INSTITUTE OF MATHEMATICS AND INFORMATICS
BULGARIAN ACADEMY OF SCIENCES

Numerical Methods and Applications

Seventh International Conference,
August 20-24, 2010, Borovets, Bulgaria

Scientific Program
Abstracts
List of Participants

Seventh International Conference on

Numerical Methods and Applications

NM&A'10

Organizer:

Institute of Mathematics and Informatics, Bulgarian Academy of Sciences

Organizing committee:

Chairperson: N. Kolkovska

I. Bazhlekov, T. Chernogorova, I. Hristov, M. Dimova, I. Georgiev, S. Stoilova, D. Vasileva

in cooperation with

- Institute of Information and Communication Technologies, Bulgarian Academy of Sciences,
- Faculty of Mathematics and Informatics, Sofia University "St. Kliment Ohridski",
- Society for Industrial and Applied Mathematics (SIAM),
- Lecture Notes in Computer Science, Springer.

Invited Speakers:

- M. Feistauer (Charles University Prague, Czech Republic),
- J.-L. Guermond (Texas A&M University, USA),
- K. Sabelfeld (Institute of Computational Mathematics and Computational Physics, Russia),
- J. Schöeberl (Vienna University of Technology, Austria),
- Bl. Sendov (Institute of Information and Communication Technologies, Bulgaria),
- P. Vabishchevich (Institute for Mathematical Modelling, Russia),
- I. Yotov (University of Pittsburgh, USA).

Keynote Speakers:

- A. Ern (University Paris-Est, France),
- R. Lazarov (Texas A&M University, USA),
- S. Parter (University of Wisconsin, USA).

August 20 - 24, 2010, Borovets, Bulgaria

Part A

Scientific Program

Friday, August 20

Plenary Session

	Lecture Hall A
08:30 – 09:15	Registration
	Chairperson: I. Dimov
09:15 – 09:30	Opening
09:30 – 10:10	**Bl. Sendov**, *New Conjectures in the Hausdorff Geometry of Polynomials* B-53
10:10 – 10:50	**K. Sabelfeld**, *Stochastic Algorithms in Linear Algebra - Beyond the Markov Chains and Neumann - Ulam Scheme* B-52
10:50 – 11:20	Coffee Break

	Chairperson: R. Lazarov
11:20 – 12:00	**J.-L. Guermond**, M. Nazarov, R. Pasquetti, B. Popov, *Entropy Viscosity for Nonlinear Conservation Laws* B-29
12:00 – 12:30	**S. Parter**, *Revisiting Preconditioning: An Interesting Result and the Lessons Learned from It* B-44
12:30 – 14:30	LUNCH
13:30 – 14:30	Registration

Parallel Sessions

Lecture Hall A *"Monte Carlo and Quasi-Monte Carlo Methods"*	**Lecture Hall B** *Contributed Talks* *"Approximation Techniques in Numerical Analysis"*
Chairperson: M. Nedjalkov	Chairperson: Bl. Sendov
14:30 – 15:00 **A. Asenov**, *Advanced Monte Carlo Techniques in the Simulation of CMOS Devices and Circuits* B-2	14:30 – 14:50 **G. P. Nikolov**, P. B. Nikolov, *Quadrature Formulae Based on Interpolation by Parabolic Splines* B-43
15:00 – 15:30 **I. Dimov,** R. Georgieva, *Monte Carlo Method for Numerical Integration Based on Sobol' Sequences* B-18	14:50 – 15:10 **N. Naidenov**, S. Kostadinova, *Bicubic Spline Recovering of Smooth Surfaces on the Basis of Irregular Data* B-42
	15:10 – 15:30 V. H. Hristov, N. V. Kyurkchiev, **A. I. Iliev**, *Global Convergence Properties of the SOR-Weierstrass Method* B-31
15:30 – 15:50 **S**. **Stefanov**, *Particle Monte Carlo Algorithms with Small Number of Partilces in Grid Cells* B-56	15:30 – 15:50 **I. Markovsky**, *Affine Data Modeling by Low-Rank Approximation* B-40

15:50 – 16:10 I. Lirkov, **S. Stoilova,** *The b-adic Diaphony as a Tool to Study Pseudo-randomness of Nets* B-38	15:50 – 16:10 **C. Meszaros**, *On Some Properties of the Augmented Systems Arising in Interior Point Methods* B-41
16:10 – 16:40	Coffee Break

Parallel Sessions

Lecture Hall A *"Environmental Modelling"*	**Lecture Hall B** *Contributed Talks " Numerical Methods for Differential and Integral Equations"*
Chairperson: A. Strunk	Chairperson: I. Yotov
16:40 – 16:50 Opening	16:40 – 17:00 M. Grote, **T. Mitkova**, *High-Order Explicit Local Time-Stepping for Damped Wave Equations* B-28
16:50 – 17:20 **K. Georgiev**, Z. Zlatev, *Specialized Sparse Matrices Solver in the Chemical Part of an Environmental Model* B-27	17:00 – 17:20 **A. Bradji**, J. Fuhrmann, *Some Error Estimates for the Discretization of Parabolic Equations on General Multidimensional Nonconforming Spatial Meshes* B-10
17:20 – 17:40 **M. C. Vila**, J. Soeiro de Carvalho, A. Fiúza, *Advanced Numerical Tools Applied to Geo-Environmental Engineering - Soils Contaminated by Petroleum Hydrocarbons, A Case Study* B-60	17:20 – 17:40 **N. Kolkovska**, *Convergence of Finite Difference Schemes for a Multidimensional Boussinesq Equation* B-35
17:40 – 18:00 **J. Březina**, P. Rálek, M. Hokr, *Parallel Simulator of Multidimensional Fracture Flow and Transport* B-11	17:40 – 18:00 **S. C. S. Rao**, S. Kumar, *An Efficient Numerical Method for a System of Singularly Perturbed Semilinear Reaction-Diffusion Equations* B-49
18:00 – 18:20 **K. Liolios**, S. Radev, V. Tsihrintzis, *A Numerical Investigation for the Optimal Contaminant Inlet Positions in Horizontal Subsurface Fllow Wetlands* B-37	18:00 – 18:20 **C. Hofreither**, *A Non-Standard Finite Element Method Based on Boundary Integral Operators* B-30
19:30	RECEPTION

Saturday, August 21

Parallel Sessions

Lecture Hall A *"Metaheuristics for Optimization Problems"*	**Lecture Hall B** *"Environmental Modelling"*
Chairperson: S. Fidanova	Chairperson: K. Georgiev
09:00 – 09:30 **C. Cotta**, *Future Generation Memetic Algorithms* B-13	09:00 – 09:20 **A. Strunk**, H. Elbern, A. Ebel, *Using Satellite Observations for Air Quality Assessment with an Inverse Model System* B-57
09:30 – 09:50 **F. Zamfirache,** M. Frîncu, D. Zaharie, *Population-based Metaheuristics for Tasks Scheduling in Heterogeneous Distributed Systems* B-61	09:20 – 09:40 **K. Ganev**, G. Gadzhev, N. Miloshev, G. Jordanov, A. Todorova, D. Syrakov, M. Prodanova, *Atmospheric Composition Studies for the Balkan Region* B-24

09:50 – 10:10 **D. Simian**, F. Stoica, C. Simian, *Evaluation of the Co-mutation Operators in Optimization of Multiple SVM Kernels* B-55	09:40 – 10:00 I. Etropolska, **M. Prodanova**, D. Syrakov, K. Ganev, N. Miloshev, K. Slavov, *Bulgarian Operative System for Chemical Weather Forecast* B-20
	10:00 – 10:20 **A. Terziyski**, N, Kochev, *Distributed Software System for Data Evaluation and Numerical Simulations of Atmospheric Processes* B-58
10:20 – 10:50	Coffee Break

Parallel Sessions

Lecture Hall A *"Metaheuristics for Optimization Problems"*	**Lecture Hall B** *"Monte Carlo and Quasi-Monte Carlo Methods"*
Chairperson: C. Cotta	Chairperson: A. Penzov
10:50 – 11:10 **S. Fidanova,** P. Marinov, K. Atanassov, *Start Strategies of ACO Applied on Subset Problems* B-21	10:50 – 11:20 M. Magdics, **L. Szirmay-Kalos**, B. Tóth, Á. Csendesi, A. Penzov, *Scatter Estimation for PET Reconstruction* B-38
11:10 – 11:30 S. Fidanova, **P. Marinov**, K. Atanassov, *Sensityvity Analysis of ACO Start Strategies for Subset Problems* B-22	11:20 – 11:40 K. Sabelfeld, **N. Mozartova**, *Sparsified Randomization Algorithms for the SVD based Low Rank Approximations* B-52
11:30 – 11:50 **A. Băutu**, H. Luchian, *Protein Structure Prediction in the 2D HP Model Using Particle Swarm Optimization* B-7	11:40 – 12:00 **M. L. Dinis**, A. Fiúza, *Using Monte-Carlo Simulation for Risk Assessment: Application to Occupational Exposure During Remediation Works* B-19
11:50 – 12:10 J. P. **Pedroso**, *Metaheuristics for the Asymmetric Hamiltonian Path* B-45	12:00 – 12:20 **T. Averina**, *Monte Carlo Simulation of Inhomogeneous Poisson Ensembles* B-5
12:20 – 14:30	LUNCH
14:00 – 14:30	Registration

Parallel Sessions

Lecture Hall A *Contributed Talks* *"Hierarchical and Domain Decomposition Methods"*	**Lecture Hall B** *Contributed Talks* *"Computational Physics, Chemistry, Biology and Engineering"*
Chairperson: S. Margenov	Chairperson: St. Radev
14:30 – 14:50 E. Karer, **J. Kraus**, L. Zikatanov, *Auxiliary Space Preconditioner for a Locking-free Finite Element Approximation of the Linear Elasticity Problem* B-34	14:30 – 14:50 **M. Hokr**, J. Kopal, J. Březina, P. Rálek, *Sensitivity of Results of the Water Flow Problem in a Discrete Fracture Network with Large Coefficient Differences* B-30
14:50 – 15:10 B. Ayuso, **I. Georgiev**, J. Kraus, L. Zikatanov, *Preconditioning of DG FEM Elasticity Systems* B-6	14:50 – 15:10 C. I. Christov, N. T. Kolkovska, **D. P. Vasileva**, *On the Numerical Simulation of Unsteady Solutions for the 2D Boussinesq Paradigm Equation* B-12
15:10 – 15:30 **P. Boyanova**, S. Margenov, *Optimal Order Multilevel Solvers in a Projection Scheme for Navier-Stokes Equations* B-9	15:10 – 15:30 **I. Hristov**, S. Dimova, *Fluxon Dynamics in Stacked Josephson Junctions* B-31

15:30 – 15:50 **P. Popov**, Y. Efendiev, Y. Gorb, *Multsacle Modeling of Poroelasticity in Highly Deformable Fractured Reservoirs* B-46	15:30 – 15:50 T. L. Boyadjiev, **H. T. Melemov**, *Merger Bound States in 0-π Josephson Structures* B-9
15:50 – 16:10 I. Georgiev, **M. Lymbery**, S. Margenov, *Analysis of the Constant in the Strengthened Cauchy-Bunyakowski-Schwarz Inequality for Quadratic Finite Elements* B-27	15:50 – 16:10 **M. Dimova**, S. Dimova, *Numerical Investigation of Self-Similar Solutions of a Reaction Diffusion Equation in a Vicinity of Critical Parameters* B-18
16:10 – 16:40	Coffee Break

Parallel Sessions

Lecture Hall A *Contributed Talks* *"Computational Mechanics"*	**Lecture Hall B** *Contributed Talks* *"Computational Physics, Chemistry, Biology and Engineering"*
Chairperson: P. Vabishchevich	Chairperson: S. Dimova
16:40 – 17:00 J.-L. Guermond, **P. D. Minev**, *A New Class of Fractional Step Techniques for the Incompressible Navier-Stokes Equations Using Direction Splitting* B-29	16:40 – 17:00 **N. N. Elkin**, A. P. Napartovich, D. V. Vysotsky, *Bidirectorial Beam Propagation Method Applied for Lasers with Multilayer Active Medium* B-20
17:00 – 17:20 A. S. Shamaev, A. A. Gavrikov, **D. U. Knyazkov**, *Some Spectral Problems of Porous Media Acoustics* B-54	17:00 – 17:20 **A. Liolios**, S. Radev, *A Numerical Approach for Obtaining Fragility Curves in Seismic Structural Mechanics: A Bridge Case of Egnatia Motorway in Northern Greece* B-36
17:20 – 17:40 **S. Radev**, N. K. Vitanov, *Application of Spectral Method for Investigation of the Profiles of the Optimum Fields for Variational Problems Connected to the Turbulent Thermal Convection* B-47	17:20 – 17:40 **G. Bencheva**, *On the Numerical Solution of a Chemotaxis System in Haematology* B-8
17:40 – 18:00 **N. K. Vitanov**, *Numerical Investigation of the Upper Bounds on the Convective Heat Trasport in a Heated From Below Rotating Fluid Layer* B-61	17:40 – 18:00 **P. Kh. Atanasova**, T. L. Boyadjiev, E. V. Zemlyanaya, Yu. M. Shukrinov, *Stability Analysis of Magnetic Flux in the LJJ Model with Double Sine-Gordon Equation* B-2
18:00 – 18:20 **S. Stoykov**, P. Ribeiro, *Forced Vibrations of 3D Beams with Large Amplitudes* B-57	

Sunday, August 22

Plenary Session

	Lecture Hall A
	Chairperson: J.-L. Guermond
08:45 – 09:25	**M. Feistauer**, *Discontinuous Galerkin Finite Element Method for Convection-Diffusion Problems and Compressible Flow* B-21
09:25 – 10:05	**J. Schöberl**, *Hybrid Discontinuous Galerkin Methods with Vector Valued Finite Elements* B-53
10:05 – 10:20	Coffee Break

	Chairperson: K. Sabelfeld
10:20 – 11:00	B. Ganis, D. Vassilev, **I. Yotov,** M. Zhong, *A Multiscale Stochastic Framework for Stokes-Darcy Flow and Transport* B-25
11:00 – 11:30	O. P. Iliev, **R. Lazarov**, J. Willems *Numerical Upscaling of Flows in Highly Heterogeneous Porous Media* B-32
11:30 – 12:30	LUNCH
12:30	EXCURSION

Monday, August 23

Plenary Session

	Lecture Hall A
	Chairperson: M. Feistauer
09:00 – 9:40	**P. Vabishchevich,** *SM Stability for Time-Dependent Problems* B-59
09:40 – 10:10	E. Burman, **A. Ern,** M. A. Fernández, *Explicit Runge - Kutta Schemes and Finite Elements with Symmetric Stabilization for First-Order Linear PDE Systems* B-12
10:10 – 10:40	Coffee Break

Parallel Sessions

Lecture Hall A *"Monte Carlo and Quasi-Monte Carlo Methods"*	**Lecture Hall B** *"Environmental Modelling"*
Chairperson: K. Sabelfeld	Chairperson: K. Georgiev
10:35 – 11:00 **D**. **Vasileska,** A. Hossain, K. Raleva, S. M. Goodnick *Is Self-Heating Important in Nanowire FETs?* B-59	10:40 – 11:00 T. Brechet, C. Camacho, **V. Veliov**, *Global Warming and Economic Behaviour* B-10
11:00 – 11:20 **K**. **Raleva,** D. Vasileska, S. M. Goodnick *Modeling Thermal Effects in Fully-Depleted SOI Devices with Arbitrary Crystallographic Orientation* B-48	11:00 – 11:20 **Tz. Ostromsky**, I. Dimov, Havasi, I. Farago, Z. Zlatev, *Richardson Extrapolated Numerical Methods for One-Dimensional Advection Schemes* B-44
11:20 – 11:40 **M**. **Nedjalkov,** S. Selberherr, I. Dimov, *Stochastic Algorithm for Solving the Wigner-Boltzmann Correction Equation* B-43	11:20 – 11:40 **E. Băutu**, A. Bărbulescu, *Mining Temperature Trends with GEP Ensembles* B-8
11:40 – 12:00 **A. Makarov**, V. Sverdlov, S. Selberherr, *Modeling of the SET and RESET Process in Bipolar Resistive Oxide-Based Memory using Monte Carlo Simulations* B-39	11:40 – 12:00 **N. Dobrinkova**, G. Jordanov, J. Mandel, *WRF-Fire Applied in Bulgaria* B-19
12:00 – 12:20 V. Baláž, **V. Grozdanov**, V. Ristovska-Dimitrieva, O. Strauch, S. Stoilova, *On the Mean Square Worst-Case Error of the Quasi-Monte Carlo Integration in Weighted Sobolev Spaces* B-6	12:00 – 12:20 **G. Dimitriu**, R.Ștefănescu *Comparative Numerical Results in 4D-Var Data Assimilation Problems Using POD Techniques* B-62
12:20 – 14:30	LUNCH
14:00 – 14:30	Registration

Parallel Sessions

Lecture Hall A *"Metaheuristics for Optimization Problems"*	**Lecture Hall B** *"Modelling and Simulation of Electrochemical Processes"*
Chairperson: K. Penev	Chairperson: O. Iliev
14:30 – 14:50 **O. Roeva**, T. Slavov, *Fed-batch Cultivation Control based on Genetic Algorithm PID Controller Tuning* B-50	14:30 – 15:00 **J. Fuhrmann**, K. Gärtner, M. Ehrhardt, A. Linke, H. Langmach, H. Zhao, *Numerical Modeling in Electrochemistry by Voronoi Finite Volume Methods* B-23
14:50 – 15:10 **F. Torrecilla-Pinero**, J. A. Torrecilla-Pinero, J. A. Gomez-Pulido, M. A. Vega-Rodriguez, J. M. Sanchez-Perez, *Parameter Estimation for a Logistic Curve. An Example of Use in an Engineering Problem* B-58	15:00 – 15:20 **O. Iliev,** A. Latz, J. Zausch, *Modeling of Species and Charge Transport in Li-Ion Batteries* B-33
15:10 – 15:30 I. Skalna, J. **Duda**, *A Comparison of Metaheurisitics for the Problem of Solving Parametric Interval Linear Systems* B-55	15:20 – 15:40 O. Iliev, S. Margenov, P. Popov, **Y. Vutov,** *Finite Volume Discretization of Nonlinear Diffusion in Li-Ion Batteries* B-33
15:30 – 15:50 **M. Angelova**, S. Tzonkov, T. Pencheva, *Genetic Algorithms Based Parameter Identification of Yeast Fed-Batch Cultivation* B-1	15:40 – 16:00 **K. Bartkowski,** O. Iliev, A. Latz, *On Numerical Simulation of 1D Problems Describing Transport Processes in Li-Ion Batteries* B-7
15:50 – 16:10 **M. Seredynski**, P. Bouvry, *Perspectives of a Selfish Behavior in Self-Policing Wireless Mobile Ad Hoc Network* B-53	
16:10 – 16:40	Coffee Break

Parallel Sessions

Lecture Hall A *"Grid Computing and Applications"*	**Lecture Hall B** *Contributed Talks"Numerical Linear Algebra"*
Chairperson: E. Atanassov	Chairperson: J. Schöberl
16:40 – 17:10 **E. Atanassov,** T. Gurov, A. Karaivanova, S. Ivanovska, D. Slavov, *Efficient Gridification of Environmental Modeling Applications* B-3	16:40 – 17:00 **J. Buša**, J. Buša, jr., E. Hayryan, *OpenCL Implementation of the Analytical Method for the Computation of the Accessible Surface Area and Excluded Volume of Overlapping Spheres* B-11
17:10 – 17:30 V. Spiridonov, **D. Syrakov**, M. Prodanova, A. Bogachev, K. Ganev, N. Miloshev, G. Jordanov, K. Slavov, *First results of See-Grid-Sci VO "Environment" Application CCIAQ* B-56	17:00 – 17:20 **M. Manguoglu**, E. Cox, F. Saied, A. Sameh, *Parallel Computation of the Fiedler Vector and Solution of Large Sparse Linear Systems via Banded Preconditioners* B-40
17:30 – 17:50 **C. Resteanu**, R. Trandafir, *Programming Problems with a Large Number of Objective Functions* B-50	17:20 – 17:40 **P. D. Michailidis**, K. G. Margaritis, *Experimental Study of Matrix Multiplication on MultiCore Processors* B-41
17:50 – 18:10 **R. Goranova**, *An Approach of Modeling ROOT Processes in Grid* B-28	17:40 – 18:00 **I. Skalna**, *Interval Dependency and the Problem of Solving Parametric Linear Systems* B-55
18:10 – 18:30 E. Atanassov, **M. Durchova,** *Efficient GPU-based Generation of the Scrambled Halton Sequence* B-3	18:00 – 18:20 P. Hr. Petkov, **M. M. Konstantinov**, N. D. Christov, *Condition and Error Estimates in Kalman Filter Design* B-46
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Tuesday, August 24

Parallel Sessions

Lecture Hall A *"Metaheuristics for Optimization Problems"*	**Lecture Hall B** *Contributed Talks* *"Numerical Methods for Differential and Integral Equations"*
Chairperson: S. Fidanova	Chairperson: N. Kolkovska
09:30 – 09:50 **N. Fujimoto**, S. Tsutsui, *A Highly-Parallel TSP Solver for a GPU Computing Platform* B-24	09:30 – 09:50 **J. D. Kandilarov**, R. L. Vulkov, *A Numerical Approach for the American Call Option Pricing Model* B-34
09:50 – 10:10 **K. Penev**, A. Ruzhekov, *Adaptive Intelligence Applied to Numerical Optimisation* B-46	09:50 – 10:10 T. Chernogorova, **R. Valkov**, *Finite-Volume Difference Schemes for the Black-Sholes Equation in Stochastic Volatility Models* B-12
10:10 – 10:30 **A. Ruzhekov,** K. Penev, *Tool for Observation, Comparison and Analysis of Advanced Search Algorithms* B-51	10:10 – 10:30 M. N. Koleva, **L. G. Vulkov**, *A Numerical Study of a Parabolic Monge-Ampere Equation in Mathematical Finance* B-35
10:30 – 10:50 **V. Atanassova**, K. Atanassov, *Ant Colony Optimization Approach to Tokens' Movement within Generalized Nets* B-5	10:30 – 10:50 N. Ishimura, **M. N. Koleva**, L. G. Vulkov, *Numerical Solution of a Nonlinear Evolution Equation for the Risk Preference* B-34
10:50 – 11:10 L. Atanassova, **K. Atanassov**, *Intuitionistic Fuzzy Interpretation of Conway's Game of Life* B-4	10:50 – 11:10 A. Andreev, **M. Racheva**, *On the Integral Type Crouzeix-Raviart Nonconforming Finite Elements* B-1
11:10 – 11:30 M. Hernández, J. J. Cáceres, **M. Pérez**, *Forecasting the Composition of Demand for Higher Education Degrees by Genetic Algorithms* B-29	11:10 – 11:30 **A. Andreev**, M. Racheva, *Postprocessing Techniques Using a Linear Nonconforming Finite Elements* B-1
DEPARTURE	

Part B

Abstracts

On the Integral Type Crouzeix-Raviart Nonconforming Finite Elements

A. Andreev, M. Racheva

We analyze some approximation properties of nonconforming piecewise linear finite elements. These elements use integral degrees of freedom which yield superclose properties and that is why they are more appropriate for postprocessing procedures. The approximate eigenvalues obtained with this method dive asymptotically lower bounds of the exact eigenvalues. Finally, computational aspects are discussed and numerical examples are presented.

Postprocessing Techniques Using a Linear Nonconforming Finite Elements

A. Andreev, M. Racheva

Two different a-posteriori techniques which improve the order of convergence of finite element solutions are presented. These methods are realized by means of an integral type Crouzeix-Raviart nonconforming finite element. Superconvergence rate is established to a second order elliptic problem by introducing nonstandard interpolated elements. We also analyze a simple postprocessing method applied to second order eigenvalue problems. Both approaches are illustrated and discussed by appropriate numerical examples.

Genetic Algorithms Based Parameter Identification of Yeast Fed-Batch Cultivation

M. Angelova, S. Tzonkov, T. Pencheva

Different kinds of genetic algorithms have been investigated for a parameter identification of a fermentation process. Altogether eight realizations of genetic algorithms have been presented four of simple genetic algorithms and four of multi-population ones. Each of them is characterized with a different sequence of implementation of main genetic operators, namely selection, crossover and mutation. A comparison of considered eight types of genetic algorithms is presented for a parameter identification of a fed-batch cultivation of S. cerevisiae. All kinds of multi-population algorithms lead to considerable improvement of the optimization criterion value but for more computational time. Among the considered multi-population algorithms the best one has an operators sequence of crossover, mutation and selection. Different kinds of considered simple genetic algorithms lead to similar values of the optimization criterion but the genetic algorithm with an operators sequence of mutation, crossover and selection is significantly faster than the others.

Advanced Monte Carlo Techniques in the Simulation of CMOS Devices and Circuits

A. Asenov

In this paper we describe advanced Monte Carlo simulation techniques that are used to study statistical variability in contemporary and future CMOS technology generations at the levels of physical transistor simulation, compact model and circuit simulation. First we will review the major sources of statistical variability in nano CMOS transistors focusing at the 45nm technology generation and beyond and will introduced the advanced 3D statistical physical statistical simulation technology and tools used to forecasts the magnitude of statistical variability. Figure 1 illustrates the statistical current-voltage characteristics of a typical 35 nm transistor.

Statistical compact models are used to transfer the variability information obtained from the physical simulations into the circuit simulation and design domain. Sensitivity analysis allows the selection of optimal statistical compact model sets of parameters. Principle component analysis (PCA) and nonlinear power method (NPM) techniques will be presented allowing statistically accurate parameters set to be generated and used in statistical circuit simulation. Fig. 2 illustrates correlation between key transistor figures of merit obtained using nave and PCA parameter generation strategies.
Finally statistical circuit simulation strategies will be presented that allow trade off between performance, power and yield in the CMOS circuit and systems design process. Fig. 3 illustrates the results of the statistical circuit simulation of an adder subject to different variability components.

Stability Analysis of Magnetic Flux in the LJJ Model with Double Sine-Gordon Equation

P. Kh. Atanasova, T. L. Boyadjiev,
E. V. Zemlyanaya, Yu. M. Shukrinov

The decrease of the barrier transparency in superconductor-insulator-superconductor Josephson junctions leads to the deviations of the current-phase relation from the sinusoidal form. The sign of second harmonics is important for many applications, in particular in junctions with a more complex structure like SFINS or SFIFS, where N is a normal metal and F is a weak metallic ferromagnet. In our work we study the static magnetic flux distributions in long Josephson junctions taking into account the higher harmonics in the Fourier-decomposition of the Josephson current. Stability analysis is based on numerical solution of a spectral Sturm-Liouville problem formulated for each distribution. In this approach the nullification of the minimal eigenvalue of this problem indicates a bifurcation point in one of parameters. At each

step of numerical continuation in parameters of the model, the corresponding nonlinear boundary problem is solved on the basis of the continuous analog of Newton's method. The solutions which do not exist in the traditional model have been found. The influence of second harmonic on stability of magnetic flux distributions for main solutions is investigated.

Efficient GPU-based Generation of the Scrambled Halton Sequence

E. Atanassov, M. Durchova

The Halton sequence is one of the first and most popular low-discrepancy sequences. Various modifications of the original construction of Halton have been developed and studied, with the purpose to improve the convergence rate of the resulting quasi-Monte Carlo algorithms. One of the most important types of modification is the scrambling, described by Owen. Since the bases of the number systems that are used are different for every coordinate, the implementation of this technique faces technical difficulties and may be unfeasible for many practical applications, involving high number of coordinates or high number of points of the sequence. In this work we describe and algorithm for efficient GPU-based generation of the Halton sequence with Owen's scrambling for each coordinate, using CUDA. We demonstrate that by employing the GPU the overhead of the scrambling becomes acceptable and we achieve overall better numerical results compared to simpler types of scrambling.

Efficient Gridification of Environmental Modeling Applications

E. Atanassov, T. Gurov, A. Karaivanova, S. Ivanovska, D. Slavov

The environmental modeling was identified as a domain of high interest for Europe, addressing practical problems related to security and quality of life. The building blocks of these applications are large-scale models like CMAQ (Community Multiscale Air Quality model), MM5 (the 5th generation PSU/NCAR Meso-Meteorological Model), SMOKE (Sparse Matrix Operator Kernel Emissions Modelling System). A number of interfaces (Linux scripts and Fortran codes) are used as to link those models with different types input information in a system capable to perform long term calculations. Running these applications on the Computational Grid faces a lot of challenge, for example: these applications are usually resource intensive, in terms of both CPU utilization and data transfers and storage; the use of applications for operational purposes poses requirements for availability of resources, which are difficult to be met on a dynamically changing Grid environment; the validation of applications is resource intensive and time consuming. This leads to a certain level of

conservatism and requires the execution environment to be predictable and controlled by the developers of the applications.
In this work we describe efficient grid implementation scheme which incorporates several grid services specifically developed by us for this type of applications. We present also a new version of the Job Track service (JTS) offering applications specific functionality, geared towards the specific needs of the Environmental Modelling and Protection applications. We used the modular design of the JTS in order to enable smoother interaction of the users with the Grid environment. Our experience shows improved response times and decreased failure rate from the executions of the application. In this work we present such observations from the use of the South East European Grid infrastructure. The new version of the JTS enables more collaborative and efficient use of the Grid resources and answers to the application requirements.

Intuitionistic Fuzzy Interpretation of Conway's Game of Life

L. Atanassova and K. Atanassov

Conway's Game of Life is a popular zero-player game, devised by John Horton Conway in 1970, and it is the best-known example of a cellular automaton. Its universe is an infinite two-dimensional orthogonal grid of square cells, each of which is in one of two possible states, live or dead. Every cell interacts with its eight neighbours, which are the cells that are directly horizontally, vertically, or diagonally adjacent. In a stepwise manner, the state of each cell in the grid preserves or alternates with respect to a given list of rules. Intuitionistic fuzzy sets (IFS) are an extension of Zadehs fuzzy sets, which introduce a degree of membership and a degree of non-membership whose sum is equal to or less than 1 and the complement to 1 is called a degree of uncertainty. The article proposes an intuitionistic fuzzy estimation of the cells state in a modified Game of Life. For each cell we can define its IF estimation as a pair consisting of the degrees l_p and l_a, namely degrees of presence and absence of life, where $l_p + l_a \leq 1$. In the classical Conway's Game of Life, the live and dead states correspond to the elementary IF estimations $< 1, 0 >$ and $< 0, 1 >$. The article presents the formulas for calculation of the IF state of liveliness of each cell, as functions of the current states of the cells neighbors. Criteria of liveliness will be also determined in terms of IFS.

Ant Colony Optimization Approach to Tokens' Movement within Generalized Nets

V. Atanassova, K. Atanassov

Generalized Nets (GNs) is a concept extending the concept of Petri nets and the rest of its modifications. One of the aspects of generalization is the fact that the GN transitions possess an index matrix of predicates, determining the conditions for tokens' transfer from any input place of the transition to any output place. On the other hand, the tokens enter the GN with their initial characteristics and during their transfer from the input to the output places of the transition, they are assigned new characteristics by means of special characteristic functions. GNs have been applied to modelling of processes in the field of artificial intelligence (expert systems, neural networks, pattern recognition, machine learning, etc.), and in particular to metaheuristic methods for solving of optimizational problems like the transportational problem, the travelling salesman problem, the knapsack problem. An important venue of application of GN is the area of Ant Colony Optimization (ACO). So far, GN have been used as a method for description of the ACO procedures. The present article for the first time adopts the opposite approach: it discusses the possibility for optimization of the GN tokens' movement, using ACO algorithms.

Monte Carlo Simulation of Inhomogeneous Poisson Ensembles

T. Averina

The Poisson law not only "controls" the points that are randomly distributed in time but also controls ensembles of points that are randomly distributed on a plane or in space with certain intensity. The simulation of Poisson ensembles is needed in many control theory problems, in queuing theory, in risk theory, and in the analysis of constructs in engineering systems.

Algorithms for modeling inhomogeneous Poisson ensembles can be designed on the basis of a majorant of the intensity function using the sequence of rejections, which are usually determined by independent values of a standard random number.

An efficient method was proposed by G. A. Mikhailov for the simulation of random variables whose probability density functions are weighted sums (mixes) of probability densities that can be efficiently modeled. For that purpose, a modified superposition method was proposed by G. A. Mikhailov. This method uses a two-step simulation for the same value of the random number.

In this paper, Mikhailov's method is extended and justified for the multistep case, and it is applied for the simulation of inhomogeneous Poisson ensembles with the use of a sequence of rejections with respect to the same random number. The corresponding modification of the well-known maximum cross-section method is developed, which

turns out to be equivalent to the standard algorithm of simulating the generalized geometric distribution.
This work was supported by the Russian Foundation for Basic Research (grants 08-01-00334, 09-01-00798)

Preconditioning of DG FEM Elasticity Systems

B. Ayuso, I. Georgiev, J. Kraus, L. Zikatanov

We will present a preconditioning techniques for interior penalty discontinuous Galerkin (IP DG) finite element methods for linear elasticity problems in primal (displacement) formulation. We will recall some of their stability and approximation properties and comment on their suitability as a discretization tool for problems with nearly incompressible materials.
Next we propose a natural splitting of the DG space, which gives rise to uniform preconditioners. The presented approach was recently introduced by B. Ayuso and L. Zikatanov (2009) in the context of designing subspace correction methods for scalar elliptic equations and is extended here to linear elasticity.
Similar to the scalar case the solution of the linear algebraic system corresponding to the IP DG method is reduced to a solution of a problem arising from discretization by nonconforming Crouzeix-Raviart elements plus the solution of a well-conditioned problem on the complementary space.

On the Mean Square Worst-Case Error of the Quasi-Monte Carlo Integration in Weighted Sobolev Spaces

V. Baláž, V. Grozdanov, V. Ristovska-Dimitrieva,
O. Strauch, S. Stoilova

In our talk, we will consider problems of the multivariate quasi-Monte Carlo integration in weighted Sobolev spaces, which are reproducing kernel Hilbert spaces. We consider a concrete weighted Sobolev space $H_{Sob,s,\gamma,\mathcal{B}_4}$, containing functions which partial derivatives up to order two have to be square integrable. This space has a reproducing kernel, based on using the Bernoulli polynomials up to fourth degree.
We will approximate the integrals through quasi-Monte Carlo algorithm with equal quadrature weights. We use a randomization of deterministic sample point nets, called (s, b)-digital shift, and consider the notion of mean square worst-case error of the integration in reproducing kernel Hilbert spaces.
As a tool of our investigation we use the Walsh functional system in base $b \geq 2$.
We obtain an exact formula for the mean square worst-case error of the integration in the space $H_{Sob,s,\gamma,\mathcal{B}_4}$. This formula is an expresion in the terms of the Walsh functions in base b and the Fourier-Walsh coefficients of the reproducing kernel, which generates the space $H_{Sob,s,\gamma,\mathcal{B}_4}$.

The formula for the mean square worst-case error is applied to two concrete choices of digital $b-$adic nets. First, we use an arbitrary $(t, m, s)-$net in base b and obtain the order of the mean square worst-case error. Second, we use the uniform lattice point net in base b and obtain the order of the mean square worst-case error. The obtained orders are compared.

On Numerical Simulation of 1D Problems Describing Transport Processes in Li-Ion Batteries

K. Bartkowski, O. Iliev, A. Latz

The modelling approaches for transport processes in Li ion batteries are presented in a companion talk in this special session. This talk concentrates on the numerical simulation of 1D problems. In order to numerically solve the resulting highly nonlinear coupled equations for ion concentrations, ion flux and electrical currents, numerical algorithms based on different versions of the Newton algorithm, the combined Newton-Picard algorithm, or the nonlinear multigrid method, are developed. A special challenge is the treatment of the nonlinear Robin like boundary conditions due to the Butler Volmer reaction kinetics at the interface of electrolyte and active particles. The performance of the numerical algorithms is studied in detail, and influence of different parameters on the convergence is numerically studied.

Protein Structure Prediction in the 2D HP Model Using Particle Swarm Optimization

A. Băutu, H. Luchian

Modern research in bioinformatics deals with large amounts of data or the simulation of complex biological processes. Many of these problems are too demanding in terms of computational and/or memory requirements for classical algorithms. Nature inspired metaheuristics can be used for finding fast and reasonably accurate solutions for them. Proteins are the most important of all the molecules found in living cells. To carry out its tasks, a protein must fold into a complex three-dimensional structure called native state, which represents the energetic ground state of the protein. Various simplified models for the protein structure exist (e.g. the Toy model, the Functional Model Protein — FMP, the Hydrophobic-Polar model — HP). The high computational complexity of predicting the folded structure of a protein recommends this problem for metaheuristics approaches.
This paper applies the Particle Swarm Optimization (PSO) algorithm to search the ground state of protein foldings. We propose a novel approach, that uses a discrete PSO variant, specially designed for protein folding in the HP model. Despite the

simplicity of the model, the protein folding problem in the HP model is $\mathcal{NP}$-hard in both 2D and 3D. Extensive experiments are performed, that cover both artificial data and real protein data, both with relative and absolute 2D folding coordinates. The results indicate that the proposed PSO method is very effective to search for ground states of the proteins structures, with respect to solution accuracy and speed.

Mining Temperature Trends with GEP Ensembles

E. Băutu, A. Bărbulescu

Changes in the statistical behavior of usual climate variables can have great impact on the occurrence of extreme weather events and finally on climate change. In this paper we tackle the problem of modeling and forecasting the direction of change in long temperature time series. The problem is usually tackled with statistical approaches, like binary autoregressive models, generalized linear models of Hidden Markov Models. We formulate the problem in terms of supervised learning. The use of ensemble techniques is known to improve the accuracy and robustness of simple classifiers.
We propose an approach that is based on the evolutionary algorithm Gene Expression Programming (GEP), combined with an ensemble technique, in order to enhance its performance. First, GEP is used to induce pools of base classifiers, which are later combined by means of a specialized weighted voting scheme. We compare the performance of the obtained models with state-of-the-art statistical and machine learning methods. The experiments performed on long time series of temperatures recorded in several meteorological stations in the South-East of Romania show that the complex ensemble models are efficient and competitive to classical methods.

On the Numerical Solution of a Chemotaxis System in Haematology

G. Bencheva

Many haematological diseases, including various types of leukaemia, are caused by abnormal production of particular blood cells. Their treatment consists mainly of two steps. The first step is chemotherapy and a whole body irradiation to eradicate the patient's haematopoietic system. The second step is the transplantation of haematopoietic stem cells (HSCs) obtained from the mobilized peripheral blood of a donor. After transplantation, HSCs find their way to the stem cell niche in the bone marrow. It has been shown that HSCs migrate *in vitro* and *in vivo* following the gradient of a chemotactic factor SDF-1 produced by stroma cells. Upon homing HSCs have to multiplicate rapidly to regenerate the blood system. Adequate computer models for these steps would help medical doctors to shorten the period in which the patient is missing their effective immune system.
Our attention at this stage is focused on the numerical solution of the mathematical model for the chemotactic movement of HSCs, proposed by A. Kettemann, M. Neuss-Radu in 2008. It consists of a nonlinear system of chemotaxis equations coupled with

an ordinary differential equation on the boundary of the domain in the presence of nonlinear boundary conditions. The unknowns of the system are the concentrations of HSCs, of SDF-1, and of the stem cells bound to the stroma cells. Various classical numerical methods applied directly to a general chemotaxis system and in particular to HSCs migration model may lead to numerical instabilities and loss of the positivity property of the solution. A finite-volume method, based on a second-order positivity preserving central-upwind scheme is proposed by A. Chertock and A. Kurganov in 2008 for a class of chemotaxis and haptotaxis models with homogeneous Neumann conditions. Their approach is applied in the current paper for the numerical solution of the HSCs migration model. Special attention is focused here on the approximation of the ODE and of the boundary conditions. Theoretical analysis of the stability, consistency, convergence and positivity properties of the modified scheme is made. Results of numerical tests illustrating the theoretical estimates are also presented.

Merger Bound States in $0 - \pi$ Josephson Structures

T. L. Boyadjiev, H. T. Melemov

The possible static distributions of magnetic flux in a $0 - \pi$ Josephson junction is described as a result of a nonlinear interaction between distributions of magnetic flux in "virtual" homogenous and π junctions. The influence of an external magnetic field on basic stability fluxons in a $0 - \pi$ Josephson junction is studied. The "virtual" junctions for basic stability fluxons are investigated.

Optimal Order Multilevel Solvers in a Projection Scheme for Navier-Stokes Equations

P. Boyanova, S. Margenov

The numerical solution of the incompressible Navier-Stokes equations has been the focus of the computational fluid dynamics community for over six decades. However, the pursuit of constructing optimal schemes, in terms of computational cost and accuracy, is still not over.

We consider the implementation of a projection scheme which is based on nonconforming Crouzeix-Raviart finite element approximation of the velocities and piece-wise constant approximation of the pressure. The most significant advantage of this approximation is that the divergence of the velocity field is zero inside each element, i.e. the approximation is locally conservative.

We show that some recently developed Algebraic MultiLevel Iteration (AMLI) preconditioners can be successfully applied to get a composite time-stepping solution method which has a total computational complexity of optimal order. ¿From computational point of view, the prediction step consists of two decoupled scalar parabolic problems. At the projection step a coupled mixed FEM problem is to be solved. Eliminating

the velocities we reduce this problem to a system with a weighted graph-Laplacian for the pressure unknowns.
The presented numerical tests aim to show both the numerical stability and the computational efficiency of the algorithm.

Some Error Estimates for the Discretization of Parabolic Equations on General Multidimensional Nonconforming Spatial Meshes

A. Bradji, J. Fuhrmann

This work is devoted to the error estimates of the discretization of parabolic equations on general nonconforming spatial meshes in several space dimensions. These meshes are recently used to approximate anisotropic heterogeneous diffusions and nonlinear equations. We present an implicit scheme based on an orthogonal projection of the exact initial function. We provide error estimates in discrete norms $L^\infty(0,T;H_0^1(\Omega))$ and $W^{1,\infty}(0,T;L^2(\Omega))$. In the particular case when the discrete flux is performed using a stabilized discrete gradient, we prove that the convergence order is $h_{\mathcal{D}}+k$, where $h_{\mathcal{D}}$ (resp. k) is the mesh size of the spatial (resp. time) discretization, in discrete norms $L^\infty(0,T;H_0^1(\Omega))$ and $W^{1,\infty}(0,T;L^2(\Omega))$ under the regularity assumption $u\in\mathcal{C}^2([0,T];\mathcal{C}^2(\overline{\Omega}))$, with u is the exact solution. These error estimates are useful because they allow us to obtain approximations for the! exact solution and its first derivatives of order $h_{\mathcal{D}}+k$.

Global Warming and Economic Behaviour

T. Brechet, C. Camacho, V. Veliov

This study is motivated by the evidence of global warming, which is caused by human activity but affects the efficiency of the economy. We employ the integrated assessment Nordhaus DICE-2007 model. Generally speaking, the framework is that of dynamic optimization of the discounted inter-temporal utility of consumption, taking into account the economic and the environmental dynamics. The main novelty is that several reasonable types of behavior (policy) of the economic agents, which may be non-optimal from the point of view of the global performance but are reasonable form an individual point of view and exist in reality, are strictly defined and analyzed. These include the concepts of "business as usual", in which an economic agent ignores her impact on the climate change (although adapting to it), and of "free riding with a perfect foresight", where some economic agents optimize in an adaptive way their individual performance expecting that the others would perform in a collectively optimal way. These policies are defined in a formal and unified way modifying ideas from the so-called "model predictive control". The introduced concepts are relevant to many other problems of dynamic optimization, especially in the context of resource economics. However, the numerical analysis in this paper is devoted to the evolution

of the world economy and the average temperature in the next 150 years, depending on different scenarios for the behavior of the economic agents. In particular, the results show that the "business as usual", although adaptive to the change of the atmospheric temperature, may lead within 150 years to increase of temperature by 2°C more than the collectively optimal policy.

Parallel Simulator of Multidimensional Fracture Flow and Transport

J. Březina, P. Rálek, M. Hokr

The granite rock represents one of the suitable sites for a nuclear waste deposit. Water in the granite massive is conducted by the complex system of fractures of various sizes. In our approach the small fractures are modeled by an equivalent permeable continuum, while the preferential flow in large geological dislocations and their intersections is considered as a 2D flow on corresponding manifolds and 1D flow on lines respectively. Hydraulic conductivity in the domains of lower dimension can be several orders of magnitude larger then effective conductivity of the 3D domain. We use mixed-hybrid discretization for the flow problem and simple finite volume up-wind scheme for the transport.
The mixed-hybrid discretization leads to a symmetric indefinite system with block diagonal leading submatrix. This allows explicit construction of the Schur complement and significant reduction of the matrix size as well as its condition number. We will show scalable parallel construction of the Schur complements and solution of the system by a two-level Schwartz domain decomposition method using the PETSC library. We will also discuss parallel solution of the transport equation.

OpenCL Implementation of the Analytical Method for the Computation of the Accessible Surface Area and Excluded Volume of Overlapping Spheres

J. Buša, J. Buša, jr., E. Hayryan

The aim of the paper is to present an OpenCL (Open Computing Language) implementation of the analytical method for the computation of the accessible surface area and excluded volume of a system of overlapping spheres, which can be used in macromolecular modelling. The algorithm of this method, based on the stereographic projection of spheres has been published formerly. This implementation allows to run the same program on all devices supporting OpenCL standard (both CPU and GPU). We will present an idea of modifications needed to the original algorithm in order to

utilize the parallelization possibilities of OpenCL and show comparison of performance of original implementation of analytical method (written in FORTRAN) with OpenCL implementation running on different platforms (AMD Opteron, NVIDIA GeForce GTX285, NVIDIA Tesla C1060). We will show that computing the accessible surface area and excluded volume on GPU is efficient.

Explicit Runge–Kutta Schemes and Finite Elements with Symmetric Stabilization for First-Order Linear PDE Systems

E. Burman, A. Ern and M. A. Fernández

We analyze explicit Runge–Kutta schemes in time combined with stabilized finite elements in space to approximate evolution problems with a first-order linear differential operator in space of Friedrichs-type. For the time discretization, we consider explicit second- and third-order Runge–Kutta schemes. We identify a general set of properties on the space stabilization, encompassing continuous and discontinuous finite elements, under which we prove stability estimates using energy arguments. Then, we establish L^2-norm error estimates with quasi-optimal convergence rates for smooth solutions in space and time. These results hold under the usual CFL condition for third-order Runge–Kutta schemes and any polynomial degree in space and for second-order Runge–Kutta schemes and first-order polynomials in space. For second-order Runge–Kutta schemes and higher polynomial degrees in space, a tightened 4/3-CFL condition is required. Numerical results are presented for smooth and rough solutions. The case of finite volumes is briefly discussed.

Finite-Volume Difference Schemes for the Black-Sholes Equation in Stochastic Volatility Models

T. Chernogorova, R. Valkov

We study numerically the two-dimensional Black-Sholes equation in stochastic volatility models (see E. Ekstrom and J. Tysk, JMAA, DOI:10.1016/j.jmaa.2010.04.014). For these models we construct finite-volume difference scheme using the appropriate boundary conditions. Numerical experiments are discussed.

On the Numerical Simulation of Unsteady Solutions for the 2D Boussinesq Paradigm Equation

C. I. Christov, N. T. Kolkovska, D. P. Vasileva

Boussinesq equation (BE) is the first model for surface waves in shallow fluid layer that accounts for both nonlinearity and dispersion. The balance between the steepening

effect of the nonlinearity and the flattening effect of the dispersion maintains the shape of the waves. In the 60s it was discovered that these permanent waves can behave in many instances as particles and they were called *solitons*. A plethora of deep mathematical results have been obtained for solitons in the 1D case, but it is of crucial importance to investigate also the 2D case, because of the different phenomenology and the practical importance. The accurate derivation of the Boussinesq system combined with an approximation, that reduces the full model to a single equation, leads to the Boussinesq Paradigm Equation (BPE):

$$u_{tt} = \Delta \left[u - F(u) + \beta_1 u_{tt} - \beta_2 \Delta u \right], \quad F(u) := \alpha u^2 \tag{1}$$

where u is the surface elevation, $\beta_1,\ \beta_2 > 0$ are two dispersion coefficients, and α is an amplitude parameter. The main difference of Eq. (1) from BE is that in the former one more term is present for $\beta_1 \neq 0$ called "rotational inertia".
It has been recently shown that the 2D BPE admits stationary soliton solutions as well. Even though no analytical formula for these solutions is available, they can be accurately constructed using either finite differences, perturbation technique, or Galerkin spectral method. Virtually nothing is known about the properties of these solutions when they are allowed to evolve in time and it is of utmost importance to answer the questions about their structural stability.
In order to devise a numerical time-stepping procedure we recast Eq. (1), as the following system:

$$v(x,y,t) := u - \beta_1 \Delta u, \quad v_{tt} = \frac{\beta_2}{\beta_1} \Delta v + \frac{\beta_1 - \beta_2}{\beta_1^2}(u - v) - \alpha \Delta F(u).$$

We design an implicit time stepping scheme for the above coupled system and solve it by the Bi-Conjugate Gradient Stabilized Method with ILU preconditioner. The scheme is second order accurate in space and time and unconditionally stable. We perform all standard tests to validate the algorithm: three different spatial grids and different time increments. The results from our numerical experiments show that for some values of the phase speed and relatively small times the unsteady solutions have a solitonic behaviour, although for large times the solution either transforms into a diverging propagating wave or blows-up. The threshold for the value of phase speed for which blow-up is observed depends mildly on the resolution of the grid, because a rougher grid has additional numerical dispersion that acts to diminish the role of the nonlinear terms.

Future Generation Memetic Algorithms

C. Cotta

The two last decades hat witnessed the emergence of memetic algorithms (MAs) as one of the weapons-of-choice for dealing with hard optimization problems. The pragmatic philosophy of MAs, open to synergistic combinations with other search techniques and any other way of incorporating problem-knowledge to the optimization

process, has led to more and more complex algorithmic models. Indeed, while early implementations of MAs were mostly based on incorporating some classical local-search strategy (such as hill climbing or simulated annealing) to an otherwise standard genetic algorithm –incidentally paving the way to a reductionist characterization of MAs as evolutionary algorithms endowed with some local-search technique– much more sophisticated models have been devised in the last years, featuring architectures and approaches that were hinted in the 80s yet unattainable until recently.

We survey these current advances in MAs, such as self-adaptation, discovery of local-search strategies, and interaction with complete techniques among other salient features, and take a look at some of the capabilities the future can bring to these techniques, focusing in particular on search completeness, and exploitation of distributed knowledge. Some important challenges stand in our way to these future generation MAs, and these will be briefly discussed as well.

Generalized Expo-rational B-splines and Isogeometric Analysis

L. T. Dechevsky

At the Seventh International Conference on Mathematical Methods for Curves and Surfaces in Tønsberg, Norway, in June 2008, at the lecture of Thomas J.R. Hughes, on which I was also present, Tom Hughes informed the geometric modelling community of the world of his vision of a united approach to geometric modelling in Computer Aided Geometric Design (CAGD) and finite element analysis (FEA) in the modelling and simulation via boundary-value problems for PDEs. The main common tool which Tom Hughes proposed was the current industrial standard in CAGD: Non-Uniform Rational B-splines (NURBS), and the NURBS-based methods proposed by him gave the start of *Isogeometric Analysis*.
On the next day of the afore-mentioned conference, I gave for the first time a communication on the topic of Generalized Expo-rational B-splines (GERBS), with Tom Hughes, Larry Schumaker, Tom Lyche and other well-known spline specialists in the audience. What seemed to impress the audience most, was the possibility to easily construct GERBS-based smooth convex partitions of unity on triangulations, where each GERBS had the support of the usual piecewise linear/affine B-spline (i.e., the star-1 neighbourhood of 'its' vertex in the triangulation) while at the same time GERBS was smooth, and multiplication of each GERBS with a coefficient which was not constant, but a Taylor polynomial 'around the vertex of the GERBS' immediately implied Hermite interpolation at this vertex of all derivatives present in the Taylor polynomial. The conversion to 'Bezier form' was also done effortlessly by simply changing the monomial basis in the Taylor polynomial around each vertex with respective *tensor-product* Bernstein basis; moreover, this conversion was done independently for every vertex in the triangulation, i.e., the procedure was readily

parallelized.
During and after the conference there was a lot of interest in the multivariate constructions based on GERBS, but I requested (at least) one year more to work on the development of the theory before starting to publish relevant results. This is why the first results on this topic began to appear in the late 2009 and in 2010.
The purpose of the present communication is to inform the Numerical Analysis community about the great potential GERBS have in CAGD and FEA, and to convince the audience that the Non-Uniform Rational Generalized Expo-Rational B-splines (NURGERBS) vastly outperform NURBS as a universal tool of Isogeometric Analysis.

First Instances of Euler Beta-function B-splines and Simplicial Finite Elements on Triangulations

L. T. Dechevsky, B. Bang, A. R. Kristoffersen, A. Lakså, P. Zanaty

In the univariate case, the derivative of an expo-rational B-spline (ERBS) between the consecutive knots t_k, $t_{k+1} : t_k < t_{k+1}$ of a strictly increasing knot-vector is either identically zero or it is an expo-rational function (i.e., a function which is the exponent of a rational function taking negative values for $t : t_k < t < t_{k+1}$ and having poles at t_k and t_{k+1}). The computation of the integral in the definition of ERBS is by fast-converging numerical quadratures. Euler Beta-function B-splines (BFBS) are an instance of generalized ERBS (GERBS) where some tradeoff has been made between the properties and the ease of computation. In the case of BFBS, the expo-rational bell-shaped function in the definition of the derivative of ERBS is replaced by a Bernstein polynomial rescaled to the interval $[t_k, t_{k+1}]$. While multiplying ERBS with a Taylor series in powers of $t - t_k$ of an analytic function makes sense and has the effect of transfinite Hermite interpolation, the same can be done with the BFBS only with a Taylor polynomial of degree not exceeding the multiplicity of t_k as a zero of the respective Bernstein polynomial. What is lost in the range of this important property is compensated in the ease of computation of the BFBS which is piecewise polynomial. This advantage considerably increases in the multivariate case, and especially on triangulated domains, since BFBS continues to be piecewise polynomial on every triangle of its support.
The purpose of this communication is to provide first instances of smooth BFBS associated with the vertices of a triangulation and supported (like the respective ERBS) on the star-1 neighbourhood of 'its'vertex (the same support as that of the respective piecewise linear/affine B-spline), as well as first instances of the corresponding BFBS simplicial finite elements associated the triangles in the triangulation, with Hermite interpolation on their boundary.

Solving Multidimensional Computational Geometric Problems on Graphics Processing Units

L. T. Dechevsky, B. Bang, A. Lakså, J. Bratlie, J. Gundersen

In previous part of this research (L.T. Dechevsky, B. Bang, J. Gundersen, A. Lakså, A.R. Kristoffersen, Solving nonlinear systems of equations on graphics processing units, In: I. Lirkov, S. Margenov, and J. Wasniewski (Eds.) LSSC'2009, LNCS 5910, Springer-Verlag, Berlin-Heidelberg, 2010, to appear) a method for isometric immersion of smooth multivariate multidimensional vector-fields onto fractal curves and surfaces was used for solving nonlinear systems of equations on graphics processing units (GPUs) used as general-purpose parallel computing architectures. From the point of view of computational geometry these results translate as solving multidimensional intersection problems where the dimension is typically higher than 3. In the present communication we consider for the first time the more general problem of computing closest points between multidimensional manifolds, where the dimension is $2, 3, 4, \ldots$. We briefly discuss also the possibility to use the same approach for solving other multidimensional geometric problems and doing comparative analysis of the geometric properties of multidimensional manifolds.

Computing n-Variate Orthogonal Wavelet Transforms on Graphics Processing Units II: Bijective Mapping Between the Local and Global Indices

L. T. Dechevsky, J. Gundersen, B. Bang

In the previous part of this study (L.T. Dechebsky, J. Gundersen, B. Bang, Computing n-Variate Orthogonal Wavelet Transforms on Graphics Processing Units, In: I. Lirkov, S. Margenov, and J. Wasniewski (Eds.) LSSC'2009, LNCS 5910, Springer-Verlag, Berlin-Heidelberg, 2010, to appear) we outlined a new algorithm for matching an n-variate orthonormal wavelet basis $b_{n,j(n)}$ obtained via multiresolution analysis up to a given resolution level $j(n)$, $n = 3, 4, \ldots$, bijectively onto 1- and 2-variate bases $b_{k,j(k)}$, $k = 1, 2$, of the same type but with lower number of variables $k < n$ and with higher resolution level $j(k) > j(n)$, so that the dimensions of the bases are the same. We termed this approach *isometric conversion between dimension and resolution*, and described the resulting algorithm up to *a bijection between respective blocks of basis functions*. This is enough to show that the algorithm provides a matching of the bases and that this matching is unique. However, for the actual computational purposes it is necessary to move one step further by elaborating the construction down to matching the individual basis functions in the blocks. This is the purpose of the present paper, whose main new result is a bijective mapping between the local indices in each of the

afore-mentioned blocks and a global set of indices which defines the number of the basis function in the basis. With the help of this bijection we define a 1-1 mapping between the indices of $b_{n,j(n)}$ and $b_{k,j(k)}$ for any two natural n and k. When $k = 2$ we use this for computing of the n-variate discrete wavelet transform (DWT) on the graphics processing unit(s) (GPU(s)) of the computer, used as a parallel processing architecture.

Generalized Expo-rational B-splines and Unconditionally Stable Explicit Finite Element Methods for Initial-Value Problems for ODEs

L. T. Dechevsky, P. Zanaty

The exposition will begin with a very concise overview of relevant recent progress in the theory of expo-rational B-splines (ERBS) and their generalizations (GERBS) including, among others, the so-called Beta-function B-splines (BFBS). The generalized Vandermonde matrix for Hermite interpolation using these new B-spline bases (which have recently been designed also for Hermite interpolation on scattered point sets in domains of any dimension) is always block-diagonal, in Jordan normal form. Thus, these B-splines provide an excellent isogeometric representation, being simultaneously a convenient and efficient tool in Computer Aided Geometric Design and a similarly convenient and efficient tool for solving initial-value and boundary-value problems for domains with difficult geometry in dimensions 2, 3, 4, and higher, and for high-order PDEs. In the present communication, which will be first on this topic, we shall start only with the simplest type of 1-variate problems: Cauchy problems for linear ODEs of any order with variable coefficients and right-hand side. As we shall show, already in this simple case the new type of B-splines makes an impact. The approximate solution is an Hermite interpolant based on GERBS over a possibly non-uniform knot-vector, and the numerical solution has the following remarkable properties: (a) The issue of stability of the numerical solution is completely eliminated. The numerical solution is always stable for any knot-vector, provided that there is an a priori estimate for the *exact* solution. (b) The ERBS-based Hermite interpolant has transfinite order of accuracy. (c) For the initial-value problems considered, the stiffness matrix is upper-triangular and band-limited, i.e., the method is explicit. (d) Modification and refining of a mesh lead to a very easy recomputation of the solution. Thus, multigrid methods with such approach are easy in implementation, cheap in computations, and very fast in convergence. (e) The method works without any modifications also when the ODE degenerates (has variable order).
If the presentation time and the publication space permits, we may briefly consider the question about preservation of order constraints by the GERBS-based approximate solution in the cases of positivity, monotonicity, convexity, k-monotonicity of the exact solution, as well as the question about one-sided approximation in these cases.

Monte Carlo Method for Numerical Integration Based on Sobol' Sequences

I. Dimov, R. Georgieva

An efficient Monte Carlo method for multidimensional integration is proposed and studied. The method is based on Sobol' sequences. Each random point in d dimensional domain of integration is generated in the following way. A Sobol' vector of dimension d ($\Lambda\Pi\tau$ point) is considered as a centrum of a sphere with a radius ρ. Then a random point uniformly distributed on the sphere is taken and a random variable is defined as a value of the integrand at that random point. It is proven that the mathematical expectation of the random variable is equal to the desired multidimensional integral. This fact is used to define a Monte Carlo algorithm with a low variance.
Numerical experiments are performed in order to study the quality of the algorithm depending of the radius ρ, and dimensionality of the problem.

Numerical Investigation of Self-Similar Solutions of a Reaction Diffusion Equation in a Vicinity of Critical Parameters

M. Dimova, S. Dimova

The self-similar problem considered is a boundary value problem for nonlinear elliptic equation. The problem has not unique solution. We focus our study on the numerical computing of the so called "spiral wave solutions".
The proposed approach is based on the continuous analog of the Newton's method and finite element methods. To reveal solutions of spiral structure appropriate initial approximations are used. The last ones are solutions of a linearized equation and are expressed by the confluent hypergeometric function ${}_1F_1(a, b; z)$. So one needs an accurate, fast and reliable computation of its values for different parameter regimes within the complex plane for the parameters a and b, as well as for different regimes of the variable z. In order to achieve this we worked out algorithms based on various methods and appropriate for different parameter ranges: Taylor expansions, asymptotic series computations, an expansion in ascending series of Chebyshev polynomials.
Another crucial point of the numerical realization is to derive a suitable boundary condition. It should be obtained from the asymptotic of the nonlinear equation. To do that one needs the asymptotic of the solution of the linearized equation, i.e. of the confluent hypergeometric function.
A detailed numerical analysis of the evolution of the "spiral wave solutions" for various medium parameters including critical values is carried out. The accuracy of this method is experimentally analyzed using embedded grids.

Using Monte-Carlo Simulation for Risk Assessment: Application to Occupational Exposure During Remediation Works

M. L. Dinis, A. Fiúza

The aim of this study was to apply the Monte-Carlo techniques to develop a probabilistic risk assessment.
The risk resulting from the occupational exposure resulting from the activities involved in the remediation of a uranium tailings disposal, in an abandoned uranium mining site, was assessed. A hypothetical exposure scenario was developed and two different exposure pathways were compared: internal exposure through radon inhalation and external exposure through gamma irradiation from the contaminated tailings material.
The input variables, such as the inhalation rate and the external exposure parameters, were considered as specific probabilistic distributions, each one characterized by its central tendency and dispersion parameters. Using the cumulative distribution function a probabilistic value for each variable can be generated using a single random number. As a consequence, this methodology allows performing a probabilistic risk assessment, generating a risk distribution.
In general terms radon inhalation contributed up to 52% of the total risk while external gamma radiation contributed up to 48%. The results showed that the median (50th percentile) of the carcinogenic annual risk of the workers directly involved in the remediation was 0,000103, while considering the individual increment lifetime risk the median was 0,0072.
Comparative risk significance with calculated deterministic doses was also performed and the results showed that the highest contribution to the dose, the external gamma irradiation, does not correspond to the highest probabilistic risk originated by radon inhalation. The latter should be taken in consideration when assessing human health exposure.

WRF-Fire Applied in Bulgaria

N. Dobrinkova, G. Jordanov, J. Mandel

WRF-Fire is a coupled atmosphere-fire behavior module of WRF (Weather Research and Forecasting Model) based on the NCAR atmosphere model equivalent to the MM5 model. WRF-Fire can be used either for research or operational system for fine calculations. In this paper we are focused on the research opportunities of the module applicable for description of a fire behavior by modifying the open source of the tool. The tool is not officially released by NCAR and a small number of the fire research community is testing it. That is why the modifications are still possible with the source code.

Bidirectorial Beam Propagation Method Applied for Lasers with Multilayer Active Medium

N. N. Elkin, A. P. Napartovich, D. V. Vysotsky

Optical devices that have piecewise continuous gain and index distributions along the main propagation direction are widespread. A typical example of such a device is the vertical cavity surface emitting laser (VCSEL). The steady-state oscillating modes of a laser are described by non-linear partial differential equations containing eigenvalues. The problem to find such modes numerically is very difficult on account of several circumstances. The eigenvalue problem of high dimension has to be solved in order to find the modal wave field and frequency of oscillations. The eigenvalue problem is non-linear in the general case because of light-medium interaction. The multilayer medium in the laser cavity complicates considerably the mathematical modeling because of partial reflections from the layer interfaces.

We present the effective numerical method for lasers with multilayer medium based on the bidirectorial beam propagation method (BiBPM). Previously, this method was developed for case of wave propagation through the multilayer structure. The applications of BiBPM for laser devices were restricted by linear eigenvalue problem neglecting influence of the light beam on gain and index of the active medium. The eigenvalue problems for a non-hermitian matrix of high dimension were solved numerically.

The round-trip operator technique is presented in the given paper based on BiBPM. Similarly to traditional Fox-Li technique our method not requires explicit calculation of matrix of the round-trip operator and suits perfectly to Krylov subspace methods of linear algebra. The presented method is extended in natural way to non-linear case taking into account light-medium interaction. The results of modeling of a VCSEL with a resonant array of quantum wells are presented.

Bulgarian Operative System for Chemical Weather Forecast

I. Etropolska, M. Prodanova, D. Syrakov,
K. Ganev, N. Miloshev, K. Slavov

In the paper, an operational prototype of the Integrated Bulgarian Chemical Weather Forecasting and Information System is presented. The system is foreseen to provide in real time forecast of the spatial/temporal Air Quality behavior for the country and (with higher resolution) for selected sub-regions and cities. The country-scale part of the system is designed, being tested and is running operationaly. It is based on the US EPA Models-3 System (MM5, SMOKE and CMAQ). The meteorological input to the system is the operational numerical weather forecast. The emission input exploits a high resolution disaggregation of the EMEP 50x50 km inventory for year 2000. When elaborated, the actual national emission inventory is foreseen to be used. The boundary conditions are prepared by a similar system running operationally in

Aristotle University of Thessaloniki, Greece. The System automatically runs twice a day (00 and 12 UTC) and produces 48-hour forecast. The results of each System's run are post-processed in a way to archive the most important pollutants' forecasts as to compare them with the respective measurements for the sake of verification of the System. Part of these pollutants is visualized as sequences of maps giving the evolution of the air quality over the country. The plots are uploaded to a specialized web-server. The web-site is constructed in a way to show both forecasts for specified moments of time and animations for all forecast period for a number of key species. In the paper, description of the System is given together with a demonstration of its products.

Discontinuous Galerkin Finite Element Method for Convection-Diffusion Problems and Compressible Flow

M. Feistauer

In this paper we shall be concerned with several aspects of the numerical solution of nonlinear, nonstationary, convection-diffusion problems by the discontinuous Galerkin finite element method (DGFEM) and applications to compressible flow. The DGFEM is based on a piecewise polynomial approximation of the sought solution without any requirement on the continuity on interfaces between neighbouring elements. It is particularly convenient for the solution of conservation laws with discontinuous solutions or singularly perturbed convection-diffusion problems with dominating convection, when solutions contain steep gradients.
In the first part we shall be concerned with theoretical analysis of error estimates of various versions of the DG discretization applied to a scalar initial-boundary value problem. We shall discuss the error estimates for space semidiscretization and some types of full space-time discretization.
In the second part, some applications of the DGFEM to the simulation of compressible flow, i.e. the solution of the compressible Euler and Navier-Stokes equations, will be presented. Our goal is to develop sufficiently accurate, efficient and robust numerical schemes allowing the solution of compressible flow for a wide range of Reynolds and Mach numbers, applicable to flow simulation in time dependent domains and to fluid-structure interaction. The efficiency and accuracy of the method will be demonstrated by computational results.

Start Strategies of ACO Applied on Subset Problems

S. Fidanova, P. Marinov, K. Atanassov

Many combinatorial optimization problems are fundamentally hard. This is the most typical scenario when it comes to realistic and relevant problems in industry and science. Examples of optimization problems are Traveling Salesman Problem, Vehicle Routing, Minimum Spanning Tree, Multiple Knapsack Problem, etc. They are NP-hard problems and in order to obtain solution close to the optimality in reasonable

time, metaheuristic methods are used. One of them is Ant Colony Optimization (ACO).
ACO algorithms have been inspired by the real ants behavior. In nature, ants usually wander randomly, and upon finding food return to their nest while laying down pheromone trails. If other ants find such a path, they are likely not to keep traveling at random, but to instead follow the trail, returning and reinforcing it if they eventually find food. However, as time passes, the pheromone starts to evaporate. The more time it takes for an ant to travel down the path and back again, the more time the pheromone has to evaporate and the path to become less prominent. A shorter path, in comparison will be visited by more ants and thus the pheromone density remains high for a longer time. ACO is implemented as a team of intelligent agents which simulate the ants behavior, walking around the graph representing the problem to solve using mechanisms of cooperation and adaptation.
Our novelty is to use estimations of start nodes with respect to the quality of the solution and thus to better menage the search process. On the basis of the estimations we offer several start strategies and their combinations. Like a benchmark problem is used Multiple Knapsack Problem (MKP), which is a representative of the class of subset problems, because a lot of real world problems can be represented by it and MKP arise like a subproblem in many optimization problems.

Sensityvity Analysis of ACO Start Strategies for Subset Problems

S. Fidanova, P. Marinov, K. Atanassov

The difficulties associated with using mathematical optimization on large-scale engineering problems, have contributed to the development of alternative solutions. Linear programming and dynamic programming techniques, for example, often fail in solving NP-hard problems with large number of variables. To overcome these problems, researchers have proposed mataheuristic methods for searching near-optimal solutions to problems. One of the most successful metaheuristic is Ant Colony Optimization (ACO).
Real ants foraging for food lay down quantities of pheromone (chemical cues) marking the path that they follow. An isolated ant moves essentially at random but an ant encountering a previously laid pheromone will detect it and decide to follow it with high probability and thereby reinforce it with a further quantity of pheromone. The repetition of the above mechanism represents the auto-catalytic behavior of a real ant colony where the more the ants follow a trail, the more attractive that trail becomes. ACO is inspired by real ant behavior to solve hard combinatorial optimization problems. The ACO algorithm uses a colony of artificial ants that behave as cooperative agents in a mathematical space where they are allowed to search and reinforce pathways (solutions) in order to find the optimal ones. The problem is represented by graph and the ants walk on the graph to construct solutions. The solutions are represented by paths in the graph. After the initialization of the pheromone trails, the ants con-

struct feasible solutions, starting from random nodes, and then the pheromone trails are updated. At each step the ants compute a set of feasible moves and select the best one (according to some probabilistic rules) to continue the rest of the tour.
The novelty in this work is the use of estimation of start nodes with respect to the quality of the solution and thus to better menage the search process. Various start strategies and their combinations are offered. Sensitivity analysis of the algorithm according strategy parameters is made. Our ideas is applied on Multiple Knapsack problem like a representative of the subset problems.

Numerical Modeling in Electrochemistry by Voronoi Finite Volume Methods

J. Fuhrmann, K. Gärtner, M. Ehrhardt,
A. Linke, H. Langmach, H. Zhao

Electrochemical devices like fuel cells and batteries are characterized by strongly coupled complex phyiscal processes. Mathematical modeling and numerical simulation of such devices, and also of supporting experiments like flow cells, are valuable tools to gain better insight into various apects of their functioning.
Due to its capability to preserve important physical properties of the continuous problem, Voronoi box based finite volume methods are our method of choice when it comes to the space discretization of such problems. We discuss advantages and challenges of this method and present results of numerical simulations of electrochemical devices.

On Finite Volume Methods for Coupled Flows on Delaunay Meshes and the Preservation of the Local Maximum Principle

J. Fuhrmann, A. Linke

We present new approaches for the discretization of coupled flow processes, in which convection-diffusion equations are coupled with the incompressible Navier-Stokes equations. The discretization aims at the discrete preservation of the local maximum principle in the convection-diffusion processes and it is based on the classical vertex-based finite volume method on boundary-conforming Delaunay meshes. The incompressible Navier-Stokes equations are discretized by a dual-grid approach, which is an extension of the classical MAC scheme to unstructured simplex meshes.

A Highly-Parallel TSP Solver for a GPU Computing Platform

N. Fujimoto, S. Tsutsui

The traveling salesman problem (TSP for short) is probably the most widely studied combinatorial optimization problem and has become a standard testbed for new algorithmic ideas. Recently the use of a GPU (Graphics Processing Unit) to accelerate non-graphics computations has attracted much attention due to its high performance and low cost.

This paper presents a novel method to solve TSP instances with a GPU based on the CUDA architecture. Especially for CUDA, the proposed method highly parallelizes a serial metaheuristic algorithm which is a genetic algorithm with the OX (order crossover) operator and the 2-OPT local search. Genetic algorithms have obvious parallelism among individuals. However, the parallelism is not enough to obtain high performance of a GPU. To utilize an advantage of "many-thread" architecture of CUDA, we extract not only the parallelism among individuals but also another parallelism in the processing of each individual. That is, we parallelize the execution of each OX operator and each 2-OPT local search, too.

To evaluate the effectiveness of the proposed method, we conduct some experiments for TSPLIB benchmark problem instances using an NVIDIA GeForce GTX285 GPU and a 3.0 GHz Intel Core 2 Duo E6850 CPU. The experimental results show that our GPU implementation is about up to 10 times faster than the corresponding CPU implementation.

Quite recently, CUDA has been successfully used to accelerate various applications in scientific fields such as fluid dynamics, image processing, and simulations. However, in the field of genetic algorithms, almost no result is known except for our QAP solver presented at the International Workshop CIGPU 2009. This is because genetic algorithms have special property of frequent random access to large data-structures, which is not the case in the other successful fields. This paper presents the first result on solving TSP with a GPU. Therefore, we believe that this paper provide considerable contribution for the workshop participants, in particular of interest in parallel metaheuristics on emerging GPU computing platforms.

Atmospheric Composition Studies for the Balkan Region

K. Ganev, G. Gadzhev, N. Miloshev, G. Jordanov,
A. Todorova, D. Syrakov, M. Prodanova

The main scientific challenge of local to regional atmospheric composition pattern modelling probably is the accounting for the strong dependence of concentrations on fluctuations of local and regional meteorological conditions, the complex interaction of transport scales (different life times of the pollutants make it even more complex), uncertainties and responses to emission forcing and boundary conditions,

both introducing information noise. Multi-scale numerical experiments have to be carried out, which to clarify to some extend different scale processes interaction, but also to further specify requirements for input data (emissions, boundary conditions, large scale forcing). Shortly speaking, extensive sensitivity studies have to be carried out, tailoring the model set-up and parameters a possible forerunner of single model ensemble forecasts. The present work aims at studying the local to regional atmospheric pollution transport and transformation processes over the Balkan Peninsula and at tracking and characterizing the main pathways and processes that lead to atmospheric composition formation in the region. The US EPA Model-3 system is chosen as a modelling tool because it appears to be one of the most widely used models with proved simulation abilities. The system consists of three components: MM5 - the 5th generation PSU/NCAR Meso-meteorological Model used as meteorological pre-processor; CMAQ - the Community Multiscale Air Quality System CMAQ; SMOKE - the Sparse Matrix Operator Kernel Emissions Modelling System the emission model. As the NCEP Global Analysis Data with 1 degree resolution is used as meteorological background, the MM5 and CMAQ nesting capabilities are applied for downscaling the simulations to a 9 km resolution over Balkans. The TNO emission inventory is used as emission input. Special pre-processing procedures are created for introducing temporal profiles and speciation of the emissions. The biogenic emissions of VOC are estimated by the model SMOKE. The air pollution transport is subject to different scale phenomena, each characterized by specific atmospheric dynamics mechanisms, chemical transformations, typical time scales etc. The specifics of each transport scale define a set of requirements for appropriate treatment of the pollutants transport and transformation processes, respectively for suitable modelling tools, data bases, scenarios and time scales for air pollution evaluation. The air pollution pattern is formed as a result of interaction of different processes, so knowing the contribution of each for different meteorological conditions and given emission spatial configuration and temporal behaviour is important for clarifying the atmospheric composition formation. Therefore the Models-3 Integrated Process Rate Analysis option is applied to discriminate the role of different dynamic and chemical processes for the pollution from road and ship transport. The processes that are considered are: advection, diffusion, mass adjustment, emissions, dry deposition, chemistry, aerosol processes and cloud processes/aqueous chemistry. Some results from several emission scenarios which make it possible to evaluate the contribution of different SNAP categories in many different terms spatial pattern, averaged over the Balkans, typical and extreme impacts, seasonal behaviour are demonstrated as well.

A Multiscale Stochastic Framework for Stokes-Darcy Flow and Transport

B. Ganis, D. Vassilev, I. Yotov, M. Zhong

We discuss a multiscale stochastic framework for uncertainty quantification in modeling flow and transport in surface-subsurface hydrological systems. The governing

flow equations are the Stokes-Darcy system with Beavers-Joseph-Saffman interface conditions. The permeability in the Darcy region is stochastic and it is represented with a Karhunen-Loève (KL) expansion. The porous media can be statistically non-stationary, which is modeled by different KL expansions in different regions. Statistical moments of the solution are computed via sparse grid stochastic collocation. The spatial domain is decomposed into a series of small subdomains (coarse grid) of either Stokes or Darcy type. The flow solution is resolved locally (on each coarse element) on a fine grid, allowing for non-matching grids across subdomain interfaces. The subdomain discretizations utilize stable Stokes or Darcy elements. Coarse scale mortar finite elements are introduced on the interfaces to approximate the normal stress and impose weakly continuity of flux. The transport equation is discretized via a local discontinuous Galerkin method. We precompute a multiscale basis, which involves solving subdomain problems with for each realization of the local KL expansion. The basis is then used to solve the coarse scale mortar interface problem in parallel for each global KL realization. The resulting algorithm is orders of magnitude faster than a global stochastic collocation approach. Error analysis for the statistical moments of the pressure, velocity, and tracer concentration is performed. Computational experiments are presented.

High Fidelity Finite Length Markov Chain Walks

J. Genoff

Given an irreducible markov chain model, what is the complete set of the highest fidelity state sequences of a given length (finite length walks), that the model is able to produce? Here, highest fidelity property means : 1) all sequences in the set have the same relative transition frequency matrix ; 2) according to some measure, the relative transition occurrence frequency matrix is as close to the model stochastic matrix as possible ; 3) each sequence starts with a state that has nonzero initial probability. A three stage approach for generation of such complete set is discussed : 1) calculation of the exact absolute transition occurrence numbers matrix, which in general, consists of non-integer values ; 2) application of controlled matrix rounding to the latter in order to obtain integer values for all transition occurrence numbers, which introduces a bias leading to the fidelity issue ; 3) generation of all sequences that satisfy the constraints for state transition occurrence numbers from the integer matrix, which can be done by any constraint preserving permutation group generating technique. This paper is focused on the first stage an original linear algebraic solution to the problem is proposed. Three distinct and mutually complementary intuitive constraint aspects of the finite length markov chain walks are formulated and formalized as three independent systems of linear equations with the exact absolute state transition occurrence numbers being the unknowns. Each system suffers from linear dependency among its equations. After proper elimination of certain part of each system and union of what is left of the three, one aggregated system is constructed. The conditions for the existence of such system's solution are investigated and its uniqueness is proven. The influence of solution's values over the existence of respective walks is considered.

Several interesting properties of the system and its solution are discussed, some of them with proofs. Since the coefficient matrix possesses a kind of sparseness, a specific optimized parallel solving procedure is devised and presented.

Analysis of the Constant in the Strengthened Cauchy-Bunyakowski-Schwarz Inequality for Quadratic Finite Elements

I. Georgiev, M. Lymbery, S. Margenov

This article considers the second order scalar elliptic boundary value problem. By discretisation using conforming quadratic finite elements, the problem can be reduced to finding a solution of a linear system of algebraic equations. Preconditioners based on various multilevel extensions of two-level finite element methods (FEM) lead to iterative methods which often have an optimal order of computational complexity with respect to the number of degrees of freedom of such a system. The key role in the derivation of optimal convergence rate estimates is played by the constant γ in the strengthened Cauchy-Bunyakowski-Schwarz (CBS) inequality, associated with the angle between the two subspaces of the splitting. More precisely, the upper bound for $\gamma \in [0, 1)$ contributes significantly to the construction of various multilevel extensions of the related two-level methods.
We study the behavior of the CBS constant for the Differences and Aggregates (DA) and First Reduce (FR) splitting of the unknowns of the system which would ultimately lead to the construction of an efficient multilevel preconditioner. The presented CBS constant estimates utilise the hierarchical basis $p - method$ for $p = 2$ where piecewise linear and piecewise quadratic basis functions are used at the vertex and mid-edge points respectively. The obtained estimates are compared with earlier results. The numerical tests are run on the software package Mathematica.

Specialized Sparse Matrices Solver in the Chemical Part of an Environmental Model

K. Georgiev, Z. Zlatev

A two-dimensional advection-diffusion-chemistry module of a large-scale environmental model (Danish Eulerian Model for studying the transport of air pollutants on large scale - UNI-DEM) is taken. The module is described mathematically by system of partial differential equations. Sequential splitting is used in the numerical treatment. The non-linear chemistry is most the time-consuming part during the computer runs and it is handled by six implicit algorithms for solving ordinary differential equations. This leads to the solution of very long sequences of systems of linear algebraic equations. It is crucial to solve these systems efficiently. This is achieved by applying four different algorithms which are developed, tested and discussed.

An Approach of Modeling ROOT Processes in Grid

R. Goranova

ROOT is an object-oriented framework, written in C++, which provides functionalities for data analysis and data visualization. It is a platform independent framework and run equally well on different operating systems as Windows or Linux. The development of ROOT services allow to the end user to use ROOT functionality without installing the environment and without knowing its specific. g-Lite is a grid middleware for access to Grid resources. It provides services for access to data storage and computational power. Data manipulation processing in Grid environment consists of the following generalized steps: data preparation, data storage, data computations and data analysis and visualization. These tasks can be presented as a process of sequential tasks, part of which uses Grid Services and the other, services provided by outside systems. Vital part of modeling of business processes is presence of service repository with registered services. The intention of current paper is to present an approach for modeling of business processes in Grid middleware based on example usage of ROOT and g-Lite services.

High-Order Explicit Local Time-Stepping for Damped Wave Equations

M. Grote, T. Mitkova

The accurate and reliable simulation of wave phenomena is of fundamental importance in a wide range of engineering applications. In the presence of complex geometry, adaptivity and mesh refinement are certainly key for the efficient numerical solution of the damped wave equation. Locally refined meshes, however, impose severe stability constraints on explicit time-stepping schemes due to the smallest elements in the mesh. When mesh refinement is restricted to a small region, the use of implicit methods, or a very small time step in the entire computational domain, are very high a price to pay. To overcome that stability restriction, local time-stepping methods are developed, which allow arbitrarily small time-steps precisely where small elements in the mesh are located. When combined with a finite element discretization in space with an essentially diagonal mass matrix, the resulting discrete numerical scheme is fully explicit.

Starting from the standard leap-frog scheme, explicit second-order local time-stepping integrators for transient wave motion have been derived. In the absence of damping these time-stepping schemes, when combined with the modified equation approach, yield methods of arbitrarily high (even) order. In the presence of damping, however, this approach cannot be used effectively. Therefore, we derive explicit local time-stepping schemes of arbitrarily high accuracy starting insted from explicit multi-step Adams-Bashforth methods. Numerical experiments validate the theoretical results and illustrate the efficiency of the proposed time integration schemes.

A New Class of Fractional Step Techniques for the Incompressible Navier-Stokes Equations Using Direction Splitting

J.-L. Guermond, P. D. Minev

A new direction-splitting-based fractional time stepping for solving the incompressible Navier-Stokes equations will be discussed. The main originality of the method is that the pressure correction is computed by solving a sequence of one one-dimensional elliptic problem in each spatial direction. The method is unconditionally stable, very simple to implement in parallel, very fast, and has exactly the same convergence properties as the Poisson-based pressure-correction technique, either in standard or rotational form.

Entropy Viscosity for Nonlinear Conservation Laws

J.-L. Guermond, M. Nazarov, R. Pasquetti, B. Popov

A new class of high-order numerical methods for approximating nonlinear conservation laws is described (entropy viscosity method). The novelty is that a nonlinear viscosity based on the local size of an entropy production is added to the numerical discretization at hand. This new approach does not use any ux or slope limiters, applies to any equation or system with one or more complementary entropy equations and does not dependent on the mesh type and polynomial approximation. Various benchmark problems are solved with finite elements, spectral elements and Fourier series to illustrate the capability of the proposed method.
The effect of the mass matrix is also discussed.

Forecasting the Composition of Demand for Higher Education Degrees by Genetic Algorithms

M. Hernández, J. J. Cáceres, M. Pérez

In this paper, a genetic algorithm is developed to forecast the relative presence of different university studies in the higher education demand in the field of economics and business/management as a whole. A selection operator is defined that assumes that the better the job opportunities associated with a specific university study, the higher the future demand for such a degree. The other element in the algorithm is a transition matrix that takes other factors into account which may influence on the changes in demand. The proposed algorithm is applied to the original populations of students enrolled on 2005/2006 to 2007/2008 courses. Then, a new algorithm, whose elements are corrected to adjust the forecasts, is applied to obtain the forecast of the demand composition on the 2009/2010 course.

A Non-Standard Finite Element Method Based on Boundary Integral Operators

C. Hofreither

We present a non-standard Finite Element Method that is based on the use of boundary integral operators and that permits polyhedral element shapes as well as grids with hanging nodes. The method can be interpreted as a local Trefftz method, i.e., the method employs element-wise PDE-harmonic trial functions. The construction principle requires the explicit knowledge of the fundamental solution of the partial differential operator, but only locally in every polyhedral element. This allows us to solve PDEs with elementwise constant coefficients. In this talk we consider the diffusion equation as a model problem, but the method can be generalized to convection-diffusion-reaction problems and to systems of PDEs like the linear elasticity system with element-wise constant coefficients.
We give rigorous error estimates for the three-dimensional case under quite general assumptions on the geometrical properties of the elements

Sensitivity of Results of the Water Flow Problem in a Discrete Fracture Network with Large Coefficient Differences

M. Hokr, J. Kopal, J. Březina, P. Rálek

This work deals with modelling of groundwater flow in a compact rock with network of discrete fractures. In a real system, it means the flow in a system of 2D planes (polygons) in the 3D space, in our 2D model problem (cross-section) it means the flow in s system of lines (abscissa) in 2D plane. The flow is governed by the Hagen-Poiseuille Law, which simply means potential flow with the coefficient (hydraulic conductivity) proportional to the width of the fracture (aperture for geologists) to the power of three.
The fracture network of the models is usually stochastically generated. The resulting problem has the features that large variations of the aperture and conductivity exist and that several very small fracture segments e.g. when three fractures cross just aside from a single point. This leads to the differences of the coefficients in the linear equations system from the finite elements up to ten orders of magnitude, with the consequence of numerical instability.
We compare two different numerical methods and simulation codes. The commercial NAPSAC using standard linear finite elements is one of the typical tools used by hydrogeologists for fractured rock problems. The code FLOW123D developed at the Technical University of Liberec (authors' group) uses mixed-hybrid finite element method with the flux mass balance by definition.
The test problem consists of 7797 fractures divided to 60052 segments. The agreement of results is quite unevenly distributed from percents for most of the values to

difference in orders of magnitude in few exceptions. The main difference is in the total mass balance error which is about 10^{-1} for NAPSAC and 10^{-5} for FLOW123D. The mentioned values with the large error are smaller contribution to the total flux and are comparable with the mass balance error, which is an argument for our code as more credible.

Fluxon Dynamics in Stacked Josephson Junctions

I. Hristov, S. Dimova

We use the Sakai-Bodin-Pedersen model – a system of perturbed sine-Gordon equations – to study numerically the dynamics of Josephson phases in stacks of inductively coupled long Josephson Junctions. The boundary conditions correspond to a stack of overlap geometry. In order to obtain appropriate initial values for the dynamic problem the corresponding static problem is solved as well. We are interested in solutions having one or two moving fluxons in each junction and seek for conditions under which a bunching of fluxons is possible. The current-voltage dependencies for different values of dissipation and coupling parameters for bunched and unbunched states are found. The regions of existence for these states with respect to the applied magnetic field and the external current are also calculated. To solve numerically the above problems Finite element method and Finite difference method are used.

Global Convergence Properties of the SOR-Weierstrass Method

V. H. Hristov, N. V. Kyurkchiev, A. I. Iliev

In this paper we give sufficient conditions for k-th approximations of the zeros of polynomial $f(x)$ under the successive over-relaxation Weierstrass method (SORW) fails on the next step. This is a further improvement of the known results. Interesting numerical examples are presented.

Message-Passing Algorithms in Markov Chains

T. Ignac, U. Sorger

The objective of this paper is to apply message-passing algorithms (e.g., belief propagation, sum-product algorithm) for investigating some properties of Markov chains. The message-passing algorithms are tools used for reasoning in the field of probabilistic graphical models (e.g., Bayesian Networks, factor graphs, etc.). Historically, Markov chains are not consider as a member of the family of probabilistic graphical models. Nevertheless, we argue that by applying tools from this field one can obtain some interesting results and conclusions related to the theory of Markov chains.
In the current paper, we focus our attention on the two following issues: a) an investigation of the passage time from a given initial state into a non-empty set of target

states; b) an analysis of the number of visits to a given set of states. In the second point, the target set can be defined dynamically, i.e., it changes with time. This is a new problem which has not been formulated before. Traditionally, such issues are considered in the context of the ergodic Markov chains, thus, one is interested in the asymptotic behavior of the chain when time goes to infinity. In contrary, we propose to consider a finite time-window. Hence, we deal with a finite vector of random variables $(X_1, ..., X_N)$ instead of an infinite chain of variables $X_1, X_2, ...$. Since in most of the practical applications the time-horizon is finite, this assumption is not strong. Moreover, the assumption of the ergodicity is not necessary for applying the proposed algorithms. The first passage time and the number of visits are random variables. We provide new algorithm for computing K first probabilistic moments of these variables. However, the most advanced result is a method for discovering probability distributions of these variables.
The novelty of the proposed work is threefold. Firstly, the methodology is new. Best to our knowledge, the message-passing algorithms have not been used in such a context before. Secondly, the computational complexity of our algorithms is often lower (and never higher) than the complexity of other existing solutions. Thus, our method can be applicable to Markov chains with a large state space. Finally, the algorithms based on the message-passing paradigm can be easily implemented. Therefore, we argue that our work may have an impact on the practical applications of Markov chains.

Numerical Upscaling of Flows in Highly Heterogeneous Porous Media

O. P. Iliev, R. D. Lazarov, J. Willems

The generalized Stokes equations (called also Brinkman equations),

$$-\mu\Delta u + \nabla p + \mu\kappa^{-1}u = f,\ \nabla \cdot u = 0 \ \text{ in } \Omega,$$

where μ is the viscosity and κ is the permeability, are used for modeling flows in highly porous media. Examples of such media are industrial open foams, filters, and insulation materials.Motivated by industrial applications of such materials we have developed a numerical method for comuting flows in heterogeneous highly porous media with complicated internal structure of the permeability.
We will present a two-scale finite element approximation of Brinkman equations. The method uses two main ingredients: (I) discontinuous Galerkin finite element method for Stokes equations, proposed and studied by J. Wang and X. Ye (2007, SINUM, v. 45) and (II) subgrid approximation developed by T. Arbogast for Darcy equations (2004, SINUM, v. 42).
There are two different applications of the proposed method: (1) numerical upscaling of Brinkman equations on coarse-grid that incorporates fine-grid features, and (2) an alternating Schwarz iteration that uses the coarse-grid in domain decomposition setting. In order to reduce coarse-grid boundary layer errors and to ensure convergence

to the global fine solution, the algorithm uses overlapping subdomains around the coarse-grid interfaces. A number of numerical examples will be presented to demonstrate the performance of both the subgrid method and the iterative procedure.

Modeling of Species and Charge Transport in Li-Ion Batteries

O. Iliev, A. Latz, J. Zausch

In order to improve the design of Li ion batteries the complex interplay of various physical phenomena in the active particles of the electrodes and the electrolyte has to be balanced. The separate transport phenomena in the electrolyte and in the active particle as well as their coupling due to the electrochemical reactions at the interfaces between the electrode particles and the electrolyte will influence the performance and the lifetime of a battery. Any modelling of the complex phenomena during the usage of a battery has therefore to be based on sound physical and chemical principles in order to allow reliable predictions for the response of the battery to changing load conditions. We will present a modelling approach for the transport processes in the electrolyte and the electrode based on non-equilibrium thermodynamics and transport theory. Numerical solution of the resulting highly nonlinear coupled equations for ion concentrations, ion flux and electrical currents, is a challenging task. Here we briefly present some simulation results obtained with our research code BEST (Battery and Electrochemistry Simulation Tool), which is developed at the Fraunhofer ITWM in cooperation with Institute for Parallel Processing, Sofia. More detailed discussions on numerical approaches for this system will be presented in two other talks in this special session.

Finite Volume Discretization of Nonlinear Diffusion in Li-Ion Batteries

O. Iliev, S. Margenov, P. Popov, Y. Vutov

Numerical modeling of electrochemical process in Li-Ion problems is an emerging topic of great practical interest. In this work we present a Finite Volume discretization of electrochemical diffusive processes occurring during the operation of Li-Ion batteries. The system of equations is a nonlinear, time-dependent diffusive system, coupling the Li concentration and the electric potential. The system is formulated at length-scale in which two different types of domains are distinguished, one for electrolyte and one for cathode/electrode. The domains can be of highly irregular shape, with the electrolyte occupying the pore space of a porous solid electrode. The material parameters in each domain differ by several orders of magnitude and can be nonlinear. Moreover, special interface conditions are imposed at the boundary separating the electrolyte from an electrode. The field variables are discontinuous across such an interface and the coupling is highly nonlinear, rendering direct iteration methods ineffective

for such problems. We formulate a Newton iteration for the coupled system. A series of numerical examples are presented for different type of electrolyte/electrode configurations and material parameters. The convergence of the Newton method is characterized both as function of nonlinear material parameters as well as the nonlinearity in the interface conditions.

Numerical Solution of a Nonlinear Evolution Equation for the Risk Preference

N. Ishimura, M. N. Koleva, L. G. Vulkov

A singular nonlinear partial differential equation (PDE), which describes the evolution of the risk preference in the optimal investment problem under the random risk process was derived by the first author in previous publications. The quantity is related to the Arrow-Pratt coefficient of relative risk aversion with respect to the optimal value function. The present paper deals with the construction of a finite difference scheme and the numerical analysis of its solution for the above mention PDE.

A Numerical Approach for the American Call Option Pricing Model

J. D. Kandilarov, R. L. Valkov

We present a numerical approach of the free boundary problem for the Black-Scholes equation for pricing the American call option on stocks paying a continuous dividend. A fixed domain transformation of the free boundary problem into a parabolic equation defined on a fixed spatial domain is performed. As a result a nonlinear time-dependent term is involved in the resulting equation. Two iterative numerical algorithms are proposed. Computational experiments, confirming the accuracy of the algorithms are discussed.

Auxiliary Space Preconditioner for a Locking-free Finite Element Approximation of the Linear Elasticity Problem

E. Karer, J. Kraus, L. Zikatanov

In this talk we consider a stable finite element discretization of the equations of linear elasticity, introduced by R. Falk (R. Falk, Nonconforming finite element methods for the equations of linear elasticity. Math. Comp., 57(196), 1991, pp. 529–550), with a focus on nearly incompressible materials. This discretization does not suffer from so-called locking effects as they are observed when using standard low(est) order conforming methods for the pure displacement formulation. In case of pure traction boundary conditions optimal order error estimates are available based on an

appropriate discrete version of Korn's second inequality. The focus of this work is on constructing uniform preconditioners for the linear systems arising from this discretization scheme. We introduce an auxiliary space method which consists in solving an auxiliary problem that involves a bilinear form on a larger auxiliary space. By defining a proper projection from this larger space to the original space a suitable preconditioner for the original problem can be set up. We discuss the details of the construction, derive spectral equivalence results based on the fictitious space lemma and present numerical experiments.

A Numerical Study of a Parabolic Monge-Ampère Equation in Mathematical Finance

M. N. Koleva, L. G. Vulkov

We propose an iterative finite difference method for solving the initial value problem of the parabolic Monge-Ampère equation, arising from the optimal investment of mathematical finance theory. We investigate the positivity and convex preservation properties of the numerical solution. Convergence results are also given. Numerical experiments demonstrate the efficiency of the algorithm and verify theoretical statements. Comparison results with classical weighted implicit method are also given.

Convergence of Finite Difference Schemes for a Multidimensional Boussinesq Equation

N. Kolkovska

We consider the Cauchy problem for the nonlinear Boussinesq equation

$$\frac{\partial^2 u}{\partial t^2} = \Delta u + \beta_1 \Delta \frac{\partial^2 u}{\partial t^2} - \beta_2 \Delta^2 u + \alpha \Delta f(u), \quad x \in \mathbb{R}^d, \ t > 0,$$
$$u(x,0) = u_0(x), \quad \frac{\partial u}{\partial t}(x,0) = u_1(x),$$

where α, β_1, β_2 are positive constants and the solution u additionally satisfies the asymptotic boundary conditions $u(x,t) \to 0$, $\Delta u(x,t) \to 0$ as $|x| \to \infty$. Typically, the nonlinear term is $f(u) = u^2$.
Depending on the way the nonlinear term $f(u)$ is approximated, we develop two families of finite difference schemes.
We obtain error estimates for these numerical methods in Sobolev space.
The extensive numerical experiments for the one-dimensional problem show good precision and full agreement between the theoretical results and practical evaluation for single soliton and the interaction between two solitons.

Evaluation of an Expo-rational B-spline for the Scalable Subset of Its Intrinsic-parameter Set

A. Lakså

Expo-rational B-splines (ERBS) provide a convenient isogeometric representation of curves, surfaces, volume deformations and higher dimensional manifolds which can be used for both geometric modeling purposes in Computer Aided Geometric Design and for computational purposes in finite and boundary element analysis.
The derivative of an ERBS between the consecutive knots $t_k, t_{k+1} : t_k < t_{k+1}$ of a strictly increasing knot-vector is either identically zero or it is an expo-rational function (i.e., a function which is the exponent of a rational function taking negative values for $t : t_k < t < t_{k+1}$ and having poles at t_k and t_{k+1}).
There is a set of parameters in the definition of ERBS which are being referred to as *the set of intrinsic parameters* of this ERBS. This name is justified by the fact that they influence the curvature of the graph of the ERBS between t_k and t_{k+1}, and for an ERBS curve in 3 and higher number of dimension these parameters influence both the curvature and the torsion of this curve.
The purpose of the present paper, and its main new result, is the identification of the exact maximal subset of the set of admissible intrinsic parameters of ERBS for which all ERBS basis functions are obtained as dilations and translates of one 'scaled' ERBS. We coin this subset to be *the scalable subset of the intrinsic-parameter set* of ERBS. The scaled ERBS can be precomputed once and forever, and can be used for fast computation of ERBS-based geometric models. In our software applications we use iterative Romberg integration for the precomputing of the scaled ERBS but the use of other positivity-preserving quadratures, such as, e.g., Gaussian quadratures, is also of interest. All of these quadrature processes are very rapidly converging, because the integrand is infinitely smooth.

A Numerical Approach for Obtaining Fragility Curves in Seismic Structural Mechanics: A Bridge Case of Egnatia Motorway in Northern Greece

A. Liolios, S. Radev

Development of vulnerability relationships for Civil Engineering structures represents a critically important step in damage estimation process. Scope of the vulnerability analysis is the creation of the so-called fragility curves, through which the probability that a specific damage level will be exceeded for a given intensity of a seismic event may be quickly estimated, supporting significantly the decision-making procedures. In the present article, a simplified numerical methodology for the evaluation of vulnerability curves for bridges is presented. The methodology is based on the Finite Element Method and combines the nonlinear static pushover procedure and the capacity spectrum method [1]. The presented methodology is applied for establishing

fragility curves for an existing reinforced concrete bridge in the Krystalopigi Psilorahi section of Egnatia Motorway, in the county of Epirus, Greece. Egnatia Odos is the Motorway that crosses northern Greece in an E-W direction. It is currently the largest and technically the most demanding highway project in Greece, and one of the biggest infrastructure ones under construction in Europe. Its main axis has a length of 670km and includes about 1900 structures (bridges and culverts). The bridge examined herein is structurally representative of hundred of bridges in Egnatia Motorway and in Greece more generally [2].
LITERATURE 1. Chopra, A.K.: Dynamics of Structures. Theory and Applications to Earthquake Engineering. Pearson Prentice Hall, New Jersey (2007). 2. ASPROGE: Research Project for the ASeismic PROtection of Bridges. Egnatia Odos S.A., Thessaloniki, Greece (2007).

A Numerical Investigation for the Optimal Contaminant Inlet Positions in Horizontal Subsurface Fllow Wetlands

K. Liolios, S. Radev, V. Tsihrintzis

A numerical treatment of flow and contaminant removal in porous media is presented. Emphasis is given to horizontal subsurface flow constructed wetlands, which are recently a good alternative solution for small settlements in order to treat municipal wastewater. The purpose here is to find their optimal design characteristics as concerns the contaminant inlet positions, in order to maximize their removal efficiency and keep their area and construction cost to a minimum. First the mathematical modelling is presented, leading to a boundary-initial value problem. Next, for the numerical simulation, the Visual MODFLOW code, based on the finite difference method, is used. Further, the numerical procedure is applied for the simulation of pilot-scale units of horizontal subsurface flow wetlands. The above pilot-scale units were constructed and operated in the Laboratory of Ecological Engineering and Technology, Department of Environmental Engineering, Democritus University of Thrace, Xanthi, Greece.

Parallel Implementation of Elasticity Solvers in Material Science Applications

I. Lirkov, S. Petrova

We consider the modeling, simulation, and implementation of parallel solution methods for design of microstructural materials whose behavior is governed by the elasticity equations. The materials are obtained by biotemplating and find various important applications in material science and engineering. The mechanical macroscopic model corresponding to our composite materials comes from the homogenization theory. The computation of the effective elasticity coefficients requires simultaneously numerical solvers in the microscopic periodicity cell which can be parallelized. We compare the

performance of the incomplete Cholesky decomposition and the algebraic multigrid method as preconditioners of the stiffness matrix. The parallel code is developed by MPI and tested on modern parallel architectures.

The b-adic Diaphony as a Tool to Study Pseudo-randomness of Nets

I. Lirkov, S. Stoilova

We consider b-adic diaphony as a tool to measure the uniform distribution of sequences, as well as to investigate pseudo-random properties of sequences. The study of pseudo-random properties of uniformly distributed nets is extremely important for Monte Carlo and quasi-Monte Carlo integration. It is known that the error of the quasi-Monte Carlo integration depends on the distribution of the points of the net. On the other hand, the b-adic diaphony gives information about the point distribution of the net.

Several particular constructions of sequences $(x_n), n = 0, 1, \ldots$ are considered. The b-adic diaphony of the two dimensional nets $\{y_n = (x_n, x_{n+1}), n = 0, 1, \ldots, M-1\}$ is calculated numerically. The numerical results show that if the two dimensional net $\{y_n\}$ is uniformly distributed and the sequence $(x_n), n = 0, 1, \ldots$ has good pseudo-random properties, then the value of the b-adic diaphony decreases with the increase the number of the points. The analysis of the results shows a direct relation between pseudo-randomness of the points of the constructed sequences and nets and the b-adic diaphony as well as the discrepancy.

Scatter Estimation for PET Reconstruction

M. Magdics, L. Szirmay-Kalos, B. Tóth, Á. Csendesi, A. Penzov

This paper presents a Monte Carlo scatter estimation algorithm for Positron Emission Tomography (PET) where positron-electron annihilations induce photon-pairs that fly independently in the medium and eventually get absorbed in the detector grid. The path of the photon pair will be a *polyline* defined by the detector hits and scattering points where one of the photons changed its direction. This polyline contains the emission point somewhere inside one of its line segments. The values measured by detector pairs will then be the total contribution, i.e. the integral of such polyline paths of arbitrary length. These high dimensional integrals need to be estimated for all detector pairs with similar relative error, thus the classical approach that would sample the source and follow photons in their natural direction is not appropriate. Instead, we should solve the adjoint problem that starts building paths at the detector pairs. We consider the contribution of photon paths to each pair of detectors as an integral over the Cartesian product set of the volume.

This integration domain is sampled globally, i.e. a single polyline will represent all annihilation events occurred in any of its points. Furthermore, line segments containing scattering points will be reused for all detector pairs. Sampling parts of photon

paths globally and *reusing* a partial path for all detector pairs allow us to significantly reduce the number of samples and consequently the computation time.
The scatter estimation is incorporated into a PET reconstruction algorithm where the scattered term is subtracted from the measurements. We also show that with this correction, the noise of the reconstructed data can be greatly reduced.

Modelling of the SET and RESET Process in Bipolar Resistive Oxide-Based Memory Using Monte Carlo Simulations

A. Makarov, V. Sverdlov and S. Selberherr

A proper fundamental understanding of the switching mechanism in resistive random access memory (RRAM) is still missing, despite the fact that several physical mechanisms based on either electron or ion switching have been recently suggested in the literature.
We associate the resistive switching behavior in RRAM with the formation (Set) and rupture (Reset) of a conductive filament (CF). The CF is formed by localized oxygen vacancies (V_o) or domains of V_o. Formation and rupture of a CF is due to a redox reaction in the oxide layer under a voltage bias. The conduction is due to electron hopping between these V_o.
For modeling of the Set and Reset process in bipolar oxide-based memory by Monte Carlo techniques, we described the dynamics of oxygen ions (O^{2-}) and electrons in an oxide layer as follows: 1) an electron hops into V_o from an electrode; 2) an electron hops from V_o to an electrode; 3) an electron hops between two V_o; 4) formation of a V_o by O^{2-} moving to an interstitial position; 5) anyhilation of a V_o by moving O^{2-} to the V_o; 6) movement of O^{2-} between the interstitials.
To verify the proposed model, we first evaluate the average electron occupations of hopping sites under different conditions. For comparison with previous work all calculations are performed on a one-dimension lattice consisting of thirty equivalent, equidistantly positioned hopping sites. The distribution of electron occupation probabilities calculated with our approach is in excellent agreement with previous work.
To simulate thermostability of a CF, we calculated the dependence of the electron occupation distribution near the anode and cathode for a system with different conditions and without taking into account the ion motion. In all types of systems the change is marginal amounting to less than 10% for a temperature increase from 25^oC to 200^oC. The proposed model contributes to for better understanding the resistive switching phenomena and it can be used for performance optimization of RRAM devices.

Parallel Computation of the Fiedler Vector and Solution of Large Sparse Linear Systems via Banded Preconditioners

M. Manguoglu, E. Cox, F. Saied, A. Sameh

The eigenvector corresponding to the second smallest eigenvalue of the laplacian of a graph, known as the Fiedler vector, has a number of applications in areas that include matrix reordering, graph partitioning, protein analysis, data mining, machine learning, and web search. The computation of the Fiedler vector has been regarded as an expensive process as it involves solving a large eigenvalue problem. We present a novel and efficient parallel algorithm for computing the Fiedler vector of large graphs based on the Trace Minimization algorithm (Sameh and Wisniewski, 1982). We compare the parallel performance of our method with a multilevel scheme, designed specifically for computing the Fiedler vector, which is implemented in routine MC73_Fiedler of the Harwell Subroutine Library (HSL).
In the second part of this talk, we will demonstrate the application of the Fiedler vector by reordering the large elements closer to the main diagonal and extracting a banded preconditioner. We will show the scalability of our banded preconditioning method using the Spike algorithm for solving systems involving the preconditioner compared to other direct and iterative solvers such as MUMPS, SuperLU, Boomer-AMG, Trilinos-ML, and others.

Affine Data Modeling by Low-Rank Approximation

I. Markovsky

The low-rank approximation problem

$$\begin{array}{ll} \text{minimize} & \text{over } \widehat{D} \quad \|D - \widehat{D}\|_{\mathrm{F}} \\ \text{subject to} & \operatorname{rank}(\widehat{D}) \leq r, \end{array} \tag{2}$$

where $\|\cdot\|_{\mathrm{F}}$ is the Frobenius norm, is a ubiquitous *linear* data modeling tool. Indeed, assuming without loss of generality that D has more columns than rows, the aim of (2) is to fit optimally the columns of D (the data) by a subspace of dimension at most r (the linear model).
This paper studies the application of low-rank approximation for *affine data modeling*, i.e., optimal data fitting by an affine set. The relevant optimization problem in this case is

$$\begin{array}{ll} \text{minimize} & \text{over } \widehat{D} \text{ and } c \quad \|D - c\mathbf{1}^\top - \widehat{D}\|_{\mathrm{F}} \\ \text{subject to} & \operatorname{rank}(\widehat{D}) \leq r, \end{array} \tag{3}$$

where $\mathbf{1}$ is the vector of appropriate dimension with all elements equal to one.
We prove that a solution for the parameter c in (3) is the mean of the columns of D. Therefore, affine data modeling reduces to linear data modeling. From an

optimization point of view, (3) decouples into two independent optimization problems:

$$\text{minimize} \quad \text{over } c \quad \|D - c\mathbf{1}^\top\|_{\mathrm{F}} \tag{4}$$

and (2), where D is replaced by $D - c\mathbf{1}^\top$, with c computed from (4).
A solution of (3), however, is *not unique* even when a solution of (2) is unique. This is due to nonuniqueness of the shift parameter c. The general solution for c is given by a particular solution plus a vector in the column span of $\widehat{D}$.

On Some Properties of the Augmented Systems Arising in Interior Point Methods

C. Meszaros

A general direct approach to compute interior point iterations for optimization problems is to solve symmetric augmeted systems. In the talk we describe the basic properties of the diagonal perturbations of these systems and the use of such perturbations to increase numerical robustness of interior point methods. We show the connection between diagonal perturbation and convexification techniques that are very important for interior point methods when solving nonconvex problems. A new efficient and computationally cheap technique is introduced for convexification and its usefulness is demonstrated by numerical experiments.

Experimental Study of Matrix Multiplication on MultiCore Processors

P. D. Michailidis, K. G. Margaritis

Matrix computations is one of the most important computational tasks in scientific computing. Two well-known parallel versions are Cannon's algorithm and the ScaLAPACK outer product algorithm. Typically, parallel implementations work well on 2D processor grids: input matrices are sliced horizontally and vertically into square blocks; there is a one-to-one mapping of blocks onto physical resources; several communications can take place in parallel, both horizontally and vertically. Even better, most of these communications can be overlapped with (independent) computations. All these characteristics render the matrix product kernel quite amenable to an efficient parallel implementation on 2D processor grids.
However, algorithms based on a 2D grid (virtual) topology are not well suited for multicore architectures. In particular, in a multicore architecture, memory is shared, and data accesses are performed through a hierarchy of caches, from shared caches to distributed caches. We need to revisit the parallel implementations of matrix computations in the context of data partitioning in order to improve the parallel execution

on multicore architectures. This work present three parallel implementations of two fundamental matrix computation kernels such as matrix - vector multiplication and matrix multiplication on multicore processors. These parallel implementations are based on the three approaches of data partitioning among the available processing units such as row-wise, column-wise and square block-wise decomposition. Furthermore, for each possible parallel implementation is analyzed experimentally using the OpenMP programming environment on a machine with 4 Intel dual-core processors - a total of 8 cores. More specifically, we examine the performance results (i.e. execution times and speedups) of the proposed parallel implementations for matrix sizes ranging from 200x200 to 5000x5000 and different number of threads ranging from 2 to 8.

Also, this work we study how to model the performance of the proposed implementations to multicore architectures by taking memory access costs into account. More specifically, we present our effort to quantify and model each parallel implementation according to a performance model. The performance model of an implementation depends on two main aspects: the computational cost and the communication cost. In the case of multicore, communications are performed through direct read/write operations in a common memory address shared by two or more threads. To determine the computational cost we use an analytical model based on the number of operations and their cost in CPU cycles. Similarly, to predict the communication cost we model the memory access times using different methods according to its behavior - linear or non-linear. The proposed performance model validates against experimental results and it shows that the model is able to predict the parallel performance slightly even if the general behavior is correct. Finally, the proposed analytical prediction model can be used to predict the performance of two matrix computations for any problem size (i.e. matrix size), number of available processors/cores and processor characteristics.

Bicubic Spline Recovering of Smooth Surfaces on the Basis of Irregular Data

N. Naidenov, S. Kostadinova

We consider a method for recovering of a smooth surface $z = f(x, y)$ on the basis of data $\{(x_i, y_i, z_i)\}_{i=1}^{N}$. The method produces a bicubic spline $s(x, y)$ with uniformly distributed knots in a rectangle $R = [a, b] \times [c, d]$, which contains the points $\{X_i(x_i, y_i)\}$. We assume that the points $\{X_i\}$ are placed arbitrarily in the plane and that $z_i = f(X_i) + \epsilon_i,\ i = 1, ..., N$, where the errors $\{\epsilon_i\}$ are independent identically distributed random variables. The main goal of the study is to clarify how the error of the approximation $f(X) \approx s(X)$ depends on the parameters of the problem and the proposed solution.

Stochastic Algorithm for Solving the Wigner-Boltzmann Correction Equation

M. Nedjalkov, S. Selberherr, I. Dimov

For the solution of convection-diffusion problems we present a multilevel self-adaptive mesh-refinement algorithm to resolve locally strong varying behavior, like boundary and interior layers. The method is based on discontinuous Galerkin (Baumann-Oden DG) discretization. The recursive mesh-adaptation is interwoven with the multigrid solver. The solver is based on multigrid V-cycles with damped block-Jacobi relaxation as a smoother. Grid transfer operators are chosen in agreement with the Galerkin structure of the discretization, and local grid-refinement is taken care of by the transfer of local truncation errors between overlapping parts of the grid.
We propose an error indicator based on the comparison of the discrete solution on the finest grid and its restriction to the next coarser grid. It refines in regions, where this difference is too large. Several results of numerical experiments are presented which illustrate the performance of the method.
The approach shows the advantages of combining adaptive meshing, multilevel techniques and discontinuous Galerkin discretization.

Quadrature Formulae Based on Interpolation by Parabolic Splines

G. P. Nikolov, P. B. Nikolov

The standard way for construction of quadrature formulae is based on polynomial interpolation. A good reason for such an approach is the Weierstrass theorem about density of algebraic polynomials in the space $C[a, b]$, with $[a, b]$ being the integration interval (supposed to be finite and closed). However, there are lot of suggestions in the literature that in many situations spline functions provide better tool for approximation than polynomials, especially when the approximated functions are of low smoothness.
In the early nineties of the last century the first named author initiated study of quadrature formulae based on spline interpolation. In 1993 he formulated a conjecture about the asymptotical optimality of the Gauss-type quadratures associated with the spaces of polynomial splines with equidistant knots in the Sobolov classes of functions. This conjecture was proved (in a joint paper with P. Köhler) in 1995, and since then several papers devoted to Gaussian quadratures associated with spaces of low degree splines appeared.
A basic difficulty in the construction of Gaussian quadrature formulae associated with a given linear space of spline functions is to determine the mutual location of the quadrature nodes and the spline knots. Moreover, the highest "spline degree of precision" is achieved at the expense of irregular nodes distribution, and hence lack of possibility for building sequences of quadratures with nested nodes.

Here we present quadrature formulae, based on interpolation with parabolic splines with equidistant knots on a regular mesh of interpolation nodes. Explicit formulae are found for the weights, which are shown to be all positive. The numerical experiments indicate that our quadratures are competitive to the classical quadrature formulae based on polynomial interpolation.

Richardson Extrapolated Numerical Methods for One-Dimensional Advection Schemes

Tz. Ostromsky, I. Dimov, A. Havasi, I. Farago, Z. Zlatev

The numerical treatment of the advection part of any large-scale air pollution model is normaly very difficult. Improving the accuracy of the computed results can be done either by refinement of the discretization grid (which is usually rather expensive in terms of computaton sesources) or by increasing the order of accuracy of the numerical method in use. The latter can often be done by a careful implementation of Richardson Extrapolation in conjunction with the numerical method chosen. In the paper, it is described how the Richardson Extrapolation can be combined with a particular numerical method (the Crank-Nicolson scheme). Three test-examples are introduced and the numerical results obtained by applying the combination of the Crank-Nicolson scheme and the Richardson Extrapolation are compared with the results obtained when the Crank-Nicolson scheme is used directly.

Revisiting Preconditioning: An Interesting Result and the Lessons Learned from It

S. V. Parter

In 1988 L. Hemmingson considered a semi-circulant preconditioner for a finite-difference discretization of the reaction diffusion equation in the unit square Ω. That is,

$$Au = \epsilon \Delta u + a\frac{\partial u}{\partial x} + b\frac{\partial u}{\partial y} + du = f, \quad (x, y) \in \Omega$$

$$u = g(x, y), \quad (x, y) \in \partial\Omega.$$

The coefficients a, b are constant and $d \leq 0$.
Her results seemed to be in conflict with earlier results of Manteuffel and Parter (1990). In 2003 Kim and Parter [KP] returned to this problem and clarified the situation. In addition, they discussed the limiting behavior of the finite-difference equations.
In this work, we explain these matters. We then use other results ($\epsilon = 1$) of [KP] to discuss the computational results of a 2001 paper by Hemmingson and Wathen on preconditioning finite-difference equations for the Navier-Stokes equations.

Then we use the techniques developed in [KP] to study the limiting behavior ($\epsilon \downarrow 0$) of the solutions of the boundary-value problem

$$\epsilon \Delta u + x \frac{\partial u}{\partial x} + y \frac{\partial u}{\partial y} = 0, \quad (x, y) \in R$$

$$u = g(x, y), \quad (x, y) \in \partial R$$

where

$$R = \{(x, y); -1 < x < 1, -1 < y < 1\}.$$

We observe that the point $(0, 0)$ is a "stagnation" point at which the reduced equation becomes singular. Finally, we discuss the behavior of the solutions of the finite-difference equations for this problem.

Metaheuristics for the Asymmetric Hamiltonian Path

J. P. Pedroso

We are dealing with the following problem: given an operation currently being done in a machine, determine the order for the set of operations to be produced next, such that the total production time is minimized. We assume that there are no precedence constraints among the operations, but there are changeover times which depend on the production sequence. Minimizing the total production time is equivalent to minimizing the time spent in changeovers, as the other times are constant.
This problem has practical relevance. In paint production, the machine cleaning times are usually dependent on the sequence; for example, producing white colour after grey requires a much more careful cleaning than the other way around. Another practical application is in food manufacturing, where strong flavours can be produced after flavourless products at a small cost, but very careful and lengthy cleaning is required in the inverse situation.
One possibility for modelling this problem is to consider a graph with a node for each of the items that must be produced. There are two arcs between every pair of nodes, one in each direction, representing the changeover time between the corresponding products. A solution to the original problem corresponds to determining a Hamiltonian path in this graph, i.e., a path going through all the nodes in the graph. The path must start with a particular node (the item being currently produced), but there is no concern about the ending node.
Given the similarity of this problem with the Travelling Salesman Problem, in particular with its asymmetric variants, we considered adapting the methods that have been developed for that problem to the current situation. Throughout this paper we will describe more formally the problem in mathematical programming, explain in detail the metaheuristics that we implemented for solving it, and present the results of applying it to a set of benchmark problems.

Adaptive Intelligence Applied to Numerical Optimisation

K. Penev, A. Ruzhekov

The article presents experimental results achieved by adaptive heuristics applied to numerical optimisation of several non-constraint test functions. The aims of the study are to identify and compare how adaptive search heuristics behave within a search space without local correlation and within a search space dominated by local optimum. The achieved results are summarised and analysed. A discussion focuses on the abilities of the adaptive heuristics to cope with non-trivial search space without local correlation between neighbour locations and on the abilities to escape from trap local optimum, which dominates more than 50% of the search space and then to reach global optimum. The article presents, also, the values of the variables for the best achieved results, which could be used for comparison to other methods and further investigation.

Condition and Error Estimates in Kalman Filter Design

P. Hr. Petkov, M. M. Konstantinov, N. D. Christov

Kalman filters play a key role in the solution of the main linear optimal control and estimation problems. The Kalman filter design consists in finding the filter gain matrix determined by a matrix Riccati equation. As it is well known the numerical solution of this equation may face some difficulties. First, the equation may be ill conditioned, i.e. small perturbations in its coefficient matrices may lead to large variations in the solution. Therefore, it is necessary to have a quantitative characterization of the conditioning in order to estimate the accuracy of solution computed.
The second difficulty is connected with the stability of the numerical method and the reliability of its implementation. It is well known that the methods for solving the Riccati equations are generally unstable. This requires to have an estimate of the forward error in the solution.
The paper deals with the computation of condition numbers and residual-based forward error estimates pertaining to the numerical solution of Riccati equations arising in the continuous-time Kalman filter design. Efficient LAPACK-based condition and error estimators are proposed involving the solution of triangular Lyapunov equations along with one-norm computation.

Multsacle Modeling of Poroelasticity in Highly Deformable Fractured Reservoirs

P. Popov, Y. Efendiev, Y. Gorb

In this work a new class of methods for upscaling fluid-structure interaction problems from the pore-level to a macroscale is proposed. We consider a fully coupled fluid-structure interaction problem for stokes fluid and an elastic solid at the pore-level. The

solid, due to coupling with the fluid, material nonlinearities, as well as macroscopic boundary conditions, can deform enough so that the pore-space is altered significantly. As a result, macroscopic properties such as the permeability of the porous media become nonlinearly dependent on the fine-scale displacements. Therefore, classical upscaled models, such as Biot's equations, can no longer be applied. We propose a series of numerical upscaling models which couple this fine-scale FSI problem to a nonlinear elliptic equation for the averaged pressure and displacements at the coase scale. The proposed multiscale methods correclty transfer the appropriate physics from the fine to the coarse scale. Moreoever they are intrinsically parallelizable on a wide variety of computer architectures. The models are applied to a two-scale media with a fracture network embedded in elastic, impermeable solid at the finer scale. We use the proposed models to upscale the fracture network to the coarse nonlinear poroelasticity. It is shown that the coarse permeability is a highly sensitive function of pressure and displacements due to their effects on changing the aperture of the fractures at the fine scale. Several numerical examples which demonstrate the method are also presented.

Application of Spectral Method for Investigation of the Profiles of the Optimum Fields for Variational Problems Connected to the Turbulent Thermal Convection

S. Radev, N. K. Vitanov

The optimum theory of turbulence is one of the few tools for obtaining analytical results for the characteristic quantities of the turbulent flows and turbulent thermal convection. This is achieved on the basis of analytical asymptotic theory which is valid for large values of the dimensionless numbers of the corresponding fluid system. For small and intermediate values of the numbers such as Rayleigh or Taylor numbers we have to solve numerically the Euler - Lagrange equations of the corresponding variational problems. The spectral methods are very suitable for obtaining the profiles of the optimum fields connected to the fluid velocity and temperature as well as for obtaining the thickness of the boundary layers of the optimum fields. In this presentation we discuss the application of the Galerkin method for solution of the Euler - Lagrange equations of a variational problem connected to the turbulent convection. We obtain several profiles of the optimum fields, describe the evolution of the thickness of the boundary layers, and finally discuss the limits of the application of Galerkin method to this system.

Water Flow Problem in Discrete Fracture Network – Algebraic Multigrid vs. Simplification of the Fracture Network

P. Rálek, J. Březina, J. Kopal, M. Hokr

This contribution deals with potential groundwater flow modelling in fractured rock. As the test problem, we used 2D stochastically generated discrete fracture network, which consists of 7797 fractures divided to 60052 segments, with large variation between largest and smallest segments. For the numerical solution, the mixed-hybrid finite element method implemented in code FLOW123D (developed at the Technical University of Liberec) was used. The discretized problem is large and numerically instable.

The first approach to improve the numerical stability of the discretized problem was the simplification of the fracture network. The fact, that the hydraulic conductivity of the fractures strongly depends on their lengths, guides to the idea of changing insignificant fractures so that it simplifies the whole fracture network. The algorithm combines deleting of small fractures, union of near intersection nodes and union of those fractures, which became (partly) identical. The originated fracture network, according optional reduction parameters, can more or less be geometrically similar to the original one, but still preserves the hydraulic behavior of the original fracture network and has better properties (e.g. disposes the small segments lying between very near intersections).

The other approach for the decrease of the computational size of the problem was algebraic multigrid preconditioning used to the discretization of the original fracture network. For the multigrid preconditioning, we used its implementation in PETSc package, which is nowadays a part of FLOW123D code.

These two approaches were used at several cases with different levels of fracture simplification or preconditioning. The contribution presents the influence of both approaches to the solution of the flow problem.

Modeling Thermal Effects in Fully-Depleted SOI Devices with Arbitrary Crystallographic Orientation

K. Raleva, D. Vasileska, S. M. Goodnick

To achieve further improvement of performance in scaled silicon devices applied mechanical stress, alternative wafer orientations, and multi-gate transistors have been actively researched or are already in production. All these options take advantage of the anisotropic nature of the silicon crystal, and therefore, of its anisotropic bandstructure, in engineering gains in the carrier transport mass and mobility. For instance, strained Si is the only new channel material which has recently made its way into the commercial integrated circuits. By straining the silicon channel, carrier mobility

can be enhanced. Also, devices fabricated on Si (110) wafer orientations has shown improved mobility characteristics over (100) devices.
The current trend in device scaling is a transition away from conventional planar CMOS to alternative non-planar technology devices, such as fully-depleted (FD), dual-gate (DG), tri-gate silicon-on-insulator (SOI) and others. The problem with SOI devices is that they exhibit self-heating effects. These self-heating effects arise from the fact that the underlying SiO2 layer has about 100 times smaller thermal conductivity than bulk Si. We have previously reported that self-heating and increased power density play important roles in the operation of fully-depleted SOI devices with channel lengths between 25 and 180 nm using 2D electro-thermal simulation based on the self-consistent solution of the Boltzmann transport equation for the electrons via Monte Carlo techniques and the energy balance equations for acoustic and optical phonons. There it was shown that due to geometry and velocity overshoot, self-heating effects are more pronounced for larger channel length devices with correspondingly larger supply voltages.
In this work we continue our investigation on the impact of the wafer crystallographic orientation on the current degradation in nanoscale FD-SOI devices due to self-heating effects. The preliminary results obtained from the simulated 25nm channel length FD-SOI structure show that the isothermal value of the on-current for (110) wafer orientation (ID=1.904mA/um for VGS=VDS=1.2V) is higher compared to the (100) wafer orientation (ID=1.772mA/um for VGS=VDS=1.2V). What is more important, the current degradation due to self-heating is slightly lower for (110) wafer orientation (2.6% versus 3.7% for (100)). From the lattice temperature profile, one can observe that the position of the hot-spot region doesnt change with the wafer orientation, but the maximum temperature is higher for (100) wafer orientation. These results are obtained by using our novel theoretical model for the temperature and thickness dependence of the thermal conductivity which is valid for (100) wafer orientation. We believe that the inclusion of the proper thermal conductivity model for (110) wafer orientation will decrease the current degradation even more. The results of these simulations will be presented at the conference.

An Efficient Numerical Method for a System of Singularly Perturbed Semilinear Reaction-Diffusion Equations

S. C. S. Rao, S. Kumar

In this work we consider a system of singularly perturbed semilinear reaction-diffusion equations. To solve this problem numerically, we construct a finite difference scheme of Hermite type, and combine this with standard central difference scheme in a special way on a piecewise-uniform Shishkin mesh. The error analysis is given and parameter-uniform error bounds are established; this shows that the present method gives better approximations than the standard central difference scheme. Moreover, it is shown that the method is third order ε-uniformly convergent, when $\sqrt{\varepsilon} \leq N^{-1}$. Numerical experiments are conducted to demonstrate the efficiency of the present method.

Programming Problems with a Large Number of Objective Functions

C. Resteanu, R. Trandafir

The paper treats the Multi-Objective Programming problem with a large set of composite objective functions, linear-hundred and nonlinear-thousand, the domain of feasible solutions being defined by a set of linear equations / inequations representing a large scale problem. Ones construct a preferred solution i.e. a non-dominated solution chosen via extending the decision-making framework. For the problems defined above, when the objective functions are all linear, there are a lot of classical,very good, solving methods based on SIMPLEX algorithm. But, if beside linear functions, the nonlinear functions appear, the classical methods do not work. Moreover, if the objective functions are in a large number, the solving becomes difficult from practical point of vue. In this particular case, a software platform, composed by a solver for Linear Programming problems and a solver for Multiple Attribute Decision Making problems in combination with Parallel and Distributed Computing techniques based on a GRID configuration, is necessary. The hardware platform has the same importance as the software platform. It is composed by a powerful server and a number of multi-processors distributed in GRID. This number is equal to the linear objective functions' number. If the server remains the same after the pervasive solving service is installed on GRID, the rest of multi-processors may differ from a solving to another solving. On server are assigned the mathematical modeling operations, i.e. the stocking of mathematical model in a format that facilitate the operations of adding / modifying / deleting its entities, the generating of the MPS problem form, the running of the first phase of the SIMPLEX algorithm and the construction of the preferred solution based on all objective functions' values. On the rest of multi-processors are assigned the optimizations upon the linear objective functions, in the re-optimization regime, which operations are scheduled by server.

Fed-batch Cultivation Control Based on Genetic Algorithm PID Controller Tuning

O. Roeva, T. Slavov

PID controller is widely used in feed-back control of industrial cultivation processes. The design of control systems requires adjustment of controller parameters, solving the control problems in an appropriate way. As a basis for the design procedure have to be defined a certain criteria evaluating the performance of the control system. In this paper a Universal discrete PID controller for the control of *Escherichia coli* fed-batch cultivation processes is designed. E. coli fed-batch culture has been widely used for production of various bioproducts including primary and secondary metabolites, proteins, and other biopolymers. Fed-batch processing is especially beneficial since a change in the nutrient concentrations affects the productivity and yield of the de-

sired product. Both overfeeding and underfeeding of nutrient are detrimental to cell growth and product formation. Development of a suitable feeding strategy is critical in fed-batch cultivation. Various strategies have been developed to control the nutrient concentration within the optimal range. For the considered process in order to prevent the growth inhibition and to maximize the biomass concentration the glucose concentration have to be controlled at low levels based on glucose measurements. The Universal discrete PID controller is used to control feed rate and to maintain glucose concentration at the desired set point. The tuning of the PID controller parameters is done applying the GA. To evaluate the significance of the tuning procedure, four criteria reflecting the performance of the PID controller are used. Additional simulations are performed for comparison of the results from the different criteria. To obtain realistic tests of the robustness of the controller and performance of the tuning procedure noise have been introduced in the simulation. As a result the optimal PID controller settings are obtained. For a short time the controller sets the control variable and maintains it at the desired set point during the process. Application of the designed controller provides maintaining of the accuracy and efficiency of the system performance.

Tool for Observation, Comparison and Analysis of Advanced Search Algorithms

A. Ruzhekov, K. Penev

The aim of this paper is to present a tool for observation and analysis of advanced algorithms such as Differential Evolution, Genetic Algorithm, Practical Swarm Optimization, Free Search and other evolutionary methods. Evolutionary techniques have a quite unpredictable output. In order to make scientific analysis without being lost in a sea full of numbers calculated by the millions every second or relying only on end results and time ratings you have to be able to visualize all the composite elements involved functions, population members, formulas, numerical values and other useful information. If this is left for the imagination to cope with there is a chance it might mislead you into false conclusions. This is where this tool comes into action with a few clicks it has the ability to customize the task to be observed and the elements to be shown. There is a detailed view of what exactly is going on population movement, mutation, current positions, goal reached and it can be paused at every point of interest. The tool is designed to work with some particular test functions of interest Michalewics, Five Hills, Step and Step Sphere, but can be extended to work with just any function that can be presented in three dimensions. With enough time and devotion I believe this tool can become a foundation for future research, analysis, education and with the ideas behind it and further future development a universal tool for visualisation of mathematical functions and algorithms. It can also help improving existing methods and developing new ones.

Stochastic Algorithms in Linear Algebra - beyond the Markov Chains and Neumann - Ulam Scheme

K. Sabelfeld

In this talk I will present some new ideas around the stochastic approach for large systems of equations, in particular, solving very large systems of linear equations, randomized singular value decomposition (SVD) based methods for solving integral equations and ' ill-posed and inverse problems. In Monte Carlo methods, one has to cope often with very large dimensions, in problems like the integration, solution of integral equations, PDEs,simulation of random fields, etc. It is customary to think that the Monte Carlo methods based on the Markov chains and Neumann - Ulam scheme are able to resolve problems for very high dimensions, however it is true only under the following restricted conditions: (1) the variance of the MC estimator is small, (2) the desired accuracy is not high, (3) the complexity of construction of the random estimator is a slow function of the dimension. The condition (3) can be often fulfilled, however the conditions (1) and (2) are of the main concern, because the convergence rate of MC methods is slow, scaling as $\sigma/N^{1/2}$ where σ is the standard deviation, and N is the sample size. In my talk I will present absolutely other approach, beyond the Markov chains and Neumann - Ulam scheme, which is much closer to deterministic methods but which uses some remarkable probabilistic properties of large matrices. So I will discuss in details the SVD based randomized low rank approximation methods which is capable to handle systems of huge dimension. Another important class of stochastic methods I am going to talk about is the randomized version of projection methods. Applications to different practical problems in random field simulation, transport in porous media, crystal structure analysis by x-ray diffraction, nucleation and coagulation of large ensembles of interacting particles.

Sparsified Randomization Algorithms for the SVD based Low Rank Approximations

K. Sabelfeld, N. Mozartova

Sparsified Randomization Monte Carlo algorithms for Singular Value Decomposition (SVD) is presented. This method is based on the Johnson-Lindenstrauss lemma which says that a large matrix can be approximated in a certain sense via random matrices of smaller size. In particular, this approach makes it possible to construct a randomized algorithm for trancated spectral decomposition for very large matrices, i.e., the top singular values and the relevant left and right singular vectors are calculated without constructing the full SVD. We extend this method for a randomized solution of integral equations of the second kind whose Neumann series converges too slow, or even diverges. Another interesting application we developed is a randomized simulation of inhomogeneous random fields, in particular, we present the results of simulations for the fractal Wiener process and 2D Lorenzian random field (for details, see [1]). In

fact, this is a randomized simulation algorithm for the Karhunen-Loève expansion for inhomogeneous random fields.

1. K. Sabelfeld, N. Mozartova. Sparsified Randomization Algorithms for low rank approximations and applications to integral equations and inhomogeneous random field simulation. *Monte Carlo Methods and Applications*, 2010, vol 16, issues 3-4.

Hybrid Discontinuous Galerkin Methods with Vector Valued Finite Elements

J. Schöberl

In this talk we discuss some recent finite element methods for solid mechanics and fluid dynamics. Here, the primary unknowns are H^1-vector fields. We show that it can be useful to treat the normal continuity and tangential continuity of the vector fields differently. One example is to construct exact divergence-free finite element spaces for incompressible flows, which leads to finite element spaces with continuous normal components. An other example is structural mechanics, where tangential continuous finite elements lead to locking free methods.
Keeping one component continuous, we arrive either at $H(curl)$-conforming, or $H(div)$ conforming methods. The other component is treated by a discontinuous Galerkin method. We discuss a generic technique to construct conforming high order finite element spaces spaces for $H(curl)$ and $H(div)$, i.e., Raviart Thomas and Nedelec - type finite elements. By this construction, we can easily build divergence-free finite element sub-spaces.

New Conjectures in the Hausdorff Geometry of Polynomials

Bl. Sendov

Let $D(C(p); R(p))$ be the smallest disk containing all zeros of the polynomial $p(z) = (z - z_1)(z - z_2) \cdots (z - z_n)$. Half a century ago, we conjectured that for every zero z_k of $p(z)$, the disk $D(z_k; R(p))$ contains at least one zero of the derivative $p'(z)$. In this paper a stronger conjecture is announced and proved for polynomials of degree $n = 3$. A number of other conjectures are announced, including a variation of the Smale's mean value conjecture.

Perspectives of a Selfish Behavior in Self-Policing Wireless Mobile Ad Hoc Network

M. Seredynski, P. Bouvry

A wireless mobile ad hoc network (MANET) consists of a number of devices equipped with wireless communication capabilities. It operates without a support from any fixed infrastructure, thus the devices are expected to cooperate on packet forwarding. Due to the fact that MANET is formed with battery constrained devices like laptops, PDAs, or smartphones, the network users are tempted to act selfishly by not participating to the packet forwarding duty. A general approach for solving the problem is referred to as a distributed cooperation

enforcement mechanism. It assumes that nodes forward packets only on behalf of those who behaved correctly in the past (i.e. cooperated on packet forwarding). However, as in MANET nodes belong to different authorities, the use of a given forwarding strategy cannot be enforced. Thus it has to be beneficial to its potential users. But what is good from a single user's point of view might not always be beneficial to other users, thus sometimes rational behavior of network participants might lead to a noncooperative network. Since the forwarding relationships between nodes are game-theoretic in nature (an optimal packet forwarding strategy of a node depends on the strategies used by others) such a network cannot be represented and analyzed as a parametric situation.
In the paper we investigate the conditions, where the development of the enforcement mechanism among MANET users is very unlikely, i.e. the reciprocity-based cooperative behavior is not beneficial to the network users. We demonstrate that in the presence of a large number of unconditionally cooperative nodes a selfish permanent defection strategy is more successful than a reciprocal tit-for-tat strategy. Firstly, a direct reciprocity-based model of packet relaying is introduced. Next, an evolutionary game-theoretical approach combining genetic algorithms and replicator equations for the search and analysis of strategies for given networking conditions is introduced. The genetic algorithm is used to discover the condition-specyfic forwarding strategies, while the replicator dynamics-based approach allows to further verify the performance of the strategies.

Some Spectral Problems of Porous Media Acoustics

A. S. Shamaev, A. A. Gavrikov, D. U. Knyazkov

The current talk concerns problems of finding natural frequency spectrum of media consisting of two fast alternating phases with different mechanical properties (e.g. elastic frame with channels filled with compressible or incompressible viscous fluid, mixture of two liquids with various viscosities and compressibilities etc). In a quite a number of cases macroscopic models of such media (they are usually called homogenized or effective models) are models of materials with dynamics described by integrodifferential equations with integral terms of convolution product by time coordinate type. In the talk (a) there are exact statements on proximity between solutions of original boundary problems for two-phase models and solutions of corresponding boundary problems for the above integrodifferential equations. In addition, (b) various natural oscillations spectra qualitative properties for the mentioned homogenized models are analyzed. It is shown that homogenized problem spectrum consists of two parts: real and complex. Complex part is a union of two complex conjugated sequences of complex numbers where real parts have a limit and imaginary parts tend to infinity or have finite limits. Real part of investigated spectrum is a union of a finite or countable number of limited sequences (lying on nonoverlapping intervals of the real axis), each having a limit. Under some conditions it is possible for some interval to contain continuous spectrum.
Analysis shows, that qualitative properties similar to described above are also valid for a number of other problems with different physical or mechanical origin: dynamics problem for viscoelastic materials with "memory", nonstandard models of heat conductivity with memory, well-known in filtration theory "double-porosity" problem.
Here we are stating a hypothesis of existence of a general operator model, with use of witch it could be possible to prove the existence of spectra of described above structure in all cases. The presented results are new and original. The work is carried out under the financial support of RFBR, grant N 08-01-00180-a.

Evaluation of the Co-mutation Operators in Optimization of Multiple SVM Kernels

D. Simian, F. Stoica, C. Simian

The aim of this paper is to present a comparative study about the effect of the genetic operators used in an original evolutionary method for optimization of SVM multiple kernels. The computation of the optimal parameter values of SVM kernels is performed using an evolutionary method based on the SVM algorithm for evaluation of the quality of chromosomes. We defined several variants of the co-mutation $LR - M_{ijn}$ operator, introduced by us in a previous paper and used them in the evolutionary algorithms. Algorithms inspired by nature are used to improve $LR-M_{ijn}$ operator performance. The evaluation of different $LR-M_{ijn}$ based co-mutation operators and their comparison with classical genetic operators was made using cross-validation, in order to estimate how accurately the computed multiple kernels will perform in practice.

Interval Dependency and the Problem of Solving Parametric Linear Systems

I. Skalna

One of the key points in interval computations is a suitable inclusion function which allows to solve the problem efficiently. Evaluation using the simplest form of interval analysis (natural extension) produces a wide interval. This is due in a large part to the fact that interval arithmetic is only sub-distributive. Another problem, commonly referred to as interval dependency, is that the multiple occurrences of a variable are considered as different variables during interval evaluation. In this study, the problem of solving parametric linear systems with coefficients dependent on interval parameters is considered. Different approaches to dealing with the interval dependency problem, suggested in the literature, are compared and used to obtain an efficient method for solving parametric linear systems. Numerical examples of structural mechanics are provided to verify and compare the performance of the proposed approaches.

A Comparison of Metaheurisitics for the Problem of Solving Parametric Interval Linear Systems

I. Skalna, J. Duda

The problem of computing a hull solution of parametric interval linear systems is considered. This problem can be reduced to the problem of solving a family of constrained optimizatiom problems. A naive evolutionary strategy turn out to be a very useful tool for computing the hull solution. However, for larger problems it seems to be not efficient enough. It requires a large number of individuals and generations to give reasonable results. In this study other metaheuristics are considered to get more efficient method for solving parametric interval linear system with both linear and nonlinear dependencies.

First Results of See-Grid-Sci VO "Environment" Application CCIAQ

V. Spiridonov, D. Syrakov, M. Prodanova, A. Bogachev,
K. Ganev, N. Miloshev, G. Jordanov, K. Slavov

The main objective of the EC FP6 project CECILIA is to deliver a climate change impacts and vulnerability assessment in targeted areas of Central and Eastern Europe. Emphasis is given to applications of regional climate modeling studies at a resolution of 10 km for local impact studies in key sectors of the region. For the purpose, intensive long-term meteorological modeling took place in Bulgarian National Institute of Meteorology and Hydrology (NIMH), in an attempt to determine climatic values for the main meteorological variables. The climatic version of the operational weather forecast model ALADIN was applied for simulating 3 time slices: 1960-2000 (Control Run, CR), 2020-2050 (Near Future, NF) and 2070-2100 (Far Future, FF), following the IPCC scenario A1B. The calculations are made for an area covering Bulgaria with resolution of 10 km. The created meteorological data base is used for two purposes. First of all, calculation of the respective modeled climates took place. The differences of climatic fields for the 3 periods are presented and interpreted. The second use of the created meteorological database is to estimate the impact of climate changes on air quality. A respective modeling System was created on the base of US EPA Models-3 tool (MM5, CMAQ and SMOKE) for a nested region with resolution of 10 km covering Bulgaria. Calculations for the last 10 years of each CR, NF and FF periods are performed, results presented and interpreted in the study.

Particle Monte Carlo Algorithms with Small Number of Partilces in Grid Cells

S. K. Stefanov

The Direct Simulation Monte Carlo (DSMC) analysis of two- and three-dimensional rarefied gas flows requires computational resources of very large proportions. One of the major causes for this is that, along with the multidimensional computational mesh, the standard DSMC approach also requires a large number of particles in each cell of the mesh in order to obtain sufficiently accurate results. In this paper we will present two modified simulation procedures which allow more accurate calculations with a smaller mean number of particles ($\langle N \rangle \sim 1$)in the grid cells. In the new algorithms, the standard DSMC collision scheme is replaced by a two-step collision procedure based on "Bernoulli trials" scheme or its simplyfied version, which is applied twice to the cells (or subcells) of a dual grid within a time step. The modified algorithms use a symmetric Strang splitting scheme that improves the accuracy of the method to $O(\tau^2)$ with respect to the time step τ making the modified DSMC method a more effective numerical tool for both steady and unsteady gas flow calculations on fine multidimensional grids. The latter is particularly important for simulation of vortical and unstable rarefied gas flows. The modified simulation schemes might be useful also for DSMC calculations within the subcell areas of a multilevel computational grid.

Forced Vibrations of 3D Beams with Large Amplitudes

S. Stoykov, P. Ribeiro

A p-version finite element and the harmonic balance methods are used to investigate the geometrically nonlinear forced vibrations of 3D beams with rectangular cross section. The beam theory used in the model is based on Timoshenko's theory for bending and Saint-Venant's for torsion. The beam may experience longitudinal, torsional and bending deformations in any plane. The equation of motion is derived by the principle of virtual work; employing the harmonic balance method it is converted into a nonlinear algebraic form and then solved by a continuation method. Because the nonlinear equation of motion presents quadratic and cubic nonlinearities, one constant term and the first three harmonics are assumed in the Fourier series. A force which excites both bending and the torsional displacements is applied and the response curves are derived and the characteristics of the motions are investigated using time plots, phase planes and Fourier spectra.

Using Satellite Observations for Air Quality Assessment with an Inverse Model System

A. Strunk, H. Elbern, A. Ebel

The operational prediction of air quality as a computationally demanding task has become an important part of the assessment of risks for our environment and health. National and international agencies and policy makers are using numerical model applications to support their activities for air pollution reduction, for decision making and for informing the general public. However, assessing air pollution levels from global to local scale still remains a challenging mission, involving parameters with large uncertainties, e.g. emissions.
As an independent source of information, observations are playing a very important role and can therefore be used to ameliorate the simulation results. This can only be achieved in a satisfying way by applying advanced data assimilation techniques, producing consistent chemical estimates on regular grids. One strongly growing amount of environmental data is available as satellite based measurements, which are widely used for both model evaluation and data assimilation purposes in the air quality modeling community.
This study aims at identifying the benefit of tropospheric NO_2 column retrievals for air quality assessment, when a state-of-the-art chemistry transport model is used together with a spatio-temporal data assimilation technique (4d-var). To this end, the European Air Pollution Dispersion - Inverse Model system (EURAD-IM) is applied to one summer and one winter episode, operating on a European domain with a spatial resolution of 15 km, jointly optimising initial values and emission rates. NO_2 data from the OMI instrument is assimilated, while European ground based in-situ and independent satellite observations (GOME-2 and SCIAMACHY) are used for evaluating the influence of assimilated observations on estimating the air quality, especially levels of nitrogen oxides. Results show a strong improvement of surface level nitrogen oxides estimates for the summer episode, sustained even after the assimilation period through emission adjustments. For the winter period, the OMI NO_2 data is of limited value due to lower boundary layer heights and thus smaller impact on emission rate optimisation.

Distributed Software System for Data Evaluation and Numerical Simulations of Atmospheric Processes

A. T. Terziyski, N. T. Kochev

A distributed software system for numerical simulations of atmospheric physicochemical processes is presented. It is a multi-layer Java based system for theoretical investigation of complex interactions of atmospheric trace gases and ice particles. The simulations are based on the fundamental theory of Langmuir adsorption and second Ficks law applied for adsorption, desorption and diffusion processes. The system consists of three basic layers: (1) input/output interface layer, (2) dispatcher layer, (3) grid-based layer for simulations distributed over multiple machines. The core software module used in level (3) is based on previously published by us software prototype for simulations of adsorption, desorption and diffusion in a closed system and Flow Tube Reactor. The main task of the current distributed system is to derive numerical estimations of several significant constants: adsorption/desorption rates, ice entry rate, ice bulk diffusion coefficient and etc. The constants are estimated by comparison of experimental signals from a Flow Tube Reactor and simulations results from the system described in this paper. The difference between both curve profiles is minimized by an exhaustive search in a multi-dimensional parameter space which represents all possible values of the physicochemical constants. The dispatcher layer of the system defines several regions of the multi-dimensional parameter space. For each region, a separate task is configured and dispatched to a node from a computer GRID or cluster. The entire parameter space is searched in a parallel manner and after that all results are united in order to find the global minimum of the difference between experimental and simulated curves. The results are printed via the input/output software layer. Example kinetic simulations performed by the software system are presented and discussed.

Parameter Estimation For A Logistic Curve. An Example of Use in an Engineering Problem

F. Torrecilla-Pinero, J. A. Torrecilla-Pinero, J. A. Gómez-Pulido, M. A. Vega-Rodríguez, J. M. Sánchez-Pérez

When you try to solve some engineering problems such as the water supply for a city or to calculate the traffic in a road, many times you will be led to make an estimation of the future population which is going to live in the city or cities that the road connects. In this situation, the most usually way to estimate the population is using a logistic curve like:

$$P = \frac{S}{1 + Me^{bt}} \tag{5}$$

where S, M and b are parameters that could be calculated like:

- $S = \frac{2P_0P_1P_2 - P_1^2(P_0+P_2)}{P_0P_2 - P_1^2}$,
- $M = \frac{S-P_0}{P_0}$,
- $b = \frac{1}{n}[\frac{P_0(S-P_1)}{P_1(S-P_0)}]$ and
- $n = (t_2 - t_1) = (t_1 - t_0)$.

taking P_0, P_1 and P_2 (populations) in equidistant times t_0, t_1 and t_2.
This way, the parameter estimation is done tanking into account only 3 populations equidistantly taken in time, and you could not take another set of data. If you want to take some others data, you should do the resolution into another way, and we propose to tackle this issue with genetic algorithms.
We have obtained some reasonable results with this approach, that represents an alternative to the classical way of estimating parameters in logistic curves.

SM Stability for Time-Dependent Problems

P. N. Vabishchevich

When time-dependent problems of mathematical physics are solved numerically, much emphasis is placed on computational algorithms of higher orders of accuracy. Along with improving the approximation accuracy with respect to space, improving the approximation accuracy with respect to time is also of interest. In this respect, the results concerning the numerical methods for ordinary differential equations (ODEs) provide an example. Taking into account the specific features of time-dependent problems for PDEs, we are interested in numerical methods for solving the Cauchy problem in the case of stiff equations.
When time-dependent problems are solved approximately, the accuracy can be improved in various ways. In the case of two-level schemes (the solution at two adjacent time levels is involved), polynomial approximations of the schemes operators on the solutions to the equation are used explicitly or implicitly. The most popular representatives of such schemes are RungeKutta methods, which are widely used in modern computations. The main feature of the multilevel schemes (multistep methods) manifests itself in the approximation of time derivatives with a higher accuracy on a multipoint stencil. A characteristic example is provided by multistep methods based on backward numerical differentiation.
Various classes of stable finite difference schemes can be constructed to obtain a numerical solution. It is important to select among all the stable schemes a scheme that is optimal in terms of certain additional criteria. In this study, we use a simple boundary value problem for a one-dimensional parabolic equation to discuss the selection of an approximation with respect to time. We consider the pure diffusion equation, the pure transport equation and combined convection-diffusion. Requirements for the unconditionally stable finite difference schemes are formulated that are related to retaining the main features of the differential problem. The concept of SM stable finite difference scheme is introduced. The starting point are difference schemes constructed on the basis of various Padé approximations.

Is Self-Heating Important in Nanowire FETs?

D. Vasileska, A. Hossain, K. Raleva, S. M. Goodnick

Modern technology has enabled the fabrication of materials with characteristic dimensions of a few nanometers. Examples are superlattices, nanowires and quantum dots. Thermal transport in these low-dimensional nanostructures is important for next-generation microelectronic cooling techniques, novel solid-state energy conversion devices, and micro-nanoscale sensors.
We have previously investigated 2D fully-depleted SOI device structures, where we observed that current degradation due to self heating effects is smaller in shorter channel length devices

due to increased non-stationary transport, and reduced thermal resistance of the underlying buried oxide. To address self-heating effects in nanowire we use the electro-thermal simulator developed at ASU, which solves the Boltzmann transport equation in a self-consistent way for electrons and the energy balance equations for acoustic and optical phonons. The thermal conductivity values for the nanowire are taken from experimental measurements reported by Li Shi et al.
In this work we focus on investigation of self-heating effect in 10 nm wide, 7 nm thick and 10 nm long channel of a silicon nanowire transistor. The difference between this structure and the previously investigated 2D fully depleted SOI transistors is that the SiO2 is now all around the structure, not just at the top and the bottom. Because SiO2 has very low thermal conductivity, and the nanowire itself has low thermal conductivity (because of phonon boundary scattering in the rectangular cross section), self heating effects are more pronounced in the nanowire transistor when compared to the same channel length fully-depleted SOI device.
At the moment we are investigating current degradation due to self-heating effects for nanowires with arbitrary crystallographic directions. In these calculations the proper thermal conductivity tensor and its geometry and temperature dependence is being taken into account.

Advanced Numerical Tools Applied to Geo-Environmental Engineering - Soils Contaminated by Petroleum Hydrocarbons, A Case Study

M. C. Vila, J. Soeiro de Carvalho, A. Fiúza

Contaminated soils can be considered as a heterogeneous, anisotropic and discontinuous geo-system, whose properties vary in time and space. Aiming the remediation of an active contaminated site (a refinery located in the north of Portugal) we performed laboratory studies with soil samples contaminated with petroleum hydrocarbons.
The experimental results concerning the kinetics of degradation led to the development of a MIMO (multiple input multiple output) model describing simultaneously the time evolution of biomass and the contaminant degradation. Several phenomena were simultaneously considered in this model: the volatilization, a fast kinetics component, a slow kinetics component and the refractoriness of some hydrocarbons for the time scale used in the experiments.
As part of the research programme we used the continuous respirometry of the contaminated soils which is a relatively unexploited subject. This procedure generated a huge amount of data as the measurements of the oxygen and carbon dioxide concentrations, as well as the temperature, are done at intervals of a second. Several mathematical tools were used for treating this data. Time series and system identification was chosen to analyze data interpreted as biological signals allowing for the detection of particularities related to daily cycles of activity, and also to analyze the temporal relationship between variables through the autocorrelation and the cross-correlation functions. The cyclic behavior of respirometric variables was analyzed using wavelets.
The combination of this set of tools, systems of ordinary differential equations, time series analysis, systems identification, Fourier analysis and wavelets theory allowed us to characterize and predict the behavior of the main variables of a geo-environmental system in progress.

Numerical Investigation of the Upper Bounds on the Convective Heat Trasport in a Heated From Below Rotating Fluid Layer

N. K. Vitanov

We apply the Galerkin method in order to obtain numerical solution of the Euler- Lagrange equations for the variational problem for the upper bounds on the convective heat transport in a fluid layer under the action of intermediate and strong rotation. The role of the numerical investigation in such kind of variational problems is to obtain the upper bounds for the case of small and intermediate values of the Rayleigh and Taylor numbers in addition to the analytical asymptotic theory which leads to the upper bounds for the case of large values of the above two characteristic dimensionless numbers. The application of the Galerkin method reduces the Euler - Lagrange equations to a system of nonlinear algebraic equations. This system is solved numerically by the Powel hybrid method. We observe that the Powel hybrid method guarantees satisfactory fast rate of convergence from the guess solution to the solution of the system of equations. We present and discuss several results from the numerical computations.

Population-based Metaheuristics for Tasks Scheduling in Heterogeneous Distributed Systems

F. Zamfirache, M. Frîncu, D. Zaharie

Tasks scheduling in heterogeneous distributed systems (e.g. grids) is known as a hard optimization problem because of the lack of reliable information about tasks and resources. In real distributed systems the tasks arrive continuosly and have to be assigned to resources either as they arrive or when a scheduling event is triggered. In this work we analyzed both the case when the scheduling event is triggered when a given number of tasks arrived and the case when the scheduling is activated at pre-specified moments of time.
Besides the traditional heuristics, a lot of population-based metaheuristics (evolutionary algorithms, memetic algorithms, ant systems) have been proposed lately. Most metaheuristics use local search operators involving either the move of a task from one machine to another one or the swap of two tasks belonging to different machines. Depending on the selection of the source and destination machines and of the task(s) to be relocated the local search can be more explorative or more exploitative. In order to make a compromise between greediness and randomness we propose a hybrid mutation operator involving both task relocation ensuring a decrease of the makespan and random relocation. Based on this mutation operator we designed an evolutionary algorithm which was tested both on a traditional benchmark based on the "expected time to compute" model and by using a simulator based on specific probability distributions. The evolutionary algorithm was compared with non-population heuristics (eg. MinMin, MaxMin, MCT, OLB, Sufferage etc.) and with other evolutionary algorithms and the results illustrate its competitiveness especially in the case highly heterogeneous and inconsistent distributed systems. Moreover population-based extensions of some heuristics used for online scheduling were designed and tested leading to improved schedules.

Comparative Numerical Results in 4D-Var Data Assimilation Problems Using POD Techniques

G. Dimitriu, R. Ştefănescu

The four-dimensional variational data assimilation (4D-Var) method has been a very successful technique used in operational numerical weather prediction at many weather forecast centers. A major difficulty in the operational use of 4D-Var data assimilation for oceanographic and atmospheric global circulation models is the large dimension of the control space, which is the size of the discrete model initial conditions, typically in the range $10^6 - 10^8$. A way to significantly decrease the dimension of the control space without compromising the quality of the final solution for the 4D-Var data assimilation, motivates us to construct the control variable on a basis of characteristic vectors capturing most of the energy and the main features of variability of the model.

Proper orthogonal decomposition (POD) technique has been used to obtain low dimensional dynamical models of many applications in engineering and science. Basically, the idea starts with an ensemple of data, called *snapshots*, collected from an experiment or a numerical procedure of a physical system. The POD technique is then used to produce a set of basis functions which spans the snapshots collection.

The first part of our work carries out a comparison approach of the accuracy of numerical solutions to data asimilation problems in the case of three advection-diffusion equations, where the proper orthogonal decomposition is defined using H^1-norm and L^2-norm, respectively. The second part of the study analyses the performance of an adaptive POD procedure with respect to the data assimilation solution obtained with the classical POD technique. The study ends with some conclusions.

Part C

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