad R = H_S\omega^2 M\, l_C/I\,, \tag{8}$$

and the natural frequency of the system corresponds to

$$\omega_0 = \sqrt{g\, M\, l_C/I}\,. \tag{9}$$

Finally, a viscous friction parameter β is also defined in (7), as

$$\beta = I^{-1}\omega_0^{-1} b \sum_{i=1}^{N} l_i^2\,. \tag{10}$$

By means of (7), the dynamics of the system of Fig. 1 can be addressed from a general viewpoint, regardless of the physical constants of each particular system. The steady response of the system depends on parameters ω, R and β, which in turn depend on the magnitudes of masses and lengths and also on the number of arms N.

3 NUMERICAL SIMULATIONS

The dynamics of pendulum systems governed by (7) is explored. Such equation is solved numerically by means of a classic Runge-Kutta method implemented in *Wolfram Mathematica*. As a general rule, a dimensionless simulation time of $t_s = 2500$, with the purpose of ensure steady state responses. To avoid transients, the first $t_d = 2300$ are discarded in the construction of all the diagrams.

To study the topology of the responses of (7), a good choice is to fix β and φ and see what happens while varying the forcing parameters R y ω, as presented in the control space Fig. 2. This choice is not arbitrary: it is demonstrated[7] that a variation of the damping parameter only shifts the multidimensional control space upwards or downwards. Meanwhile, φ is just a phase angle which does not alter the dynamics, except for a shift in the rest position of the pendulum. Thus, nothing too interesting happens while varying β and φ. Figure 2 clearly shows that topology may change dramatically as R and/or ω are varied. The coexistence of stable periodic and chaotic solutions is possible, depending on initial conditions. The map of Fig. 2 is constructed as follows: for each fixed pair (R, ω), several simulations are performed with different initial conditions; the topology of each steady state is computed to give the color classification of the corresponding point (R, ω) in the control space. One can observe that, if the excitation amplitude is sufficiently low (low R), the rest position is the only possible stable solution and the system behaves as a linear one. As R increases, oscillations, rotations and tumbling chaos[5] appear, unveiling a rich nonlinear dynamics. In the construction of Fig. 2, steps

of 1/100 were employed for R and ω, while 63 initial states were considered for each pair (R, ω), producing a total of $5.67 \cdot 10^6$ simulations.

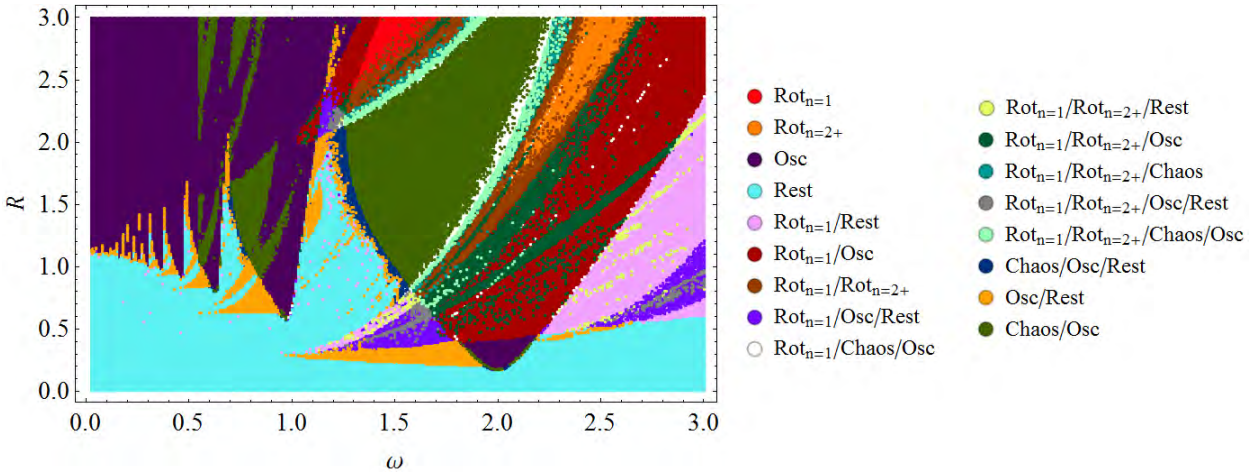


Figure 2. Control space R-ω showing the most significant physical responses of a system with $\beta = 0.1$ and $\varphi = 0$. Rot$_{n=1}$ means "pure rotations of period 1" while Rot$_{n=2+}$ means "pure rotations of period 2 or higher".

The rest position is always a solution of (7), either stable or unstable. Contours of Fig. 3 indicate the probability of occurrence of a stable rest solution. The resonance zones are those regions of the control space inside which the rest position is unstable (i.e. probability is zero in Fig. 3, since unstable solutions are not captured by numerical simulations). Resonance zones are represented by the blue "tongues" in Fig. 3, centered around $\omega = 2/p$, being p a positive integer. The largest resonance zone lies around $\omega = 2$ ($p = 1$) and is called the *main resonance zone*. For energy harvesting purposes, it is convenient to lie inside the resonance zones since the rest solution is the less energetic state (recall that the parametric pendulum is a potential well system).

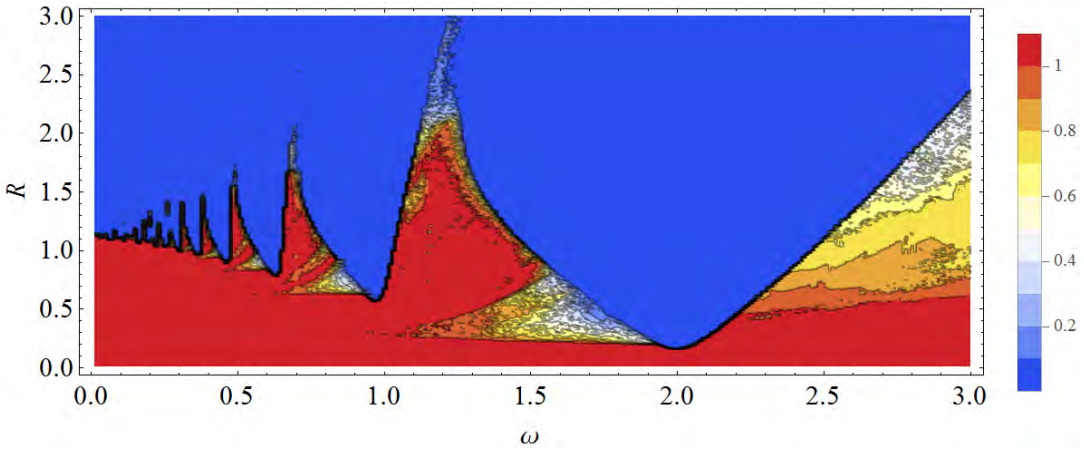


Figure 3. Stability diagram showing the resonance zones (blue tongues). Contours indicate the probability of occurrence of a stable rest solution. $\beta = 0.1$ and $\varphi = 0$.

As stated in the Introduction, period-1 rotations are desired since they are the most energetic motion of a parametric pendulum. Contours of Fig. 4 show the probability of occurrence of

stable period-1 rotations, given a random initial state. Such magnitude represents a measure of the robustness of rotations since it quantifies the ease of a trajectory to stick to the rotating attractor (blue: low robustness; red: high robustness). In practical terms, rotational motion cannot take place for $\omega < 1$. Moreover, there is a wide range of the control space where rotations are not possible, irrespective of the initial conditions (blue areas). On the other hand, the red area located at $R > 2.1$ and $1.2 < \omega < 1.7$ means that all initial states produce rotations. This implies that rotation is the only stable steady state. Consequently, a design of a pendulum WEC with such settings of R and ω would not require an external control to reach and maintain rotations, thus strongly simplifying energy extraction. Sadly, such high values of R cannot be reached by the forcing of the sea waves[8,9]. However, a suitable design of a WEC can be obtained in the vicinity of the main resonance zone, where rotation is also a common response, as can be checked from Fig. 3. Comparing Fig. 4 and Fig. 5, one can verify the increase in the probability of obtaining stable rotations when the period-1 restriction is removed.

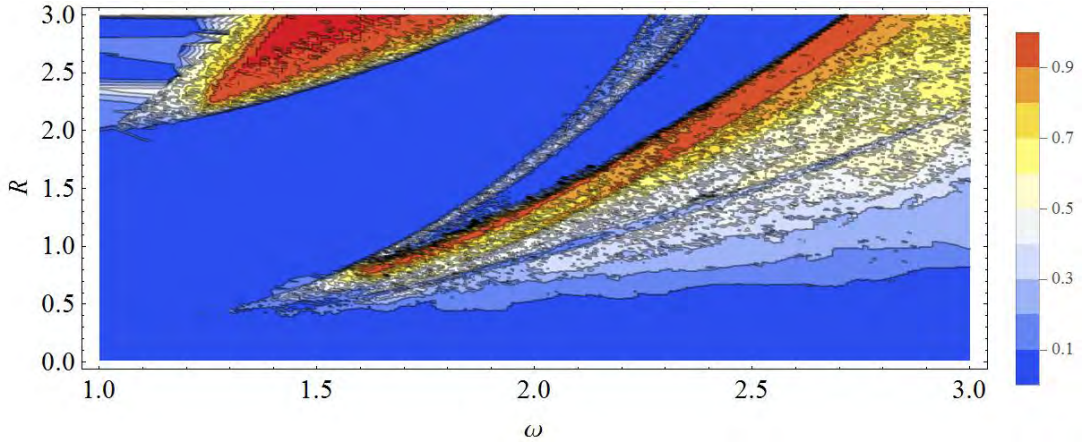


Figure 4. Period-1 rotation zones in the control space. $\beta = 0.1$ and $\varphi = 0$.

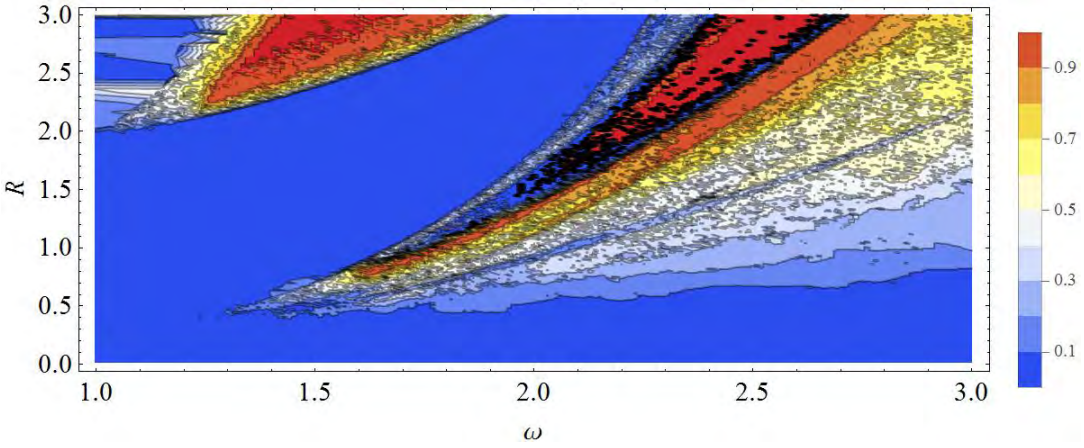


Figure 5. Rotation zones in the control space, regardless of the period. $\beta = 0.1$ and $\varphi = 0$.

The topology of the response for $\omega = 2$ can be studied by means of a bifurcation diagram, as the one presented in Fig. 6. The first qualitative observation is that rotations can be obtained for a wide range of R: they suddenly appear at $R = 0.450$ by a fold (or saddle-node) bifurcation, and

vanishes by a crisis at $R = 1.810$ after a period-doubling cascade. The values of R must be taken as indicative, since they can shift with a modification of damping. Nevertheless, the topology does not change. Period-1 rotating attractors always coexist with oscillatory attractors. This implies that initial conditions and robustness play an important role in order to reach a stable rotation.

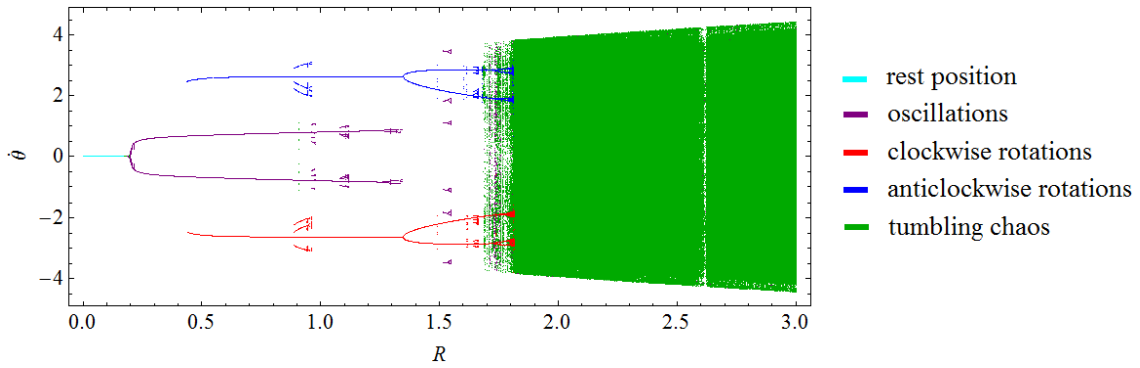


Figure 6. Bifurcation diagram of $\dot{\theta}$ for the main parametric resonance ($\omega = 2$), $\beta = 0.1$, $\varphi = 0$.

Fig. 7 presents a sequence of rotational responses in the phase plane as R is varied, with transients included. These phase planes are associated to the bifurcation diagram of Fig. 6. The sequence shows the topological evolution of the period-1 rotating attractors in the phase plane, from their birth at $R = 0.450$ until their disappearance at $R \approx 1.810$, as well as its interaction with other attractors. Fig. 7a shows the situation previous to the birth of the stable rotating attractor: an oscillation is the only possible response, since the rest position has just lost stability by means of a supercritical Hopf bifurcation (at $R = 0.196$). Fig. 7b shows how the stable branches of both symmetric period-1 rotating attractors suddenly appear, by a fold bifurcation. From $R = 0.450$ up to $R = 0.900$, period-1 rotations and period-2 oscillations coexist, being Fig. 7b the phase portrait of the system. From $R = 0.900$ (Fig. 7c), a pair of period-3 rotating attractors attempt against robustness of period-1 rotations. This is because all initial states captured by the period-3 attractors are *stolen* from period-1 attractors. This is also evidenced in the control space of Fig. 3, as a blue stripe extended approximately from $(R, \omega) = (0.5, 1.5)$ to $(R, \omega) = (2.3, 3.0)$. This pair of period-3 attractors run into cascade by a supercritical flip (period doubling) bifurcation at $R = 0.945$ (Fig. 7d) and finally vanish in a crisis at $R = 0.960$. From this point on, the topological structure of Fig. 7b is recovered, as period-1 rotations and period-2 oscillations are the only possible steady states. Up to $R = 1.350$, rotatory responses remain unchanged and only oscillatory responses undergo topological changes. As an example, Fig. 7e shows how the period-2 oscillating attractor has doubled its period. An interesting event takes place between $R = 1.331$ and $R = 1.350$: the oscillatory attractor has suddenly vanished after a rapid cascade and period-1 rotation is the only possible steady state (Fig. 7f). This is of course an ideal scenario for energy harvesting, as all initial conditions produce stable rotations. Sadly (again) the interval of R is too short, being practically impossible to tune, especially if the external forcing presents variations as in the case of the sea waves. At $R = 1.350$ a flip bifurcation occurs, doubling the period of the rotating attractor (Fig. 7g). Period-2 rotations take place, thus initiating the inevitable Feigenbaum cascade. Phase plane of Fig. 7h is associated to the period-6 oscillating motion that can be clearly observed in Fig. 6 at $R = 1.550$. This attractor appears briefly as R is varied, and corresponds to an oscillating rotation (in the sense of Garira and Bishop[3]), as can be

checked from Fig. 7h. Finally, Fig. 7i shows the rotating attractor at the edge of the crisis that will trigger its disappearance. A high periodic rotation can be obtained after very long transients, but most of the initial conditions give rotating chaos: an unpredictable aperiodic rotation. After R = 1.810, no periodic solution survives, being tumbling chaos the only possible response of the system.

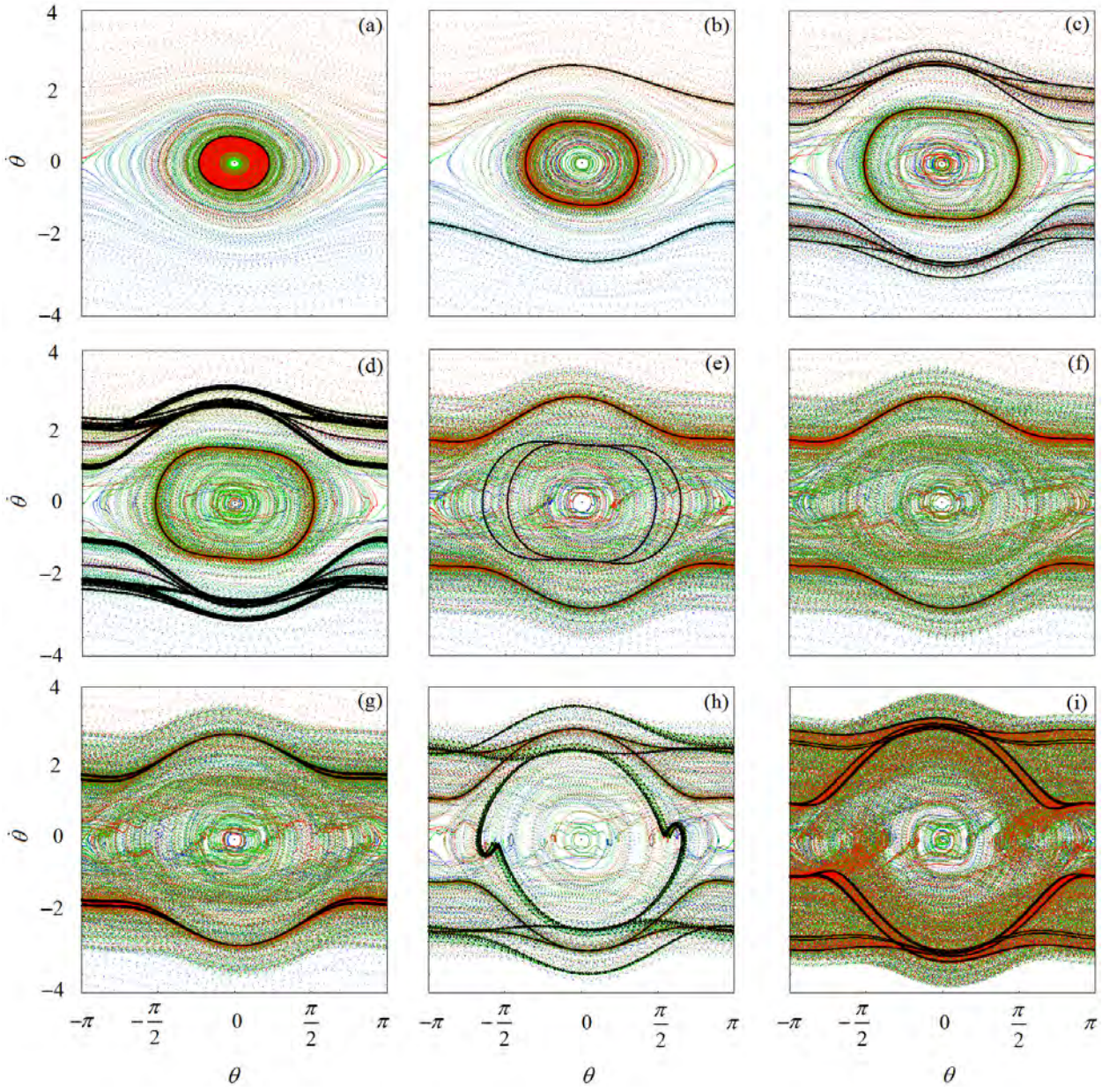


Figure 7. Sequence of the rotational responses, for $\omega = 2$, $\beta = 0.1$ and $\varphi = 0$. (a) $R = 0.250$; (b) $R = 0.450$; (c) $R = 0.900$; (d) $R = 0.945$; (e) $R = 1.329$; (f) $R = 1.331$; (g) $R = 1.350$; (h) $R = 1.550$; (i) $R = 1.750$;

It is worth noting that, between R = 1.331 and R = 1.810, and except for some small interference, rotations represent the only possible response of the pendulum.

4 CONCLUSIONS

This article aims to contribute to the development of pendulum systems for energy extraction from ocean waves. By means of numerical simulations, the dynamics of a parametric pendulum with multiple concentric masses, i.e. a *N*-pendulum, is addressed. The importance of such configuration lies in the need of reaching very low natural frequencies of the system, to mate with the excitation frequencies of the sea waves. The study is focused on how to achieve and maintain rotating motions of the *N*-pendulum, as period-1 rotations represent the most energetic motion of a pendulum.

A main conclusion of this work is that with a correct configuration of non-dimensional excitation and damping parameters, steady rotations can be easily reached and predicted. Such parameters are closely related to an adequate design of the pendulum harvester. Although damping parameters can be estimated in a relatively easy way, forcing parameters depend on sea wave motion and only can be bounded between certain limits, and statistically known. However, with an adequate design of the harvester, period-1 rotating attractors are robust against changes in excitation. In addition, for some specific combinations of the parameters, all initial conditions produce the most energetic rotating motion: a period-1 rotation. This is very interesting for energy harvesting because, theoretically, no external control action would be needed to reach rotating motion.

Energy harvesting by means of pendulum rotations is a very attractive idea because high amounts of energy could be recovered with simple and relatively small devices. The present work contributes to the knowledge on the field, but it is only a step aiming to understand the dynamics of the mechanical system in a simplified way. Further research is needed, including: active control of rotations to cope with variations of external forcing, optimization of the harvester devices for a maximum energy extraction, development of a suitable generator for the conversion of kinetic to electric energy, influence of the proper generator dynamics, influence of the synchronization phenomenon, and several others.

REFERENCES

[1] Wiercigroch, M., A new concept of energy extraction from waves via parametric pendulor. UK Patent Application, 2010.

[2] Yurchenko, D. y Alevras, P., Dynamics of the *N*-pendulum and its application to a wave energy converter concept. International Journal of Dynamics and Control, 1:290–299, 2013.

[3] Garira, W. y Bishop, S.R., Rotating solutions of the parametrically excited pendulum. Journal of Sound and Vibration, 263:233–239, 2007.

[4] Thompson, J., Stewart, H., Nonlinear dynamics and chaos. John Wiley & Sons, 2002.

[5] Clifford, M. y Bishop, S., Rotating periodic orbits of the parametrically excited pendulum. Physics Letters A, 201:191–196, 1995.

[6] Chow, T., Classical mechanics. John Wiley & Sons, 1995.

[7] Leven, R., Pompe, B., Wilke, C. y Koch, B., Experiments on periodic and chaotic motions of a parametrically forced pendulum. Physica D, 16:371–384, 1985.

[8] LeMéhauté, B., An introduction to hydrodynamics and water waves. Springer, 1976.

[9] Reguera, F., Dotti, F., Sosa, M. and Machado, S., Applicability of parametric *N*-pendulum wave energy converters in the Argentine Sea. To appear in Renewable Energy, 2019.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

On the Connection between Possibility Theory and Probability-box Theory in Structural Mechanics

Alex Dridger*, Ismail Caylak**, Rolf Mahnken***, Eduard Penner****

*Chair of Engineering Mechanics, Paderborn University, North rhine westphalia, Germany, **Chair of Engineering Mechanics, Paderborn University, North rhine westphalia, Germany, ***Chair of Engineering Mechanics, Paderborn University, North rhine westphalia, Germany, ****Chair of Engineering Mechanics, Paderborn University, North rhine westphalia, Germany

ABSTRACT

In many engineering applications the uncertainty quantification has become important in order to obtain authentic results. In general physical parameters are influenced by different types of uncertainty, where basically aleatory and epistemic types are distinguished. The first type is of intrinsic nature and may be described by stochastic methods based on randomness. The epistemic uncertainty, as the second type, arises due to a lack of knowledge. In practice, e.g. a safety assessment in the engineering sector both types of uncertainty occure simultaneously. Thus, in order to describe the corresponding uncertainty characteristic referred to as ``imprecise probability'' different techniques were introduced [1]. A commonly used approach in structural mechanics is called the probability-box (p-box) ansatz [2] using probability bound analysis capturing uncertain information with pairs of lower and upper distribution functions. Moreover, a possibilistic approach [3] based on the fuzzy set theory may be used in order to describe impresice probability using alpha-level discretization techniques. Compared to the first approach, the second one is rarely applied in structural mechanics. Furthermore, advocates of the p-box approach are criticizing the possibilitsitc approach and vice versa. This work examines both approaches in structural mechanics. For this, due to sparse available information, material parameters are characterized by imprecise probability. To this end, a p-box defined by two cumulative distribution functions and a possibility distribution comprising a family of probability distributions are generated. The probability bound analysis and the alpha-level discretization technique, respectively, are used to calculate a quantity of interest considering the sparse information of input material parameters. We investigate the relation between both approaches, e.g. that a p-box can be encoded by a pair of possibility distributions. Furthermore, the advantages and disadvantages are discussed extensively in order to understand why especially the possibility theory is rarely applied in the ingeneering sciences in contrast to, e.g. the computer sciences. Finally, our results are clarified in a numerical example. [1] Coolen F, Troffaes M, Augustin T. Imprecise probability 2011 (pp. 645-648), International encyclopedia of statistical science: Springer. [2] Traffaes M, Miranda E, Destercke S. On the connection between probability boxes and possibility measures. Information Sciences. 2013:224(Supplement C):88-108. [3] Dubois D, Prade H. Possibility theory and its applications: Where do we stand?. In: Kacprzyk J, Pedrycz W, eds. Springer handbook of computational intelligence. Berlin Heidelberg: Springer 2015 (pp. 31-60).

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Thermo-mechanical Behaviour of Fire Protected Steel Structures Using Coupled Multiphysics Finite Element Analysis

Georgios Drosopoulos*, Iksha Singh**, Siphesihle Motsa***, Georgios Stavroulakis****

*Structural Engineering and Computational Mechanics Group (SECM), University of KwaZulu-Natal, Durban, South Africa, **Structural Engineering and Computational Mechanics Group (SECM), University of KwaZulu-Natal, Durban, South Africa, ***Structural Engineering and Computational Mechanics Group (SECM), University of KwaZulu-Natal, Durban, South Africa, ****Computational Mechanics and Optimization Institute (COMECO), Technical University of Crete, Chania, Greece

ABSTRACT

A numerical modelling approach is proposed for the simulation of the structural performance of steel structures in fire conditions. Coupled, transient, temperature-displacement non-linear finite element analysis is used to describe the steel structure and passive fire protection (concrete/gypsum boards), under both thermal and mechanical loading. The main concept, which is under investigation in this work, is the consideration of the gradual damage of the passive fire protection due to fire conditions, on the evaluation of the structural performance of the steel structure. Both concrete and gypsum boards, are expected to develop cracks and fail at elevated temperatures, after a duration of the fire event. Delamination between boards and the structure may also appear. Then, their contribution to the fire protection is reduced or totally vanished. This work proposes a simple finite element modelling and analysis scheme, to take into account this gradual damage of the fire protection. Principles taken from contact mechanics are applied to the steel - protection interface, to account for thermal and mechanical contact. A standard fire (temperature – time) curve is considered to be the thermal loading of the structures under investigation. Mechanical loads varying linearly over the time, are considered simultaneously to thermal loads. Applications to simple structural elements (steel column-beam) and more complex systems (steel connection) are presented. Force-displacement diagrams are used to quantify the strength of the systems and compare the unprotected and the protected structures. Yielding of the considered structures, after each loading scenario and fire protection configuration, is recorded. Among the main concepts under investigation, are mentioned here the consideration of bi-axial loads and the application of fire loading in one or more surfaces of the unprotected and fire protected steel structures. The gradual loss of the fire protection under a fire event results in the drastic reduction of the strength of steel structures. This is quantified in the presented research. References 1. Arablouei, A., and Kodur, V. (2016a). “Effect of fire insulation delamination on structural performance of steel structures during fire following an earthquake or an explosion.” Fire Safety Journal, 84, 40-49. 2. Zografopoulou, K., and Mistakidis E. (2017). Numerical simulation of the behaviour of steel members with damaged SFRM fire protection coatings at elevated temperatures, EUROSTEEL 2017, September 13–15, Copenhagen, Denmark.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

An Accurate and Effective Local Average Contact Method

Guillaume Drouet*, Patrick Hild**, Mickaël Abbas***

*Electricité De France R&D;, **Mathematical Institute of Toulouse, Paul Sabatier University, ***Electricité De France R&D;

ABSTRACT

Finite element methods are often used to approximate the unilateral contact problems. Such problems show a nonlinear boundary condition, which roughly speaking requires that the solution u is non-positive on a part of the boundary of the domain ?. This nonlinearity leads to a weak formulation written as a variational inequality which admits a unique solution and the regularity of the solution shows limitations whatever the regularity of the data is. A consequence is that only finite element methods of order one and of order two are of interest. In this work we are interested in contact problems of two bodies whose respective meshes not coincide on the contact interface using finite element methods of order one and two in two and three space dimensions. In this case it is now known that the local node-on-segment contact conditions are not satisfactory in comparison with more global approaches inspired from the mortar domain decomposition method adapted to contact problems. But, these more global approaches are most of the time complicated to implement in a generic way in an industrial FEM software. The goal of this work is to define a local and develloper-friendly method that is as efficient as standard mortar approaches, the Local Average Contact (LAC) method. This approach handles in a local way the contact constraint by averaging locally on some well defined patches the jump of the normal displacement independently of the space dimension and of the degree and type of the finite elements. The LAC method can be seen as a Lagrange method in which the multiplier representing the contact pressure is piecewise constant independently of the degree (one or two) of the finite elements chosen for the displacements, this method then satisfies the inf-sup condition thanks to the definition of the local patches. In this work we show that the method provides optimal convergence results in the energy norm in the general case of non-matching meshes and therefore combines both the advantages of locality and accuracy and is as efficient as the original mortar approach. The locality is a key point to implement efficiently in a generic way on all elements the method on the targeted FEM software. We exhibit several numerical experiments, both academics and industrials, the results are obtained with the official implementation of the method in the open-source FEM software code_aster. The extension of the method to the contact-friction case is in progress.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Comparative Study of B-Spline- and Lagrange- FEM in Solving Acoustic Scattering Problems

Shaima Magdaline Dsouza*, Tahsin Khajah**, Stéphane P.A. Bordas***, Sundararajan Natarajan****

*Indian Institute of Technology Madras, Chennai, India, **University of Texas at Tyler, ***University of Luxembourg, Luxembourg, ****Indian Institute of Technology Madras, Chennai, India

ABSTRACT

We compare the performance of B-Spline- and Lagrange- Finite Element Methods in solving acoustic problems. The space truncation error is artificially excluded from the numerical solution by modifying the exact solutions. Hence, the numerical error is reflecting the pollution, and discretization errors and therefore a true indicator of the numerical performance. The comparison is performed based on the error per degree of freedom in low and high order analysis. The pollution error is studied by comparing the evolution of the numerical error for increasing frequencies in both methods. Then, the structure and the condition number of the resulted linear systems are compared to clarify the strength and weakness of each method.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Multiphysics Topology Optimization Using DCT-based Compression

Jianbin Du*, Pingzhang Zhou**, Zhenhua Lv***

*Tsinghua University, **Tsinghua University, ***Tsinghua University

ABSTRACT

Abstract Traditional topology optimization methods often need to deal with a large number of design variables equivalent to the number of finite elements analyzed, the quantity could be from a number of thousands to even hundreds of millions. The latter normally means that in order to obtain an effective design with enough details, a lot of computing resources need to be consumed [1], which increases to a great extent the cost of topology optimization in large-scale engineering applications. In this work, we developed a novel topology optimization method based on DCT (Discrete Cosine Transform) compression technique [2], which can greatly reduce the number of both the design variables and the computational scale of finite element analysis in topology optimization under the premise of maintaining a certain accuracy of optimization design. As one of the most popular transform technique in digital image compression, the DCT may effectively filter the high frequency components in a set of spatially distributed data without (or with very less) loss of the main characteristics of the data, which provides the solid foundation of the present method. Numerical examples on multiphysics designs including static, dynamic and thermal structural topology optimization are performed to validate the proposed method and show its advantage in improvement of computational efficiency of large scale designs. Interesting features of the present method and further possible development of the method in the future are discussed. Keywords: Multiphysics topology design; Discrete cosine transform; Computational efficiency; Finite element; High frequency filter; Acknowledgement The research is supported by NSFC (11772170, 11372154) which is gratefully acknowledged by the authors.
References [1] Niels Aage, Erik Andreassen, Boyan S. Lazarov & Ole Sigmund, Giga-voxel computational morphogenesis for structural design, Nature. 2017, 550: 84–86. [2] P. Zhou, J. Du, Z. Lu, Highly efficient density-based topology optimization using DCT-based digital image compression, Structural and Multidisciplinary Optimization. 2018, 57: 463-467.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Comparison between Truncation and Stabilizing Error in Multiphase Moving Particle Semi-implicit Method Based on Corrective Matrix

Guangtao Duan*, Seiichi Koshizuka**, Akifumi Yamaji***, Bin Chen****

*Department of Systems Innovation, The University of Tokyo, 7-3-1, Hongo, Bunkyo-ku, Tokyo 113-8656, Japan, **Department of Systems Innovation, The University of Tokyo, 7-3-1, Hongo, Bunkyo-ku, Tokyo 113-8656, Japan, ***Cooperative Major in Nuclear Energy, Graduate School of Advanced Science and Engineering, Waseda University, Tokyo 169-8555, Japan, ****State Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University, Xi'an 710049, PR China

ABSTRACT

The moving particle semi-implicit (MPS) method has great advantages in simulating free surface, multiphase and fluid-solid interaction flows owing to its Lagrangian nature. However, the Lagrangian motion of particles also brings two challenges: the anisotropic particle distribution and the particle clumping. The former can decrease the accuracy of original MPS models and cause some random discretization error. The corrective matrix is effective to reduce such error to the level of truncation error. The latter can trigger instability easily due to particles' continuous approaching and thus some adjustment strategies for stability have to be adopted, thereby resulting in stabilizing error. The purpose of this paper is to compare the relative magnitude of the truncation and stabilizing error, which is of great significance to understand the reliability as well as capability of particle methods and further to compensate discrepancy. Due to the difficulty in separating different kinds of error from total error in dynamic simulations, an indirect approach is developed for the comparison. The basic idea is to check whether significant decline of the total error takes place after the truncation error is further reduced by high-order schemes. First, new discretization schemes based on second order corrective matrix (SCM) are proposed for MPS to reduce the truncation error further. Second, the SCM schemes are coupled with the our previous MMPS methods and stabilizing strategies. Then, various typical free-surface/multiphase flows, including Taylor-Green vortex, excited pressure oscillation flow, elliptical drop deformation and bubble rising flow, are simulated to test the variance of total error between using the FCM (first order corrective matrix) and SCM schemes. It is found that the SCM schemes did not remarkably reduce the total error, implying that the stabilizing error is dominant compared to the truncation error. Therefore, reducing the error due to stabilizing strategies is of more significance to reduce the total error.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Consistent Element-free Galerkin Method for Crack Growth

Qinglin Duan*, Xin Gao**, Zeyang Feng***, Xikui Li****

*Dalian University of Technology, **Dalian University of Technology, ***Dalian University of Technology, ****Dalian University of Technology

ABSTRACT

Prediction of material failure by fracture is of major concern in many engineering problems. In the past decades, several types of computational methods have been developed to model fracture. Among them, the element-free Galerkin (EFG) method [1] is one of the major methods developed for this purpose at the earliest stage. In comparison with the traditional finite element method, EFG is more convenient to construct high order approximation and to implement h-adaptive computations. This provides certain advantages in numerical modelling of cracks. However, the EFG method is computational inefficient since a large number of integration points is required and even worse, it is not able to exactly pass patch tests. In recent years, Duan et al. [2] developed an improved EFG method by correcting nodal derivatives at quadrature points based on the Hu-Washizu three-field variational principle. The number of integration points is significantly reduced, whereas the solution accuracy and convergence are greatly improved. This leads to a significant increase in computational efficiency. In particular, the method is able to exactly pass patch tests in a consistent manner and thus it is named as consistent element-free Galerkin (CEFG) method. In addition, the method can obtain very accurate stress fields. This work extends the CEFG method to crack problems in which the accuracy of stress solutions is crucial. Background integration mesh is used to describe cracks geometrically. The description of the discontinuity in displacement at cracks is based on the phantom node method [3] which does not need to add additional nodal degrees of freedom. The algorithm to introduce the phantom nodes and the method to evaluate the domain integral in cracked “element” are proposed. Numerical results show that the developed method is able to exactly pass the discontinuous patch test and to accurately predict crack paths. Adaptive refinement at the tip of extending cracks is also presented. References 1. Belytschko T, Lu YY, Gu L. Element-free Galerkin methods. International Journal for Numerical Methods in Engineering 1994; 37:229–256. 2. Duan QL, Gao X, Wang BB et.al. Consistent element-free Galerkin method. International Journal for Numerical Methods in Engineering 2014; 99:79–101. 3. Song JH, Areias Pedro M. A. and Belytschko T. A method for dynamic crack and shear band propagation with phantom nodes. International Journal for Numerical Methods in Engineering 2006; 67:868–893.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Hierarchical Non-Intrusive Algorithm for the Generalized Finite Element Method

Armando Duarte*, Travis Fillmore**

*University of Illinois at Urbana-Champaign, **University of Illinois at Urbana-Champaign

ABSTRACT

An algorithm for non-intrusively coupling a commercial finite element software with a research code implementing a hierarchical enrichment of finite element spaces is presented. Examples of hierarchical methods supported by the algorithm are the Generalized or eXtended FEM (GFEM), the scale-bridging GFEM with numerically defined enrichment functions (GFEMgl), and the p-version of the FEM. The proposed Hierarchical Non-Intrusive Algorithm (HNA) combines the vast library of classical elements available in commercial FEM platforms with the ability of the GFEMgl to analyze localized phenomena like cracks and spot welds, on coarse meshes. The algorithm does not require iterations between the standard and Generalized FEM platforms and is simple to implement. Examples showing the application of the HNA to the coupling of Abaqus with a 3-D GFEMgl software are presented. They also demonstrate the benefits of combining finite elements available only in a commercial platform with a GFEM.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Framework Design Methodology and Experience with FLASH

Anshu Dubey*

*Argonne National Laboratory

ABSTRACT

Scientific software used for simulation of complex multiphysics phenomena has many characteristics that make it uniquely challenging to architect and maintain. The models being computed have multiple operators which can have diverse requirements from the system hardware and software. Often the operator requirements are at cross-purpose with one another, where what is good for one is bad for another. Similarly, data structures and data layout that are optimal for one operator need not be the best for another. Additionally, there exists a positive feedback loop between scientific understanding and more demands on both simulation software and system resources needed to run the simulations. Greater understanding leads to higher fidelity models that usually imply greater diversity in methods and solvers used, and/or greater resolution, which implies more resources being utilized. The key framework design elements in face of such complexity are separation of concerns, and a collection of encapsulated building blocks that interoperate with one another through well defined interfaces. These two basic elements of design philosophy have been deployed in most successful multiphysics codes such as FLASH, Uintah, Amber, NWChem and many others. These codes have served their respective scientific communities for a decade or more, and have even branched out to serve other communities. We use FLASH as an example to illustrate how these basic design principles have resulted in an extensible framework that has been exploited by several research communities to adopt FLASH for their own use. FLASH is a composable, multiphysics, multiscale simulation software with a large and varied international user base in several research communities. FLASH was originally developed for simulating thermonuclear runaways in astrophysics. It has undergone three major version revisions, and a fourth one is underway to prepare the code for the forthcoming heterogeneity in platforms. This presentation will highlight the challenges in maintaining separation of concerns during various revisions to the code all the way to the current ongoing revision, and the corresponding variations in our approach to framework design.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

On the Performance of the Numerical Manifold-based Mass Lumping Scheme in Comparison to Standard Diagonalization Methods

Sascha Duczek*, Hauke Gravenkamp**

*Otto von Guericke University Magdeburg, **University of Duisburg-Essen

ABSTRACT

The application of explicit time integration schemes is an indispensable prerequisite for solving highly dynamic problems such as wave propagation or impact events. However, to fully harness the advantages of explicit time stepping algorithms, the mass matrix needs to be in diagonal form. This can be achieved by a variety of different methods known as mass lumping techniques [1]. The row sum technique is an intuitive procedure where all components of a row of the mass matrix are summed, and the result is placed on the main diagonal. In the context of Serendipity-type finite elements, this approach is unfortunately only viable for nodal-based linear shape functions. Otherwise negative components arise which have detrimental effects on the solution of transient problems. Here, an impaired convergence or even a divergence of the results is observed. Another heuristic approach proposed by Hinton, Rock, and Zienkiewicz is the HRZ method (diagonal scaling) [2]. This technique guarantees positive entries on the main diagonal of the mass matrix but is still only applicable to (higher order) nodal-based shape functions. A mathematically appealing approach to mass lumping is the so-called nodal quadrature technique also referred to as optimal lumping [1]. This method can be deployed in connection with tensor product shape functions defined on Gauß-Lobatto-Legendre (GLL) or Chebyshev-Gauß-Lobatto (CGL) points. Considering a trunk space formulation (Serendipity-type finite elements) of higher order finite elements, the optimal lumping scheme is not applicable as it is generally not possible to construct an integration rule of the required accuracy that guarantees positive weighting. Therefore, a different mass lumping scheme based on the numerical manifold method has recently been proposed. It is important to note that also in this case mass lumping is only applicable to nodal shape functions. Considering modal or hierarchic shape functions, a diagonal mass matrix is physically meaningless and leads to an impaired convergence of the results. In the present contribution, all properties of this method are discussed and its performance is compared to the aforementioned conventional mass lumping methods. Guidelines on the recommended use of each method are then derived from the numerical results. References [1] Cook, R. D.; Malkus, D. S. & Plesha, M. E. Concepts and Applications of Finite Element Analysis, John Wiley & Sons, 1989 [2] Hinton, E.; Rock, T. & Zienkiewicz, O. C. A Note on Mass Lumping and Related Processes in the Finite Element Method, Earthquake Engineering and Structural Dynamics, 1976, 4, 245-249

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22–27, 2018, New York City, NY, USA

DIRECT COMPUTATION OF ABSORBING BOUNDARY CONDITIONS AT THE DISCRETE LEVEL

D. DUHAMEL*

*Laboratoire Navier, Ecole des Ponts ParisTech,
IFSTTAR, CNRS, UPE, UMR 8205, Champs-sur-Marne, France

Key words: Finite Element, absorbing boundary, wave, Helmholtz equation, discrete method

Abstract. The calculation of wave radiation in exterior domains by finite element methods can lead to large computations. A large part of the exterior domain is meshed and this computational domain is truncated at some distance where local or global boundary conditions are imposed at this artificial boundary. These conditions at finite distance must simulate as closely as possible the exact radiation condition at infinity and are generally obtained by discretizing an operator on the boundary.

Here, we propose a different approach, still based on the finite element method. Instead of finding an absorbing operator and then discretizing it, we will estimate the absorbing operator directly at the discrete level and build a sparse matrix approximating the absorbing condition. This discrete absorbing matrix is added to the dynamic stiffness matrix of the problem which is then solved in a classical way. The problem is considered for acoustics in the frequency domain and is described by the Helmholtz equation. The coefficients of the absorbing matrix are found from the solutions of small size linear systems for each node on the radiating boundary. This is done using a set of radiating functions for which a boundary condition is written. The precision of the method is estimated from the number of functions in the test set and from the number of coefficients allowed in the sparse matrix. Finally, some examples are computed to validate the method.

1 INTRODUCTION

Solving the Helmholtz equation in unbounded domains is important in many problems of mechanics and physics, for instance for the acoustic radiation or the diffraction around a body immersed in a fluid. Using the finite element method to solve the problem, one has to define a finite truncated domain on which the solution should be as close as possible to the solution on the unbounded domain. For this, it is necessary to define a boundary condition at the exterior of this truncated domain. These conditions at finite distance must simulate as closely as possible the exact radiation condition at infinity. This boundary condition could be global or local depending if all the degrees of freedom on the boundary are connected or if a given node is only coupled to a limited number of nodes around it. Among the global approaches we find the Dirichlet to Neumann (DtN)

proposed by [1, 2], or the boundary element method described in many classical textbooks like [3, 4, 5]. Both methods lead to full matrices and generate heavy computations.

In local methods, on the contrary, the condition at a boundary node involves only a limited number of neighbouring nodes. They can be classified into mainly three sets: those involving only the degrees of freedom of the domain, those with additional degrees of freedom at nodes on the boundary and those with an additional domain. Concerning the absorption conditions which do not involve additional variables or domains, a first possibility is using infinite elements as proposed by [6, 7, 8, 9]. These are elements extending at infinity and satisfying the Sommerfeld radiation condition. However, it needs the development of special elements based on functions with outwarding propagation wave-like behaviour in the radial direction. Other absorbing boundary conditions involving differential operators of different orders on the boundary were proposed by different authors [10, 11, 12]. These relations were improved by Bayliss and Turkel [13, 14] using sequences of local non-reflecting boundary conditions in spherical and cylindrical coordinates. However, all these conditions are difficult to implement above the second order because of the high order derivatives involved in their formulations. More efficient boundary conditions can be obtained by the addition of variables on the exterior surface such as in [15, 16]. They involve only second derivatives of the auxiliary variables and so can be efficiently implemented. Surrounding the computational domain by absorbing layers was also proposed by [17, 18] with the perfectly matched layer in which the wave equation is analytically continued into complex coordinates. This however can add a non negligible number of degrees of freedom to the problem and the optimal parameters in the absorbing layer are not so easy to find.

Most of the previous absorbing boundary conditions are written at the continuous level, but it can be interesting to write them at the discrete level. For instance, boundary conditions at the discrete level using the properties of periodic media were proposed by [19]. In [20] boundary conditions based on the PLM were written after discretisation of the equations and were found to be more efficient than their continuous versions. Such a discrete approach is used in this paper. The following section presents the problem formulation and the building of the discrete absorbing matrix. Then some examples are presented before the conclusion.

2 PROBLEM FORMULATION

2.1 Helmholtz equation

We consider the two-dimensional acoustic equation in the frequency domain in the exterior Ω_e of a bounded domain Ω_i of boundary Γ_i, see Fig.1. The Helmholtz equation with a Neumann boundary condition on Γ_i and a radiation condition at infinity is

$$\begin{aligned} \Delta p + k^2 p &= f \quad on\ \Omega_e \\ \frac{\partial p}{\partial n} &= g \quad on\ \Gamma_i \\ \frac{\partial p}{\partial r} - ikp &= o(\frac{1}{\sqrt{r}})\ when\ r \to \infty \end{aligned} \tag{1}$$

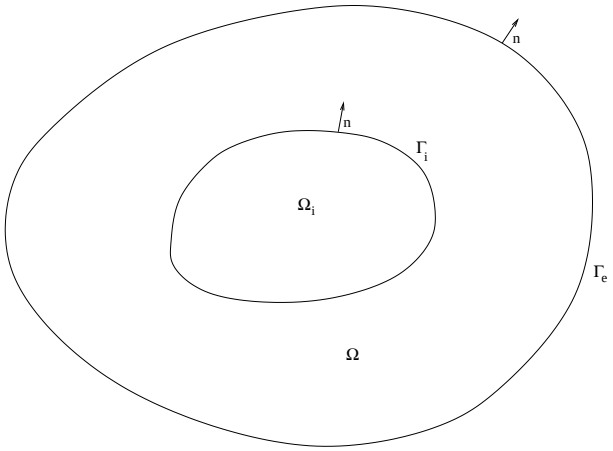


Figure 1: Exterior domain.

with f and g given functions representing the sources in the domain and at the boundary. The domain Ω_e is truncated at some finite distance by the boundary Γ_e and the discrete problem is posed on the bounded domain Ω located between the surfaces Γ_e and Γ_i. Its variational formulation is

$$\int_\Omega (\Delta p + k^2 p) q dx = \int_\Omega f q dx \tag{2}$$

$$-\int_{\Gamma_i} \frac{\partial p}{\partial n} q ds + \int_{\Gamma_e} \frac{\partial p}{\partial n} q ds + \int_\Omega (-\nabla p.\nabla q + k^2 pq) dx = \int_\Omega f q dx \tag{3}$$

with q a test function and the exterior normals n on surfaces Γ_i and Γ_e. One assumes that the absorbing boundary condition can be written on the surface Γ_e as

$$\frac{\partial p}{\partial n} = Ap \tag{4}$$

where A is an operator acting on the pressure p inside Ω. So the variational formulation is now

$$\int_{\Gamma_e} (Ap) q ds + \int_\Omega (-\nabla p.\nabla q + k^2 pq) dx = \int_\Omega f q dx + \int_{\Gamma_i} \frac{\partial p}{\partial n} q ds \tag{5}$$

2.2 Discretisation of the absorbing operator

The absorbing operator is such that

$$\begin{aligned} \int_{\Gamma_e} \frac{\partial p}{\partial n}(s) q(s) ds &= \int_{\Gamma_e} (Ap)(s) q(s) ds \\ &= \int_{\Gamma_e} \int_\Omega A(s,x) p(x) q(s) dx ds \end{aligned} \tag{6}$$

The discrete form can be written as

$$\mathbf{M}^s \mathbf{q} = \mathbf{M}^s \mathbf{A} \mathbf{M}^v \mathbf{p} \tag{7}$$

with

$$\begin{aligned} M^s_{lj} &= \int_{\Gamma_e} N^s_l(s) N^s_j(s) ds \\ M^v_{im} &= \int_{\Omega} N^v_i(x) N^v_m(x) dx \end{aligned} \tag{8}$$

$\mathbf{q}$ is the vector of the normal derivatives of the pressure at the nodes of Γ_e and $\mathbf{p}$ the vector of the pressures at nodes in Ω. N^s and N^v are the usual interpolation functions on the boundary and in Ω respectively. Finally the vectors $\mathbf{p}$ and $\mathbf{q}$ are linked by

$$\mathbf{q} = \mathbf{A}\mathbf{M}^v\mathbf{p} \tag{9}$$

and one has to identify the matrix $\mathbf{AM}^v$.

2.3 Determination of the absorbing matrix

The solution of the problem can be expanded as

$$p(r,\theta) = \sum_{-\infty}^{+\infty} a_n H_n(kr) e^{in\theta} \tag{10}$$

The completeness of the expansion on the boundary was proved by [21, 22, 23]. One now has to find an approximation of the matrix $\tilde{\mathbf{A}} = \mathbf{AM}^v$. One looks for a discrete operator acting on the pressure at nodes inside Ω such that the matrix $\tilde{\mathbf{A}}$ is sparse and the relation (9) is satisfied for outgoing waves.

For a node i at point $\mathbf{x}_i$ on the boundary, one considers nodes i_j at points $\mathbf{x}_{i_j}$ in Ω with $j = 1...n_i$ in the neighborhood of $\mathbf{x}_i$ and such that $\mathbf{x}_{i_1} = \mathbf{x}_i$. So the line i of the matrix $\tilde{\mathbf{A}}$ will have non zero coefficients only at nodes i_j. To find these coefficients, one writes equation (9) for Hankel functions of different orders n. Choosing a point $\mathbf{o}$ interior to Ω_i, one should have

$$\frac{\partial}{\partial n_i}(H_n(k|\mathbf{x}_i - \mathbf{o}|)e^{in\theta_i}) = \sum_{j=1...n_i} a^i_j (H_n(k|\mathbf{x}_{i_j} - \mathbf{o}|)e^{in\theta_{i_j}}) \tag{11}$$

for $-N \leq n \leq N$ and n_i the exterior normal at node i. Denoting the vectors

$$\mathbf{f}_i = \begin{bmatrix} \frac{\partial}{\partial n_i}(H_{-N}(k|\mathbf{x}_i - \mathbf{o}|)e^{-iN\theta_i}) \\ ... \\ \frac{\partial}{\partial n_i}(H_0(k|\mathbf{x}_i - \mathbf{o}|) \\ ... \\ \frac{\partial}{\partial n_i}(H_N(k|\mathbf{x}_i - \mathbf{o}|e^{iN\theta_i})) \end{bmatrix} \quad and \quad \mathbf{a}_i = \begin{bmatrix} a^i_{i_1} \\ ... \\ a^i_{i_{n_i}} \end{bmatrix} \tag{12}$$

and the matrix

$$\mathbf{H}_i = \begin{bmatrix} H_{-N}(k|\mathbf{x}_{i_1} - \mathbf{o}|)e^{-iN\theta_{i_1}} & ... & H_{-N}(k|\mathbf{x}_{i_{n_i}} - \mathbf{o}|)e^{-iN\theta_{i_{n_i}}} \\ ... & & ... \\ H_0(k|\mathbf{x}_{i_1} - \mathbf{o}|) & ... & H_0(k|\mathbf{x}_{i_{n_i}} - \mathbf{o}|) \\ ... & & ... \\ H_N(k|\mathbf{x}_{i_1} - \mathbf{o}|)e^{iN\theta_{i_1}} & ... & H_N(k|\mathbf{x}_{i_{n_i}} - \mathbf{o}|e^{iN\theta_{i_{n_i}}} \end{bmatrix} \tag{13}$$

Relation (11) can be put under the form

$$\mathbf{f}_i = \mathbf{H}_i \mathbf{a}_i \tag{14}$$

Its solution is

$$\mathbf{a}_i = (\mathbf{H}_i^* \mathbf{H}_i)^{-1} \mathbf{H}_i^* \mathbf{f}_i \tag{15}$$

with * denoting the hermitian transpose of a matrix. The vector $\mathbf{a}_i$ gives the ith line of the matrix $\tilde{\mathbf{A}}$. Considering these relations for all nodes at the boundary, one gets the sparse matrix $\tilde{\mathbf{A}}$ describing an approximate absorbing boundary condition on Γ_e.

The discretisation of the other parts of the variation formulation (5) leads to the final discrete equation.

$$(\mathbf{K} - \tilde{\mathbf{A}} - k^2 \mathbf{M})\mathbf{p} = \mathbf{f} \tag{16}$$

which can be solved by classical solvers.

3 NUMERICAL EXAMPLES

3.1 Test problem

As example we consider an annular domain limited by an interior circle of radius $0.15m$ and an exterior circle of radius $0.3m$ (see Fig.2). The sound velocity is $c = 340m/s$. A boundary condition is defined at the interior circle as the normal derivative of the sound pressure generated by a point source located at point $\mathbf{x}_s = (0.1, 0)$ and is given by

$$q(\mathbf{x}) = -\frac{ik}{4} \frac{\mathbf{n}.(\mathbf{x} - \mathbf{x_s})}{|\mathbf{x} - \mathbf{x_s}|} H_1(k|\mathbf{x} - \mathbf{x_s}|) \tag{17}$$

with $\mathbf{x}$ the position of a node on the interior boundary and $\mathbf{x_s}$ the position of the point source. The analytical solution is given by

$$p(\mathbf{x}) = \frac{i}{4} H_0(k|\mathbf{x} - \mathbf{x_s}|) \tag{18}$$

and will be compared to various numerical solutions.

We define the errors e_g on the whole domain Ω and e_b on the exterior boundary Γ_e by

$$\begin{aligned} e_g^2 &= \frac{\sum_{i \ node \ on \ \Omega} |p_i^{num} - p_i^{ana}|^2}{\sum_{i \ node \ on \ \Omega} |p_i^{ana}|^2} \\ e_b^2 &= \frac{\sum_{i \ node \ on \ \Gamma_e} |p_i^{num} - p_i^{ana}|^2}{\sum_{i \ node \ on \ \Gamma_e} |p_i^{ana}|^2} \end{aligned} \tag{19}$$

with the superscripts ana and num denoting respectively the analytical and numerical solutions.

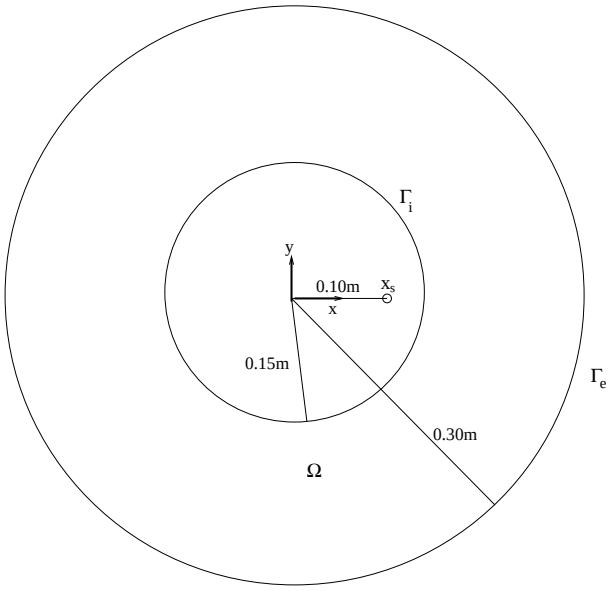


Figure 2: Annular domain.

3.2 Influence of different parameters

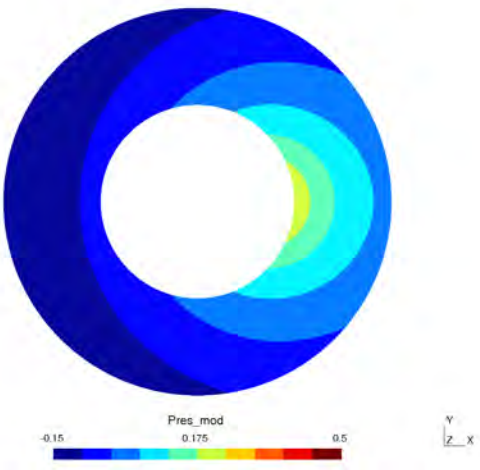
We begin by estimating the influence of the truncation order N on the error. In Fig.3 four solutions are plotted. The first one is obtained with the crude boundary condition $\frac{\partial p}{\partial n} = ikp$ (denoted as the ik solution), two solutions are obtained by the present method with respectively $N = 0$ and $N = 1$ and the last one is the analytical solution for the frequency $100Hz$. These solutions are obtained by taking $n_i = 20$ coefficients for each boundary node in the building of the matrix $\tilde{A}$. As can be seen the ik solution leads to large errors while the solutions with the present method lead to rather good solutions even for the simplest one with $N = 0$. The numerical errors are given in table 1 with similar conclusions.

condition	global error	boundary error
ik	0.837	0.956
N=0	0.059	0.078
N=1	0.003	0.005

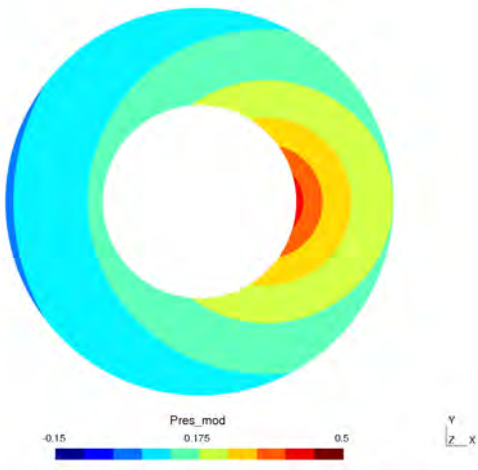
Table 1: Errors for the different boundary condition at 100Hz

In Fig.4 the solution is plotted versus the number of points n_i used to build $\tilde{A}$ with $N = 1$. Using $n_i = 2$ is clearly not enough. However, one can see that $n_i = 5$ gives a rather good solution which is still improved by using more points. Numerical values are given in table 2.

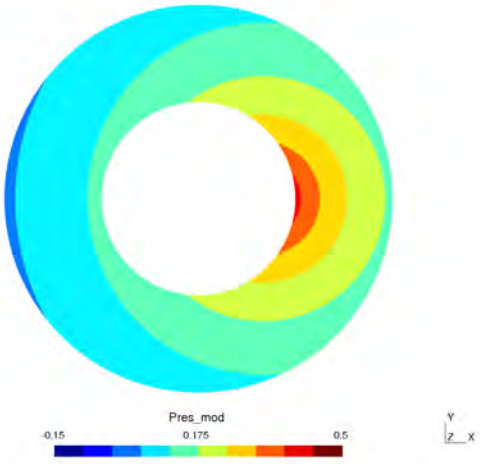
Finally Fig.5 compares the analytical solutions and the numerical ones for different frequencies. Only $n_i = 2$ points are used which leads to crude estimates. While the



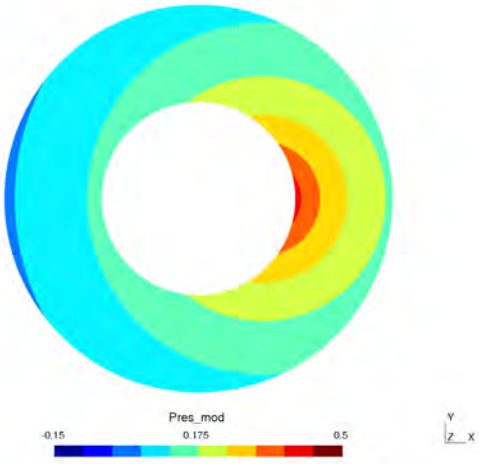
(a) ik boundary condition



(b) N=0



(c) N=1



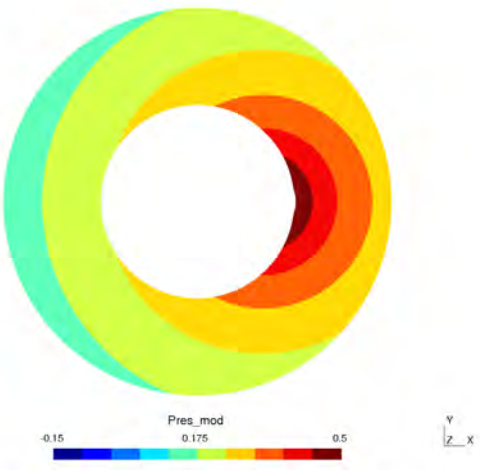
(d) Analytical solution at 100Hz

Figure 3: Comparison of solutions at 100Hz

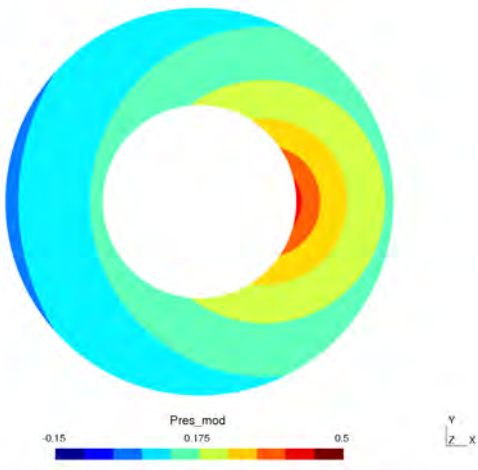
solution at $100Hz$ shows important errors, the results at $300Hz$ and $1000Hz$ are much better. This shows that the condition is more efficient as the frequency increases as for other absorbing boundary conditions.

4 CONCLUSION

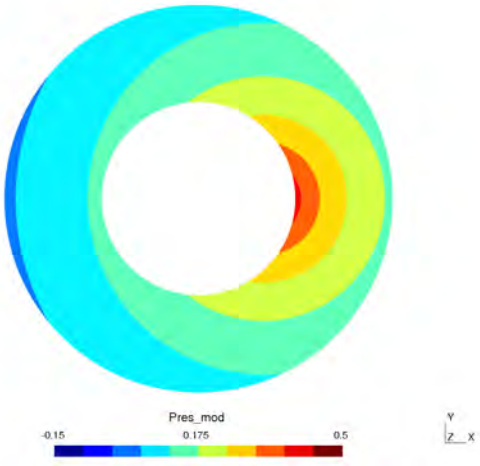
A new numerical method has been presented for computing absorbing boundary conditions for the Helmholtz equation. It builds a discrete absorbing matrix directly from



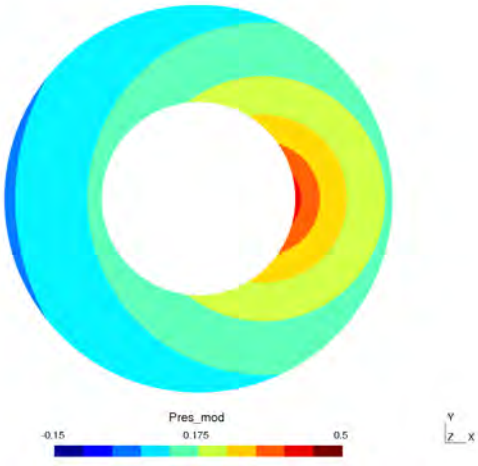
(a) $n_i = 2$



(b) $n_i = 5$



(c) $n_i = 10$



(d) $n_i = 20$

Figure 4: Solutions for different numbers of nodes used to define the matrix $\tilde{A}$

the finite element discretisation of the problem. This can be applied to any shape and does not require additional variables or additional domains. So the number of degrees of freedom is the same as for the problem without absorbing boundary conditions. Examples show the accuracy of the method. Similar approaches could be used for other wave propagation problems such as for the propagation of elastic waves. Future works will include comparisons with other classical absorbing boundary conditions and the consideration of more complex domains such as domains with corners.

Number of nodes	global error	boundary error
$n_i = 2$	0.459	0.522
$n_i = 5$	0.010	0.013
$n_i = 10$	0.005	0.006
$n_i = 20$	0.003	0.005

Table 2: Error for different numbers of nodes used to build the matrix $\tilde{A}$

REFERENCES

[1] J.B. Keller and D. Givoli. Exact non-reflecting boundary conditions. *Journal of computational physics*, 82(1):172–192, 1989.

[2] D. Givoli and J.B. Keller. A finite element method for large domains. *Computer Methods in Applied Mechanics and Engineering*, 76(1):41–66, 1989.

[3] C.A. Brebbia and S. Walker. *Boundary Element Techniques in Engineering*. Newnes-Butterworths, 1980.

[4] R.D. Ciskowski and C.A. Brebbia. In *Boundary element methods in acoustics*. Computational mechanics publications, Elsevier Applied Sciences, 1991.

[5] M. Bonnet. *Boundary Integral Equation Methods for Solids and Fluids*. John Wiley and Sons, 1995.

[6] P. Bettess. Infinite elements. *International Journal for Numerical Methods in Engineering*, 11(1):53–64, 1977.

[7] P. Bettess. *Infinite Elements*. Penshaw Press, 1992.

[8] D.S. Burnett. A three-dimensional acoustic infinite element based on a prolate spheroidal multipole expansion. *Journal of the Acoustical Society of America*, 96:2798–2816, 1994.

[9] R.J. Astley. Infinite elements for wave problems: a review of current formulations and an assessment of accuracy. *International Journal for Numerical Methods in Engineering*, 49(7):951–976, 2000.

[10] B. Engquist and A. Majda. Absorbing boundary conditions for numerical simulation of waves. *Proceedings of the National Academy of Sciences*, 74(5):1765–1766, 1977.

[11] R. Clayton and B. Engquist. Absorbing boundary conditions for acoustic and elastic wave equations. *Bulletin of the Seismological Society of America*, 67(6):1529–1540, 1977.

[12] A. C. Reynolds. Boundary conditions for the numerical solution of wave propagation problems. *Geophysics*, 43(6):1099–1110, 1978.

[13] A. Bayliss and E. Turkel. Radiation boundary conditions for wave-like equations. *Communications on Pure and Applied Mathematics*, 33(6):707–725, 1980.

[14] A. Bayliss, M. Gunzburger, and E. Turkel. Boundary conditions for the numerical solution of elliptic equations in exterior regions. *SIAM Journal on Applied Mathematics*, 42(2):430–451, 1982.

[15] F. Collino. High-order absorbing boundary conditions for wave propagation models. straight line boundary and corner cases. In *Proc. 2nd Int. Conf. on Mathematical & Numerical Aspects of Wave Propagation, R. Kleinmanet al.SIAM*, pages 161–171, Delaware, USA, 1993.

[16] T. Hagstrom and S.I. Hariharan. A formulation of asymptotic and exact boundary conditions using local operators. *Applied Numerical Mathematics*, 27(4):403 – 416, 1998.

[17] J.P. Berenger. A perfectly matched layer for the absorption of electromagnetic waves. *Journal of computational physics*, 114(2):185–200, 1994.

[18] J.P. Berenger. Three-dimensional perfectly matched layer for the absorption of electromagnetic waves. *Journal of computational physics*, 127(2):363–379, 1996.

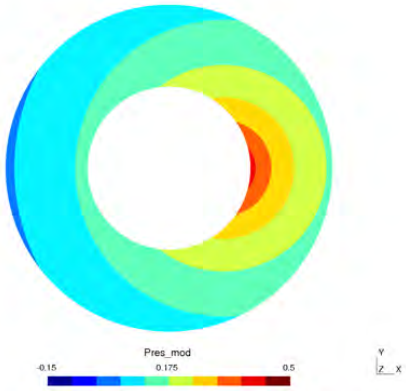
[19] D. Duhamel and T.M. Nguyen. Finite element computation of absorbing boundary conditions for time-harmonic wave problems. *Computer Methods in Applied Mechanics and Engineering*, 198(37):3006–3019, 2009.

[20] S. Thirunavukkarasu and M.N. Guddati. Absorbing boundary conditions for time harmonic wave propagation in discretized domains. *Computer Methods in Applied Mechanics and Engineering*, 200(33):2483 – 2497, 2011.

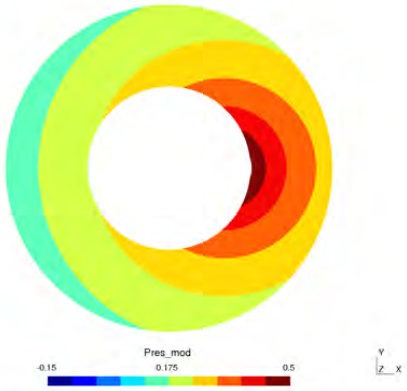
[21] D. Colton. Runges theorem and far field patterns for the impedance boundary value problem in acoustic wave propagation. *SIAM Journal on Mathematical Analysis*, 13(6):970–977, 1982.

[22] R.F. Millar. On the completeness of sets of solutions to the helmholtz equation. *IMA Journal of Applied Mathematics*, 30(1):27–37, 1983.

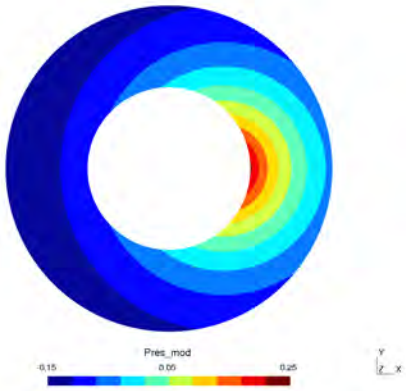
[23] Y. Liu and J.S. Bolton. On the completeness and the linear dependence of the cartesian multipole series in representing the solution to the helmholtz equation. *The Journal of the Acoustical Society of America*, 140(2):EL149–EL153, 2016.



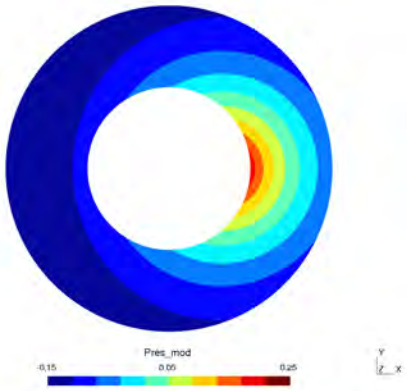
(a) Analytical solution 100Hz



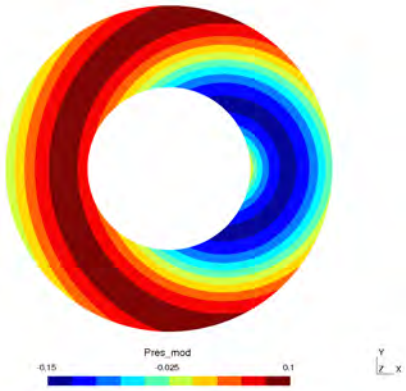
(b) Numerical solution 100 Hz



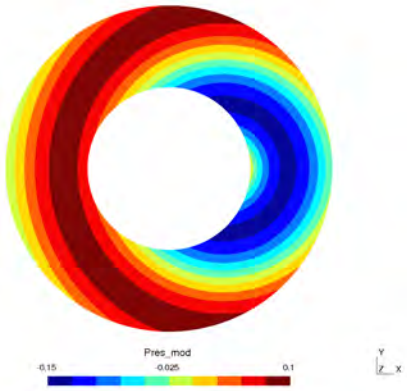
(c) Analytical solution 300Hz



(d) Numerical solution 300 Hz



(e) Analytical solution 1000Hz



(f) Numerical solution 1000 Hz

Figure 5: Solutions for different frequencies

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Microstructural Origins of Fatigue Crack Nucleation

Fionn Dunne*, Bo Chen**, Jun Jiang***

*Imperial College, **Imperial College, ***Imperial College

ABSTRACT

An integrated experimental, characterization and computational crystal plasticity study of cyclic plastic beam loading has been carried out for nickel single crystal (CMSX4), oligocrystal (MAR002) and polycrystal alloys in order to assess quantitatively the mechanistic drivers for fatigue crack nucleation. The experimentally validated modelling provides knowledge of key microstructural quantities (accumulated slip, stress and GND density [1]) at experimentally observed fatigue crack nucleation sites and it is shown that while each of these quantities is potentially important in crack nucleation, none of them is in its own right is sufficient to be predictive. However, the local (elastic) stored energy density, measured over a length scale determined by the density of GNDs, has been shown to predict crack nucleation sites in the single and oligocrystal tests. In addition, once primary nucleated cracks develop and are represented in the crystal model, the stored energy correctly identifies where secondary fatigue cracks are observed to nucleate in experiments [2]. This (Griffith-Stroh type) quantity also correctly differentiates and explains intergranular and transgranular fatigue crack nucleation. Further, for the polycrystal containing an oxide agglomerate, multiple crack nucleations occurred at the nickel matrix-inclusion interface and both nucleation and growth were found to be crystallographic with highest slip system activation driving crack direction. Local slip accumulation was found to be a necessary condition for crack nucleation, and that in addition, local stress and density of geometrically necessary dislocations are involved. Fatemi-Socie and dissipated energy were also assessed against the experimental data, showing generally good, but not complete agreement. However, the local stored energy density (of a Griffith-Stroh kind) identified all the crack nucleation sites as those giving the highest magnitudes of stored energy. [1] Yongjun Guan, Bo Chen, Jinwen Zhou, Ben Britton, Jun Jiang, Fionn Dunne. Crystal Plasticity Modelling and HR-DIC Measurement of Slip Activation and Strain Localisation in Single and Oligo-crystal Ni Alloys under Fatigue. Intl. Jnl. Plasticity. 88, 70-88, 2017. [2] Bo Chen, Jun Jiang, Fionn Dunne. Microstructurally-sensitive fatigue crack nucleation in Ni-based single and oligo crystals. Jnl. Mech. Phys. Solids. 106, 15-33, 2017. [3] Bo Chen, Jun Jiang, Fionn Dunne. Is Stored Energy Density the Primary Meso-scale Mechanistic Driver for Fatigue Crack Nucleation? Intl. Jnl. Plas. 101, 213-229, 2018.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Data-Driven and Reduced Order Modeling : An Attempt at a Taxonomy of Problems and Approaches

Karthik Duraisamy*

*University of Michigan, Ann Arbor

ABSTRACT

With the growing interest in data-driven and reduced order modeling approaches, there is a pressing need to classify different problem formulations and approaches using a consistent language. Since this field is inherently multi-disciplinary, even the use of basic terms tend to be confusing and often misused. In this talk, an attempt is made at establishing a taxonomy of approaches in data-driven and reduced order modeling. Different classes of problems that are addressed by these approaches will also be categorized and examples from literature will be provided. The intent of this talk is to set the stage for the use of a common terminology such that the community can - in the future - efficiently navigate literature and more easily exchange ideas.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Multi-scale Method for a Three-Phase Reservoir Simulator Considering Gravity Effects

Omar Y. Duran Triana*, Philippe Devloo**, Sonia M. Gomes***

*Researcher, **Professor, ***Professor

ABSTRACT

The scope of this work is to develop and implement a fast integration point mixed finite element -- finite volume scheme, that can solve fine detailed geological realizations by the use of a new multi--scale approach- that allows the fast generation of computational reservoir models taking in account gravity effects. The strong formulation being considered is the weighted pressure formulation for the black--oil model. Using a integration point mixed finite element -- finite volume discretization scheme, that stores all the required data at integration points and the multi--scale hybrid mixed method MHM with local mass conservation at any scale, it is possible to solve efficiently conservative fluxes on both coarse and fine scales. Once theses fluxes are determined, they are used to solve the transport equations of the flowing phases. The nonlinearities associated with black--oil model are treated with a segregated multi--physics solver. We present how to account the buoyancy effects, as well evaluations for computational efficiency and accuracy on a series of full and corresponding multi-scale reservoir models with a high degree of realism, highly heterogeneous rock properties distributed in an representative domain considering complex reservoir and wells geometric descriptions. The multi-scale simulation with integration point mixed finite element method allow us to compute every simulation states in a reasonable time, and it represents a robust and fast approach that enable us to simulate a detailed geological realizations not allowed be possible with current upscaling methods.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A General Mesh Smoothing Approach for Finite Elements

Raul Durand*

*University of Brasilia

ABSTRACT

The elements geometry in finite element meshes can be enhanced by means of smoothing procedures. This paper presents a smoothing technique based on ideal shapes and the use of finite element deformation analyses. Initially, it is assumed that the ideal shape for a particular element corresponds to a regular shape, e.g. polygon or polyhedron with the highest quality metric, with the same area or volume. Based on the initial element coordinates and thanks to the singular value decomposition (SVD) properties, a desired location for the ideal shape is found. Assuming a given mechanical stiffness, the nodal forces required to transform an element into its ideal version is calculated. Once the corresponding nodal forces for all elements are found, a deformation analysis is carried out aiming to transform the elements geometry into the desired ones. The solution provides a deformed mesh with elements with improved quality. The whole process can be applied iteratively to get better improvements. In practice, just few iterations (e.g. two or three) are enough to obtain significant enhancements. The method is applicable to improve finite element meshes constituted by linear and quadratic elements in two and three dimensions.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Energy Stable Discontinuous Galerkin Approximations of the Perfectly Matched Layer for Linear Wave Equations

Kenneth Duru*, Alice-Agnes Gabriel**, Gunilla Kreiss***, Leonhard Rannabauer****

*Munich University, Germany, **Munich University, Germany, ***Uppsala University, ****Technical University of Munich

ABSTRACT

Computational procedures based on discontinuous Galerkin (dG) schemes can be flexible, high order accurate, provably stable, and well-suited for complex large scale wave propagation problems. However, real world wave propagation problems are often formulated in large or unbounded domains. An effective and reliable domain truncation scheme becomes essential, since it enables efficient and high fidelity numerical simulations. The perfectly matched layer (PML) has emerged as an efficient and robust technology to simulate the absorption of waves in many applications. However, previous attempts to effectively include the PML in many modern numerical methods, such as the dG method, proved to be a nightmare for practitioners. Exponential and/or linear growth is often seen in numerical simulations. We present a provably energy-stable dG approximation of the perfectly matched layer (PML) for the three and two space dimensional (3D and 2D) linear wave equations, in first order form. Our approach is rooted in a rigorous mathematical analysis, beginning from the continuous model down to the discrete problem. We derive continuous energy estimates for the 3D PML in the Laplace space. By emulating the energy estimate in the discrete setting we construct asymptotically stable dG approximation of the PML for the wave equation. The analysis will focus on the 3D linear acoustics wave equation. But, we will demonstrate extensions of our method to the 3D linear elasto-dynamic equations. These have been implemented in the dG code, ExaHyPE, a simulation engine for hyperbolic PDEs on adaptive Cartesian meshes, for exascale supercomputers. Finally, we present a large scale numerical simulation of a geophysical wave propagation problem, involving the scattering and interactions of acousto-elastic waves, in a complicated Earth model, with geologically constrained complex free-surface topography.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Towards Exa-scale Multi-physics Simulations of Earthquakes

Kenneth C. Duru*, Alice-Agnes Gabriel**, Leonhard Rannabauer***, Michael Bader****

*LMU Munich, **LMU Munich, ***TUM, ****TUM

ABSTRACT

Realistic earthquake scenarios combine spontaneous dynamic rupture propagation on pre-existing fault interfaces according to non-linear friction laws with seismic wave propagation. The up-to-date largest (1500 km of faults) and longest (500 s) dynamic rupture simulation is modeling the 2004 Sumatra-Andaman earthquake on the curved mega-thrust and a system of splay faults validated by geodetic, seismological and tsunami observations. Such dynamic earthquake sources can be readily coupled to tsunami simulations to analyse tsunami generation and propagation. Whereas these earthquake simulations are based on the Discontinuous Galerkin method exploiting unstructured meshes to account for complex geometries (e.g. high resolution topography and bathymetry, 3D subsurface structure, and fault networks) feature preserving meshing poses limitations for large-scale problems. We present a first application scenario of the ExaHyPE engine, an hyperbolic PDE engine designed to enable exascale (10^18 FLOPs/sec) simulations for conservation laws on future supercomputers without manual meshing.

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

High-Order Finite Element Methods for Acoustics

Fabian Duvigneau*, Ulrich Gabbert**, Sascha Duczek***

*Otto von Guericke University Magdeburg, **Otto von Guericke University Magdeburg, ***Otto von Guericke University Magdeburg

ABSTRACT

The acoustic behavior of structures has lately been in the focus of industrial applications, due to the fact that the acoustic emission of a product is one major parameter which significantly influences the customer perception with respect to comfort and functionality. In this context, the numerical simulation of vibroacoustic problems needs to provide reliable information in order to be able to evaluate the acoustic behavior of new products already in an early stage of the product development process. With the help of a suitable simulation model expensive experimental studies can be reduced and acoustically improved designs can be developed. However, there are already commercial software tools available which offer the opportunity to solve coupled vibroacoustic problems. These tools are typically based on conventional low-order finite element methods (h-FEM) for solving the governing partial differential equations (PDEs) of the problem. In this contribution the advantages of high-order finite element methods (p-FEM), such as a possibly exponential convergence rate [1], will be exploited. In such an approach the same accuracy can be obtained by using significantly less degrees of freedom (dof) compared to classical h-FEM simulations. Consequently, the required computational time required for the analysis can be significantly reduced for a given target accuracy. This property is of special importance when complex structures of practical relevance are under investigation. Even today the overall efficiency of the simulation process is still an issue, despite the ever growing computational power. To exploit the described advantages, high-order FEMs have to be extended to acoustical problems. In the current contribution the vibration analysis and the fluid-structure-interaction are also taken into account. The advantage of high-order methods has been demonstrated by the authors in previous studies, e.g. in the context of wave propagation analysis [2] and multi-physics applications such as piezoelectricity [3]. In this contribution the developed high-order simulation approach is discussed and the received results are compared both with commercial finite element solutions as well as with measurements. Here, the focus is placed on the accuracy and the required computational effort of the different methods. References [1] Szabó, B. & Babuška, I.: “Finite Element Analysis”, John Wiley and Sons, 1991 [2] Willberg, C.; Duczek, S.; Vivar Perez, J. M.; Schmicker, D. & Gabbert, U.: “Comparison of Different Higher Order Finite Element Schemes for the Simulation of Lamb Waves”, Computer Methods in Applied Mechanics and Engineering, 2012, Vol. 241-244, pp. 246-261 [3] Duczek, S. & Gabbert, U.: “Anisotropic Hierarchic Finite Elements for the Simulation of Piezoelectric Smart Structures”, Engineering Computations, 2013, Vol. 30, pp. 682-706

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

Contact Pressure Solution Deformation in Phase Field Models

Branislav Dzepina*, Daniele Dini**, Daniel Balint***

*Imperial College London, **Imperial College London, ***Imperial College London

ABSTRACT

Pressure solution is a deformation mechanism experienced by non-hydrostatically stressed elastic bodies whose primary mode of material transport is diffusive mass transfer. Although originally investigated within the geology community to describe the enhanced compaction of rock and soil particles, the pressure solution mechanism is also applicable to the high pressure sintering of advanced metals and ceramics. During the ultra-high pressure liquid phase sintering of diamond grains, which is the focus of the study, it is estimated that inter-particle contact pressures can approach 100 GPa at some of the contacts. Within the vicinity of such contacts, significant elastic strain energy is stored in the material. As a result of diffusive transfer through the liquid phase, material is transported along energy gradients from the centre of the contact to the lesser-stressed surrounding particle surface. Tracking of the particle interfaces due to this deformation mechanism is not trivial, especially when other processes such as bonding are considered. Thus a phase field model for this process is justified. Elastic energy in phase field models have previously been reported in literature, however, these models are usually concerned with the strain energy resulting from elastic mismatch at the interfaces, phase transformation or strain fields applied to the entire simulation domain. The presented work is an extension of the advection-diffusion sintering phase field model initially proposed by Wang [1]. The original sintering model is modified by the incorporation of contact mechanics and an elastic strain energy term in the free energy functional. The particles are initiated by scalar fields which represent their concentration within the simulation domain. Given a starting configuration, the diffuse interfaces of the particles are allowed to evolve in time in order to minimise the energy of the system. Contact pressure distribution within the contact is approximated by the overlap of the scalar fields that represent the respective particles. Rigid particle motion by advection velocity fields is used to maintain contact between the deforming particles. The effect of pressure solution deformation on the shape of a single particle pressed onto a non-interacting wall is presented. The proposed model is also applied to the demonstration of high pressure sintering between two particles and finally to a cluster of several interacting particles. [1] Yu U. Wang, Computer modeling and simulation of solid-state sintering: A phase field approach, Acta Materialia, Volume 54, Issue 4, 2006, Pages 953-961

13th World Congress on Computational Mechanics (WCCM XIII)
2nd Pan American Congress on Computational Mechanics (PANACM II)
July 22-27, 2018, New York, NY, USA

A Coupled Phase-field/Diffusion/Deformation Model for Upper and Lower Bainitic Transformation

Martin Düsing*, Rolf Mahnken**

*Paderborn University, **Paderborn University

ABSTRACT

The bainitic transformation in steel leads to two different morphologies, upper and lower bainite, which distinguish due to different carbon diffusion mechanisms [1]. The constant temperature during the displacive transformation from austenite to bainitic ferrite influences the mobility of the carbon during the subsequent diffusion. The movement of the carbon determines the location of the carbides, which precipitate at accumulations of carbon. In upper bainite the carbon atoms succeed in leaving the supersaturated bainitic ferrite by diffusing across the interface while in lower bainite most of the carbon stays within the bainitic ferrite and accumulate there [1]. In this contribution we present a new model simulating the above described phase transformation. A phase-field method is applied to govern the three phases austenite, bainitic ferrite and carbide while an elaborate diffusion model considers the separation of carbon within the supersaturated bainitic ferrite and the diffusion across the interface. It is based on a Cahn-Hilliard diffusion equation. To describe the slim shape of the bainitic ferrite phase the model is coupled with deformations. The simulation is based on a thermodynamic framework of generalized stresses as introduced by Gurtin [2] for a two phase Ginzburg-Landau system and a Cahn-Hilliard equation. We extend this framework for multiphase-field models coupled to a viscous Cahn-Hilliard equation and deformations. The framework distinguishes between basic balance laws which are universal and constitutive equations which depend on the specific material. The Clausius-Duhem inequality is used to impose restrictions to the constitutive equations. The numerical examples show the transformation from austenite to bainitic ferrite, the subsequent diffusion and the precipitation of carbides [3]. Depending on the constant temperature the different diffusion mechanisms are weighted. For low temperatures most of the carbon starts to separate within the bainitic ferrite while only a minor part succeed in leaving the supersaturated phase. Subsequently carbides precipitate at accumulations of carbon. For higher temperatures the carbon diffuses across the interface into the austenite phase. In the example one can see how the concentration within the austenite between two phases of bainitic ferrite grows until carbides precipitate. [1] Bhadeshia, H. K. D. H. Bainite in steels, Cambridge, Second Edition (2001). [2] Gurtin, M. E., Physica D: Nonlinear Phenomena (1996) 92:178–192. [3] Düsing, M. and Mahnken, R., Int J Solids Struct (2017) doi:10.1016/j.ijsolstr.2017.11.018