A DISCUSSION OF LOW ORDER NUMERICAL INTEGRATION FORMULAS FOR RIGID AND FLEXIBLE MULTIBODY DYNAMICS

Dan Negrut, Naresh Khude, and Toby Heyn

Department of Mechanical Engineering
University of Wisconsin, 1550 Engineering Drive, Madison, WI, 53706, USA
e-mails: negrut@engr.wisc.edu, khude@wisc.edu, heyn@wisc.edu

Abstract. *The premise of this work is the observation that real-life mechanical systems limit the use of high order integration formulas due to the presence in the associated models of friction and contact/impact elements. High-order numerical integration methods are impractical in these cases, and producing a numerical solution relies on the use of low order integration formulas. The latter methods are generally robust and expeditious; their major drawback is the fact that they usually require small integration step-sizes in order to meet a user prescribed accuracy. This paper looks at several low order numerical integration methods that draw on both the Hilber-Hughes-Taylor (HHT) formulas and Backward Differentiation Formula (BDF) method, in an effort to assess their behavior. The first objective is to briefly indicate the theoretical results available in the literature regarding the stability and convergence properties of these low order methods when applied in the context of multibody dynamics simulation (MBS). The second objective is to perform a set of numerical experiments to compare these integration formulas in terms of several metrics: (a) efficiency, (b) energy preservation, and (c) velocity constraint drift. A set of simple mechanical systems are used to this end: a double pendulum, a slider crank with rigid bodies and a slider crank with a flexible body represented in the floating frame formulation.*

1 INTRODUCTION

A multitude of phenomena, processes, and applications are described in terms of mixed systems of differential equations combined with linear and nonlinear algebraic equations, most often corresponding to models coming from engineering, physics, and chemistry. Differential equations relate certain quantities to their derivatives with respect to time and/or space variables. Algebraic equations usually model conservation laws and the constraints present in the system. When there are derivatives with respect to only one independent variable (usually time) the equations are called differential-algebraic equations (DAEs). DAEs are basically differential equations defined on submanifolds of $\mathbb{R}^n$. The constrained equations of motion can be expressed in the form (see, for instance, Haug (1989), Shabana (2005))

$$\begin{aligned} \dot{\mathbf{q}} &= \mathbf{v} \\ \mathbf{M}(\mathbf{q})\dot{\mathbf{v}} &= \mathbf{Q}\left(t,\mathbf{q},\mathbf{v},\boldsymbol{\lambda},\boldsymbol{\mu},\mathbf{u}(t)\right) - \boldsymbol{\Phi}_{\mathbf{q}}^{T}(\mathbf{q},t)\boldsymbol{\lambda} - \boldsymbol{\Gamma}_{\mathbf{v}}^{T}(\mathbf{v},\mathbf{q},t)\boldsymbol{\mu} \\ 0 &= \boldsymbol{\Phi}(\mathbf{q},t) \\ 0 &= \boldsymbol{\Gamma}(\mathbf{v},\mathbf{q},t), \end{aligned} \tag{1}$$

where $\mathbf{q}\in\mathbb{R}^n$ are generalized coordinates, $\mathbf{v}\in\mathbb{R}^n$ are generalized velocities, $\boldsymbol{\lambda}\in\mathbb{R}^m$ and $\boldsymbol{\mu}\in\mathbb{R}^p$ are Lagrange multipliers, and $\mathbf{u}:\mathbb{R}\rightarrow\mathbb{R}^c$ represent time dependent external dynamics; e.g., control variables. The matrix $\mathbf{M}(\mathbf{q})$ is the generalized mass matrix, $\mathbf{Q}(t,\mathbf{q},\mathbf{v},\boldsymbol{\lambda},\boldsymbol{\mu},\mathbf{u}(t))$ represents the vector of generalized forces, $\boldsymbol{\Phi}(\mathbf{q},t)$ is the set of m holonomic constraints, i.e., position-level kinematic constraints, and $\boldsymbol{\Gamma}(\mathbf{v},\mathbf{q},t)$ is the set of p nonholonomic constraints, i.e., velocity-level kinematic constraints (Abraham and Marsden 1985; Arnold 1989; Haug 1989). Differentiating the kinematic constraints with respect to time leads to the additional equations

$$\begin{aligned} \mathbf{0} &= \boldsymbol{\Phi}_{\mathbf{q}}(\mathbf{q},t)\,\mathbf{v} + \boldsymbol{\Phi}_{\mathbf{t}}(\mathbf{q},t) \\ \mathbf{0} &= \boldsymbol{\Phi}_{\mathbf{q}}(\mathbf{q},t)\,\dot{\mathbf{v}} + (\boldsymbol{\Phi}_{\mathbf{q}}(\mathbf{q},t)\mathbf{v})_{\mathbf{q}}\,\mathbf{v} + 2\boldsymbol{\Phi}_{\mathbf{q}t}(\mathbf{q},t)\mathbf{v} + \boldsymbol{\Phi}_{tt}(\mathbf{g},t) \\ \mathbf{0} &= \boldsymbol{\Gamma}_{\mathbf{v}}(\mathbf{v},\mathbf{q},t)\dot{\mathbf{v}} + \boldsymbol{\Gamma}_{\mathbf{q}}(\mathbf{v},\mathbf{q},t)\mathbf{v} + \boldsymbol{\Gamma}_{t}(\mathbf{v},\mathbf{q},t). \end{aligned} \tag{2}$$

Equations (1) and (2) form an over-determined system of DAEs, having strictly more equations than variables. The ability to solve such systems is relevant for several classes of applications such as multibody dynamics and molecular dynamics.

When finding the solution of Eqs. (1) and (2), most numerical solvers currently used in industry share some or all of the following major drawbacks: numerical drift that occurs when the solution does not stay on the manifold of constraints at the position and/or velocity levels and as such might become nonphysical; inability to deal efficiently with stiffness; loss of underlying properties of the exact flow and trajectories; no preservation of invariants such as energy; introduction of undesired numerical damping; and the reduction of convergence order when solving stiff problems that arise often in applications. Whereas techniques for the numerical solution of ordinary differential equations (ODEs) go back more than three centuries and are well established, the numerical solution of DAEs has a comparatively short history (Brenan, Campbell et al. 1989; Hairer, Lubich et al. 1989; Haug 1989; Hairer and Wanner 1996). The first class of numerical techniques subsequently applied to DAEs was published by Gear (1971) for the solution of ODEs. Since then DAEs have widely penetrated the numerical analysis, engineering, and scientific computing communities and are increasingly encountered in practical applications. Still, numerically solving DAEs poses fundamental difficulties not encountered when solving ODEs. Therefore, specialized numerical techniques have been developed, typically belonging to one of two classes: state-space methods or direct methods.

State-space methods first reduce the DAEs to a smaller dimension ODE problem, thus benefiting from the extensive body of knowledge associated with ODE solvers. Specifically, the DAEs induce differential equations on the constraint manifold Potra and Rheinboldt (1991), which can be reduced on a subspace of the *n*-dimensional Euclidean space. The resulting state-space ODEs (SSODEs) are integrated using classical numerical integration formulas. The one-to-one local mapping from the manifold to the subspace of independent coordinates is then used to determine the point on the manifold corresponding to the solution of the SSODEs. This framework formalizes the theory of numerical solution of DAEs using the language of differential manifolds (Rheinboldt 1984). Practical approaches in this class of methods are due to Wehage and Haug (1982), Liang and Lace (1987), Potra and Rheinboldt (1991), and Yen (1993). The main factor that differentiates these approaches is the choice of manifold parameterization. State-space methods have been subject to criticism in two aspects. First, the choice of parameterization generally is not global. Second, poor choices of the projection space result in SSODEs that are numerically demanding, mainly at the expense of overall efficiency and robustness of the algorithm (Alishenas 1992). Although the theoretical framework for these methods was outlined several years ago (Mani, Haug et al. 1985; Potra and Rheinboldt 1991), it was only recently that implicit numerical integration methods for DAEs have been proposed in the context of SSODEs for multibody dynamics analysis (Haug, Negrut et al. 1997; Negrut, Haug et al. 2003). The major intrinsic drawback associated with state-space methods remains the expensive DAE to ODE reduction process that is further exacerbated in the context of implicit integration, which is the norm in industry applications.

Alternatively, direct methods discretize the constrained equations of motion (1), after possibly reducing the index of the DAEs by considering some or all of the kinematic constraint equations in (2). Original contributions in this direction are found in the work of Orlandea (1977), Gear et al. (1985), Brenan et al. (1989), Ascher and Petzold (1993), Führer and Leimkuhler (1991), Lubich et al. (1995), Ascher et al. (1994; 1995), and Bauchau et al. (2003). When dealing with systems that include flexible substructures and bodies, numerical methods have been sought that are capable of introducing controllable numerical dissipation to damp out spurious high frequencies, which are an artifact of the spatial discretization, without affecting the low frequencies of the system and the accuracy of the method (Hughes 1987; Geradin and Rixen 1994). Several methods have been proposed for structural dynamic simulation, such as the HHT method (also called α-method, (Hilber, Hughes et al. 1977)) and the generalized α-method (Chung and Hulbert 1993). These are order two methods proposed in conjunction with ODE problems associated with structural dynamics. For constrained multibody systems few methods capable of addressing the nonlinear algebraic component associated with the DAE problem have been reported (Cardona and Geradin 1989; Cardona and Geradin 1994; Yen, Petzold et al. 1998). Recent theoretical and implementation aspects related to an HHT-based numerical integrator for the simulation of large mechanical systems with flexible bodies and contact/impact have been discussed by Negrut et al. (2007). One of the salient attributes of their algorithm is the good condition number of the Jacobian associated with the implicit numerical integrator. Extending on a scaling idea introduced in conjunction with BDF methods by Brenan et al. (1989) and recently discussed by Bottasso et al. (2007), the condition number remains bounded when $h \to 0$. Furthermore, the proposed method effectively "filters out" errors in certain partial derivatives that might be introduced, for instance, by approximations of external loading (tires, aerodynamic forces, etc.), thanks to the scaling by h^2. The method, released in the latest version of the commercial simulation package ADAMS is equipped with numerical integration error estimation, integration step-size control, and Newton iteration stopping criteria. A benchmark test of several thousand

models of various complexities indicated an average reduction factor of two to three in simulation time when compared with the previous integrators in ADAMS. The very attractive attributes of the method proposed by Negrut et al. (2007) are overshadowed by two drawbacks. First, there is no global proof of convergence associated with the method, although extensive numerical experiments indicate second order convergence. Second, the method imposes only the position-level constraint equations, which leads to a violation of the velocity-level constraint equations.

2 INTEGRATION FORMULAS

The first numerical integration method considered here draws on the Newmark formulas (Newmark 1959). It requires the selection of two parameters $\gamma \geq 1/2$, $\beta \geq (\gamma + 1/2)^2/4$ based on which, given the acceleration $\ddot{q}_{n+1}$ at the new time step t_{n+1}, the new position and velocity are obtained as

$$\mathbf{q}_{n+1} = \mathbf{q}_n + h\dot{\mathbf{q}}_n + \frac{h^2}{2}\left[(1-2\beta)\ddot{\mathbf{q}}_n + 2\beta\ddot{\mathbf{q}}_{n+1}\right] \tag{3}$$

$$\dot{\mathbf{q}}_{n+1} = \dot{\mathbf{q}}_n + h\left[(1-\gamma)\ddot{\mathbf{q}}_n + \gamma\ddot{\mathbf{q}}_{n+1}\right] \tag{4}$$

In the context of a multibody dynamics, using an integration step size h, the discretization scheme operates on the constrained equations of motion and position kinematic constraint equations to lead to the nonlinear system:

$$\left(\mathbf{M}\ddot{\mathbf{q}}\right)_{n+1} + \left(\mathbf{\Phi}_{\mathbf{q}}^T\boldsymbol{\lambda}\right)_{n+1} = \mathbf{Q}_{n+1} \tag{5}$$

$$\mathbf{\Phi}(\mathbf{q}_{n+1}, t_{n+1}) = 0\,. \tag{6}$$

The method, called hereafter NEWMARK, is first order, unless $\gamma = 1/2$ and $\beta = 1/4$. This choice leads to the trapezoidal method, which is known in the literature to have stability problems when used on index-3 DAEs.

Referred to as HHT-I3, the second method considered in this study draws on the HHT method (Hilber, Hughes et al. 1977), which has been widely used in the structural dynamics community and later used in the context of MBS (Cardona and Geradin 1989). HHT-I3 represents a slight variation of the NEWMARK method in that it still uses the same discretization formulas of Eqs. (3), (4) but alters the equation of motion:

$$\left(\mathbf{M}\ddot{\mathbf{q}}\right)_{n+1} + (1+\alpha)(\mathbf{\Phi}_{\mathbf{q}}^T\boldsymbol{\lambda} - \mathbf{Q})_{n+1} - \alpha(\mathbf{\Phi}_{\mathbf{q}}^T\boldsymbol{\lambda} - \mathbf{Q})_n = 0 \tag{7}$$

Recently, the method was analyzed by Negrut, Rampalli et al. (2007) (local error control, step-size selection, Newton stopping criteria), and implemented in MSC.ADAMS, a commercial simulation package.

The third integration method considered in this study is essentially the BDF method of order two proposed by Gear (1971). This method is cast into a form similar to the Newmark formula:

$$\mathbf{q}_{n+1} = \frac{4}{3}\mathbf{q}_n - \frac{1}{3}\mathbf{q}_{n-1} + h\left(\frac{8}{9}\dot{\mathbf{q}}_n - \frac{2}{9}\dot{\mathbf{q}}_{n-1}\right) + \frac{4}{9}h^2\ddot{\mathbf{q}}_{n+1} \tag{8}$$

$$\dot{\mathbf{q}}_{n+1} = \frac{4}{3}\dot{\mathbf{q}}_n - \frac{1}{3}\dot{\mathbf{q}}_{n-1} + \frac{2}{3}h\ddot{\mathbf{q}}_{n+1} \tag{9}$$

These formulas used in conjunction with Eq. (5) and (6) lead to a second order method referred to in the sequel as NSTIFF.

The next three numerical integration methods investigated herein take into account the velocity kinematic constraint equations to prevent drift in velocity constraints and improve the overall quality of the solution. One of these methods introduces a correction into the New-

mark formulas based on the constraint accelerations and was shown to have global convergence order two (Jay and Negrut 2006). Given an initial configuration $(\mathbf{q}_0, \dot{\mathbf{q}}_0, \ddot{\mathbf{q}}_0)$, defining $\mathbf{f}(t,\mathbf{q},\dot{\mathbf{q}}) := \mathbf{M}^{-1}(\mathbf{q})\mathbf{Q}(t,\mathbf{q},\dot{\mathbf{q}})$ and $\mathbf{r}(\mathbf{q},\boldsymbol{\lambda}) := -\mathbf{M}^{-1}(\mathbf{q})\boldsymbol{\Phi}_{\mathbf{q}}^T\boldsymbol{\lambda}$,

$$\mathbf{q}_1 = \mathbf{q}_0 + h\dot{\mathbf{q}}_0 + \frac{h^2}{2}\left((1-2\beta)\ddot{\mathbf{q}}_0 + 2\beta\ddot{\mathbf{q}}_1\right) + \frac{h^2}{2}((1-b)\mathbf{R}_0 + b\mathbf{R}_1) \tag{10}$$

$$\dot{\mathbf{q}}_1 = \dot{\mathbf{q}}_0 + h\left((1-\gamma)\ddot{\mathbf{q}}_0 + \gamma\ddot{\mathbf{q}}_1\right) + \frac{h}{2}\left(\mathbf{R}_0 + \mathbf{R}_1\right) \tag{11}$$

$$\boldsymbol{\Phi}\left(\mathbf{q}_{n+1}, t_{n+1}\right) = 0 \tag{12}$$

$$\boldsymbol{\Phi}_{\mathbf{q}}(\mathbf{q}_1, t_1)\dot{\mathbf{q}}_1 + \boldsymbol{\Phi}_t(\mathbf{q}_1, t_1) = 0 \tag{13}$$

$$\ddot{\mathbf{q}}_1 = (1+\alpha)\mathbf{f}(t_1,\mathbf{q}_1,\dot{\mathbf{q}}_1) - \alpha\mathbf{f}(t_0,\mathbf{q}_0,\dot{\mathbf{q}}_0) \tag{14}$$

where $b \neq 1/2$ is a free coefficient, $\mathbf{R}_0 := \mathbf{r}(t_0,\mathbf{q}_0,\boldsymbol{\psi}_0)$, $\mathbf{R}_1 := \mathbf{r}(t_1,\mathbf{q}_1,\boldsymbol{\psi}_1)$, and $\boldsymbol{\psi}_0$, $\boldsymbol{\psi}_1$ are determined at each time step by imposing that the position and velocity kinematic constraint equations hold at time t_1. This method is referred as HHT-ADD and discussed at length in (Jay and Negrut 2006).

The fifth integration method investigated, HHT-SI2, is a variation on the above formula (Jay and Negrut 2007). Preliminary theoretical and numerical results indicate that using the following discretization formulas, in conjunction with the position and velocity kinematic constraint equations leads to a second order method:

$$\mathbf{q}_1 = \mathbf{q}_0 + h\dot{\mathbf{q}}_0 + \frac{h^2}{2}\left((1-2\beta)\ddot{\mathbf{q}}_\alpha + 2\beta\tilde{\mathbf{a}}_{1+\alpha}\right) \tag{15}$$

$$\dot{\mathbf{q}}_1 = \dot{\mathbf{q}}_0 + h\left((1-\gamma)\ddot{\mathbf{q}}_\alpha + \gamma\ddot{\mathbf{q}}_{1+\alpha}\right) \tag{16}$$

$$\mathbf{M}_{1+\alpha}\tilde{\mathbf{a}}_{1+\alpha} = (1+\alpha)\mathbf{f}\left(t_1,\mathbf{q}_1,\dot{\mathbf{q}}_1,\tilde{\boldsymbol{\lambda}}_1\right) - \alpha\left(t_0,\mathbf{q}_0,\dot{\mathbf{q}}_0,\boldsymbol{\lambda}_0\right) \tag{17}$$

$$\mathbf{M}_{1+\alpha}\ddot{\mathbf{q}}_{1+\alpha} = (1+\alpha)\mathbf{f}\left(t_1,\mathbf{q}_1,\dot{\mathbf{q}}_1,\boldsymbol{\lambda}_1\right) - \alpha\left(t_0,\mathbf{q}_0,\dot{\mathbf{q}}_0,\boldsymbol{\lambda}_0\right) \tag{18}$$

where $\mathbf{M}_{1+\alpha} := \mathbf{M}\left(t_{1+\alpha}, \mathbf{q}_0 + h(1+\alpha)\dot{\mathbf{q}}_0\right)$ and $\tilde{\mathbf{a}}_{1+\alpha}$, $\tilde{\boldsymbol{\lambda}}_1$ are auxiliary variables which are local to the current time step.

Finally, the sixth and last integration method investigated in this work is the so called stabilized index 2 formulation of Gear, Gupta, and Leimkuhler (1985), which uses the discretization formulas of Eqs. (8) and (9) and solves the following system of nonlinear equations to recover the state of the mechanical system at time-step t_{n+1}:

$$\mathbf{v}_{n+1} = \dot{\mathbf{q}}_{n+1} + \left(\boldsymbol{\Phi}_{\mathbf{q}}^T\boldsymbol{\mu}\right)_{n+1} \tag{19}$$

$$(\mathbf{M}(\mathbf{q})\dot{\mathbf{v}})_{n+1} = \mathbf{Q}(t_{n+1},\mathbf{q}_{n+1},\mathbf{v}_{n+1}) - \boldsymbol{\Phi}_{\mathbf{q}}^T(\mathbf{q}_{n+1},t_{n+1})\boldsymbol{\lambda} \tag{20}$$

$$\boldsymbol{\Phi}(\mathbf{q}_{n+1},t_{n+1}) = \mathbf{0} \tag{21}$$

$$\boldsymbol{\Phi}_{\mathbf{q}}(\mathbf{q}_{n+1},t_{n+1})\,\mathbf{v}_{n+1} + \boldsymbol{\Phi}_t(\mathbf{q}_{n+1},t_{n+1}) = \mathbf{0} \tag{22}$$

Like HHT-SI2, this integration method relies on the discretization of the kinematic velocity constraint equations and the use of an auxiliary variable $\boldsymbol{\mu}$ to prevent velocity drift. This method is referred to as NSTIFF-SI2 and, according to theoretical results due to Gear, Gupta et al. (1985) is a second order integration method.

Among these integration methods, NSTIFF, HHT-ADD, HHAT-SI2, and NSTIFF-SI2 have global convergence proofs for the class of differential algebraic equations associated with multibody dynamics (Lötstedt and Petzold 1986; Brenan and Engquist 1988; Jay and Negrut 2006; Jay and Negrut 2007). However, theoretical global convergence results for NEWMARK and HHT-I3 are, to the best of our knowledge, not known yet. Nonetheless, numerical experiments carried out suggest that even in case of index 3 DAEs, these methods

display convergence orders that have been proved for the ODE case (one and two, respectively). A formal proof for this is yet to be produced.

3 MODELS CONSIDERED

The models considered for testing and comparison of algorithm performance are the double pendulum, slider crank, and slider crank with flexible link using floating frame of reference formulation. The model parameters and the initial conditions used are summarized below.

a. Double Pendulum

Figure 1 shows the schematic of a double pendulum. Torsional spring and dampers are included in the model at the pin joints. The parameter values used in this model are m_1 = 3 kg, L_1 = 1m, k_1 = 400N/m, c_1 = 15 Ns/m, m_2 = 0.3 kg, L_2 = 1.5 m, k_2 = 300000 N/m and $c_2 = 5000$ Ns/m. The initial conditions were $\theta_1(0) = 2\pi, \theta_2(0) = 0, \dot{\theta}_1(0) = 0$ and $\dot{\theta}_2(0) = 10$. Units throughout the paper are SI unless indicated otherwise.

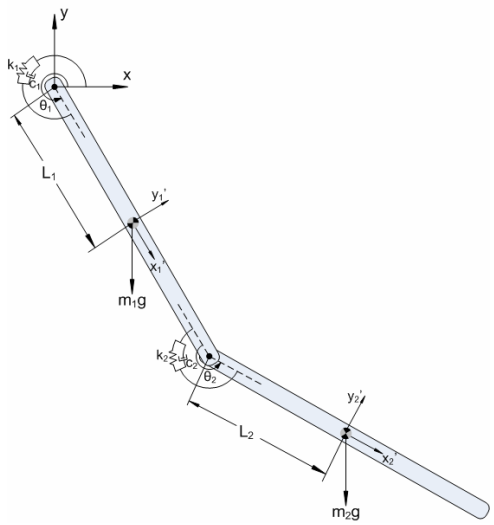

Figure 1: Double Pendulum

b. Slider Crank

The schematic of a slider crank model including a spring-damper element is shown in Figure 2. The parameters associated with the model are m_1 = 3 kg, L_1 = 0.3 m, m_2 = 0.9 kg, L_2 = 0.6 m, k = 100 N/m and c = 5 Ns/m.

The initial conditions used for simulation of motion were $\theta_1(0) = 3\pi/2$, $\dot{\theta}_1(0) = 0$ rad/s.

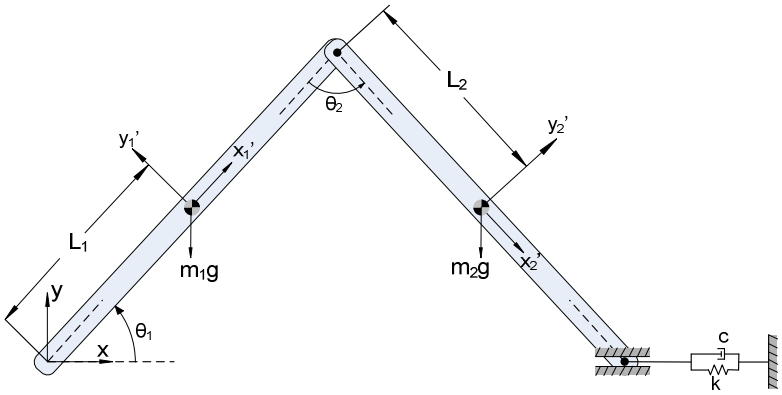

Figure 2: Slider Crank

c. Flexible Slider Crank

This model is similar to the rigid model shown in Figure 2, except that the spring and damper are not included. The parameter values used in this model are m_1 = 3 kg, L_1 = 0.3 m, m_2 = 0.9 kg and L_2 = 0.6 m. In this model, the connecting rod is made flexible with floating frame of reference, which has the properties, cross-section area A = 5.74E-6 m^2, moment of inertia I = 2.765E-8 m^4 and Young's modulus E = 200 GPa. The initial conditions are $\theta_1(0) = 3\pi/2$, $\dot{\theta}_1(0) = 1$ rad/s.

4 NUMERICAL EXPERIMENTS

The numerical algorithms were implemented on each model and several experiments were run to evaluate their performance and compare them in terms of order of convergence, energy preservation, constraint satisfaction and efficiency.

4.1 Order analysis

To assess the convergence order of each numerical method, a reference solution for each model is determined using the Runge-Kutta method (RK4) with a step size of 1e-6. Each model is simulated for 2 seconds and the results are compared to the reference solution based at the final time. Results show that, as expected, NSTIFF, HHT-SI2, HHT-ADD, NSTIFF-SI2 exhibit order 2 convergence. However, HHT-I3 and NEWMARK show order 2 and order 1 convergence respectively, for all the models. The convergence order plots for each numerical method using considered models are shown in Figure 3 through Figure 10.

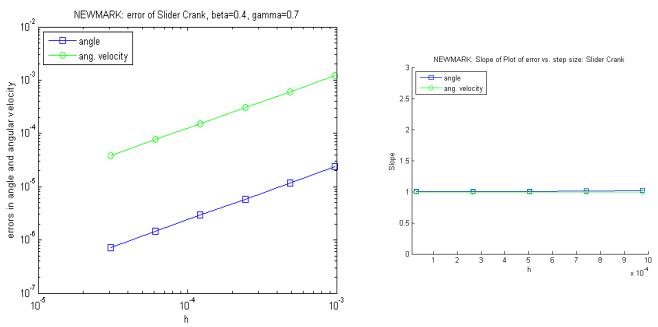

Figure 3: Global Convergence Order – Newmark: Slider Crank

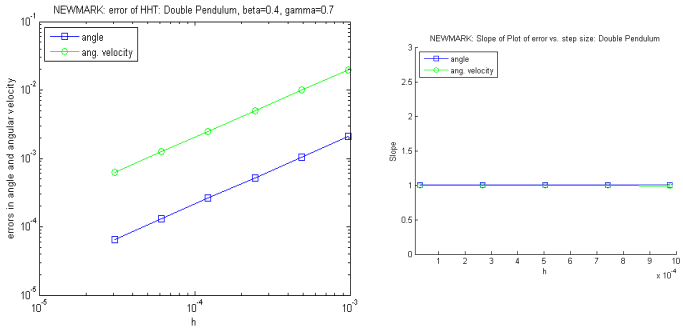

Figure 4: Global Convergence Order – Newmark: Double Pendulum

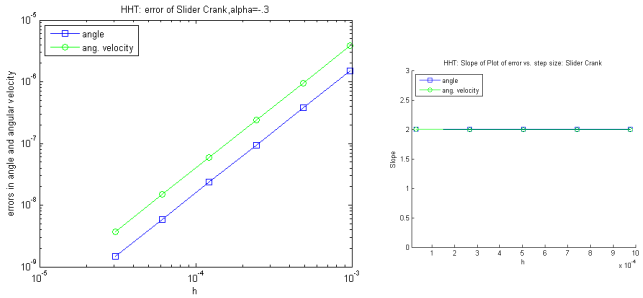

Figure 5: Global Convergence Order – HHT-I3: Slider Crank

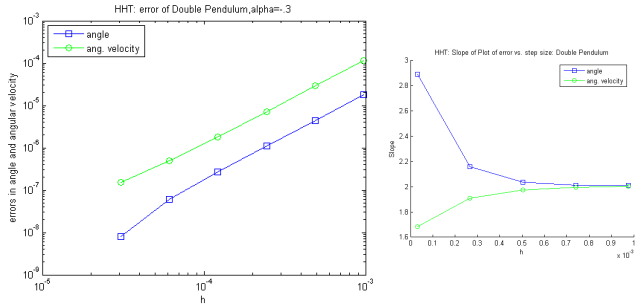

Figure 6: Global Convergence Order – HHT-I3: Double Pendulum

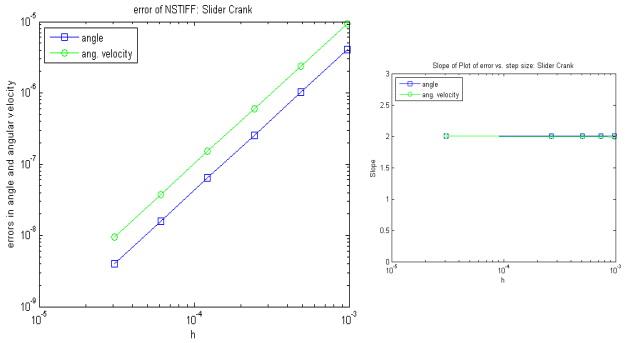

Figure 7: Global Convergence Order – NSTIFF: Slider Crank

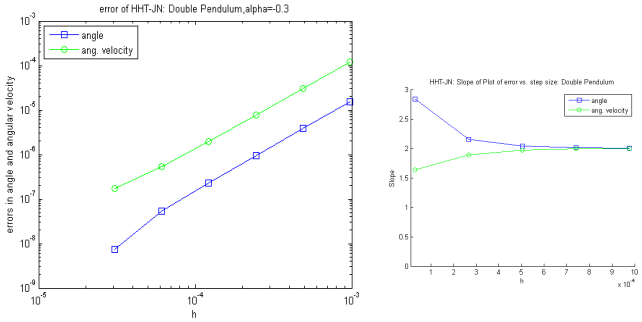

Figure 8: Global Convergence Order – HHT-ADD: Double Pendulum

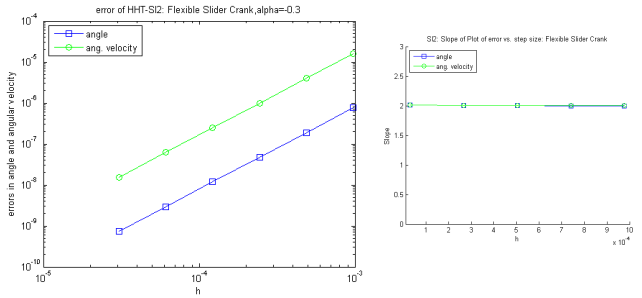

Figure 9: Global Convergence Order – HHT-SI2: Flexible Slider Crank

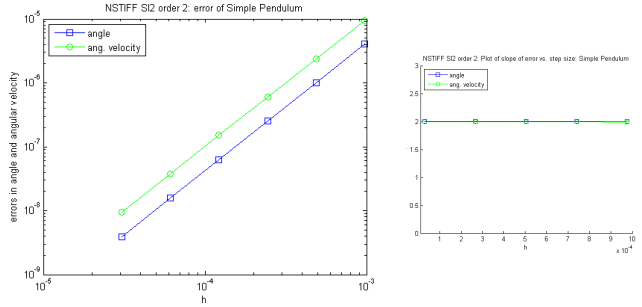

Figure 10: Global Convergence Order – NSTIFF-SI2: Slider Crank

4.2 Energy preservation

The HHT method came as an improvement over Newmark formulas because it preserved the A-stability and numerical damping properties while achieving second-order accuracy in solving DAEs. In this method, high-frequency oscillations that are of no interest as well as parasitic high-frequency oscillations that are a byproduct of the finite element discretization are damped with the parameter α. The choice of α is based on the desired level of damping for a particular model. The smaller the value of α, the more damping is induced in the numerical solution. Note that the choice $\alpha = 0$ leads to the trapezoidal method with no numerical damping. The effect of this damping can be seen from energy preservation plots shown in Figure 11 and Figure 12. These energy plots are for the slider-crank model from which the translational damper was removed. The system is conservative, and for the particular reference system employed, the total energy should be constant and equal to zero.

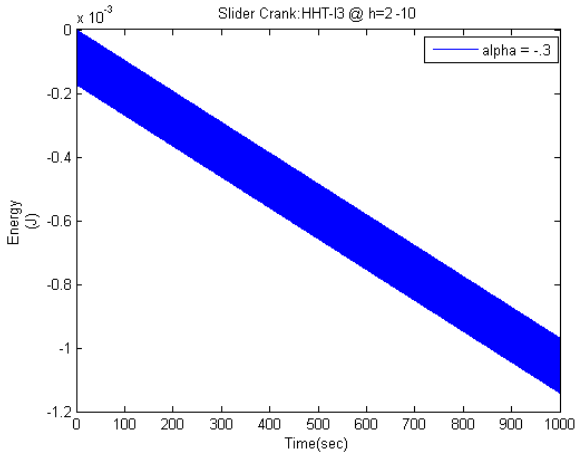

Figure 11: Energy Dissipation at α = - 0.3

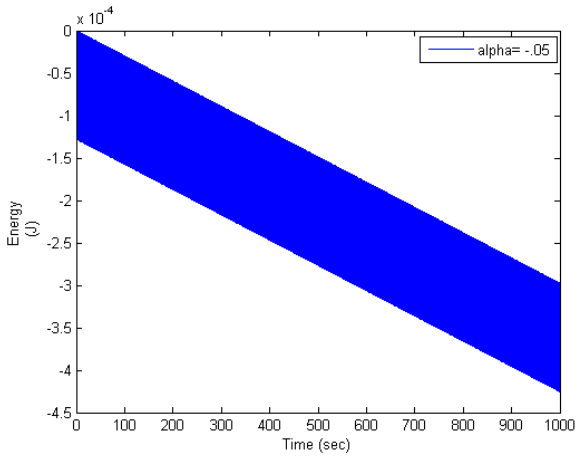

Figure 12: Energy Dissipation at α = - 0.05

As anticipated, when $\alpha = -0.3$ the numerical damping-induced dissipation is more pronounced than the $\alpha = -0.05$ case. Even more relevant is an investigation of how the numerical energy dissipation changes with the step-size. Results in Figure 12 indicate a highly oscillatory pattern. To capture the degree to which a numerical scheme dissipates energy, an average energy dissipation over an interval $[0,T]$ is computed as

$$\varepsilon(T) = \frac{1}{T}\int_0^T |E_{tot}(t)|dt\,. \tag{23}$$

If no numerical dissipation was present in the system then $\varepsilon(T) = 0$, $\forall T > 0$. On a log-log scale, Figure 13 shows $\varepsilon(10)$ for the rigid slider crank model with no physical damping. Surprisingly, this average total energy error converges to zero like $O(h^q)$, where q is the order of the method. In other words, for NEWMARK it converges to zero like $O(h)$, while for all the other methods the average energy error converges like $O(h^2)$.

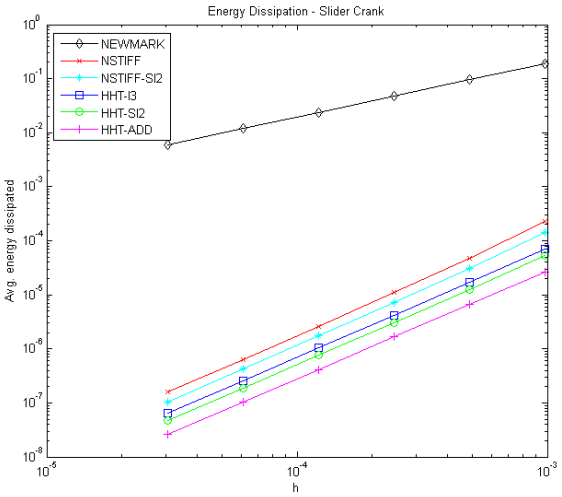

Figure 13: Energy Dissipation Characteristics – Slider Crank

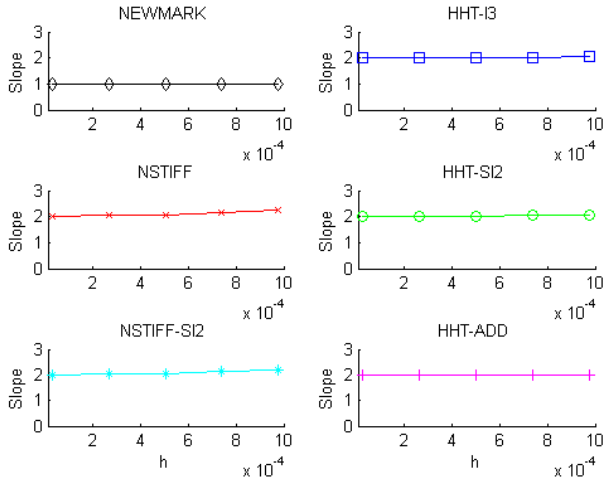

Figure 14: Slope- Energy Dissipation

It remains for this observation vis-à-vis the behavior of $\varepsilon(T)$ to be formally proven. This would be an interesting result, since $\varepsilon(T)$ is a global error that captures the energy drift over the entire simulation. Such a result could be relevant, for instance, in the context of Molecular Dynamics (MD) simulation. Since one of the reasons for which entire classes of integrators are disqualified in MD simulation is that they do not preserve energy. However, with values in the femtosecond range, the step-size for MD simulations might be so small that HHT, Newmark, and BDF type methods might in fact be viable candidates in the MD simulation arena. This question is currently under investigation (Schafer, Serban et al. 2007).

4.3 Kinematic constraint drift

The rationale behind stabilizing the numerical solution of the index 3 DAE of multibody dynamics using the velocity kinematic constraint equations is to prevent drift in satisfying this set of algebraic constraints. Three of the six methods analyzed in this study, namely HHT-ADD, HHT-SI2, and NSTIFF-SI2, enforce these equations. As such, no velocity constraint drift is expected in the numerical solution. This is confirmed by the plots in Figure 15 through

Figure 17. These figures display a plot of the velocity constraint violation in the X direction against the velocity constraint violation in the Y direction for the rigid slider-crank mechanism. Data was plotted at each time step and, as anticipated, confirms that the velocity kinematic constraint equations are satisfied within machine precision.

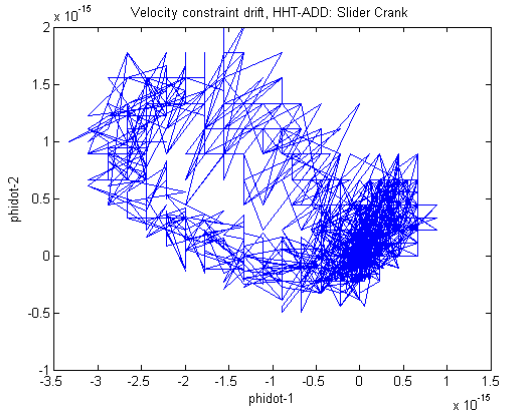

Figure 15: Velocity Constraint Drift - HHT-ADD

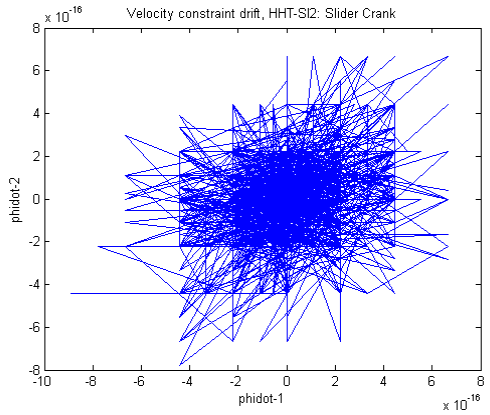

Figure 16: Velocity Constraint Drift - HHT-SI2

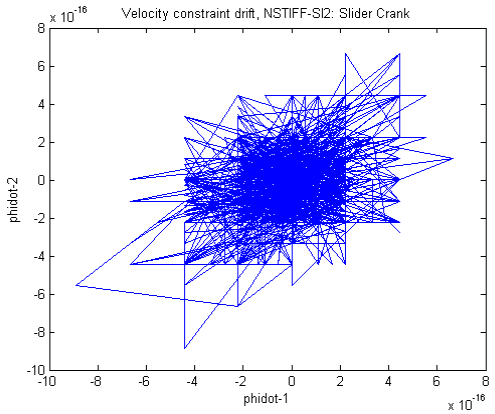

Figure 17: Velocity Constraint Drift - NSTIFF-SI2

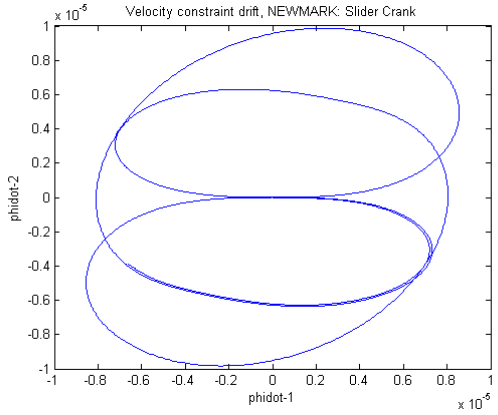

Figure 18: Velocity Constraint Drift - NEWMARK

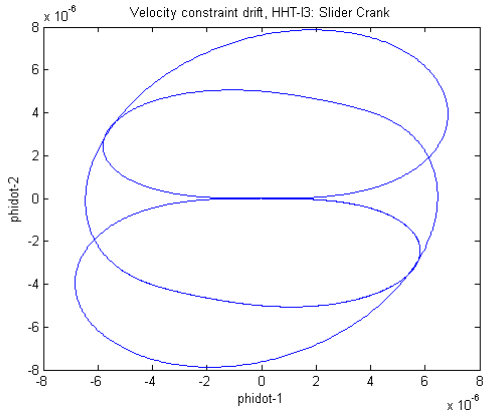

Figure 19: Velocity Constraint Drift - HHT-I3

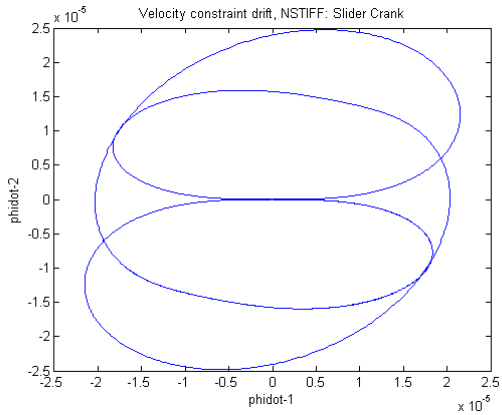

Figure 20: Velocity Constraint Drift - NSTIFF

Figure 18 through Figure 20 show the same information for the rigid slider crank with no damping; the plots report data obtained during a 10 second long simulation, with a step-size $h = 2^{-10}$ s. The most remarkable thing is that NEWMARK, HHT-I3, and NSTIFF display the same error behavior. Moreover, as the step-size decreases, the box that bounds the plot shrinks but the shape of the curves remains the same for all three integration methods. The root cause of this behavior remains to be investigated. For now, it should be pointed out that numerical experiments indicate that the error in satisfying these constraints converges like

$O(h^q)$, where q is the order of the method. A more formal investigation of these observations remains to be done in the future.

4.4 Efficiency comparison

For an early comparison of CPU efficiency, the six methods investigated in this work were used to run a 2 second-long simulation of the slider crank model with a constant step-size $h = 2^{-10}$. The timing results are reported in Table 1, while Figure 21 compares these CPU times normalized to the time it takes the HHT-I3 method to finish the simulation. The figure suggests that having the kinematic velocity constraint equations enforced usually leads to a 30% simulation slowdown. These are, however, preliminary results that remain to be confirmed in the case of the other models.

Numerical Integration Method	CPU time for 2 Sec simulation of Slider Crank
NEWMARK	1.880573
NSTIFF	1.937542
HHT-I3	2.086842
NSTIFF – SI2	2.333389
HHT- SI2	2.720254
HHT- ADD	3.544779

Table 1: Slider crank timing results

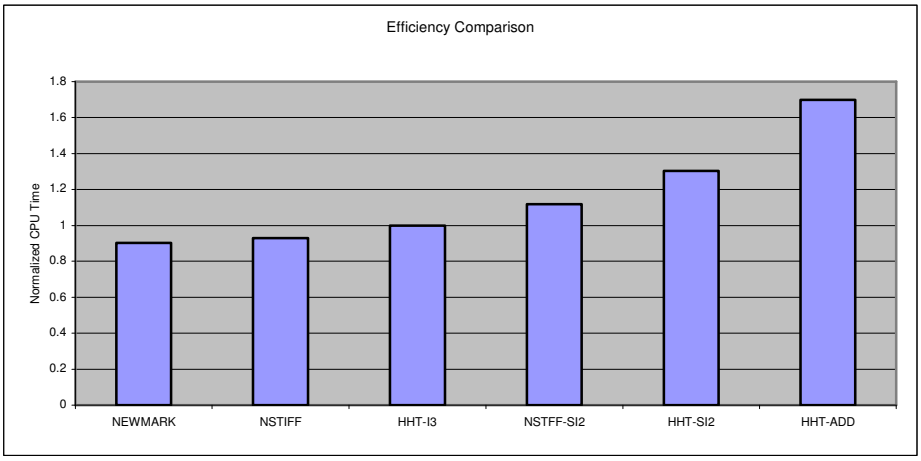

Figure 21: Comparison of efficiency (normalized to performance of HHT-I3)

5 CONCLUSIONS AND FUTURE WORK

This paper investigates several low-order numerical integration formulas. The motivation for this effort is twofold. First, the vast majority of large real-life models contain discontinuities, friction, and contacts that effectively make low-order integration formulas the only viable robust candidates capable of handling these classes of problems. Secondly, although less relevant, compared to higher-order implicit formulas, the numerical methods investigated herein are straightforward to implement and some of them are already commonly used in practice. Based on the order convergence and timing results presented, for problems where accurately satisfying the velocity kinematic constraint equations is not a priority, HHT-I3 is a good

choice. It is a second order method that has the ability to change the amount of numerical damping that enters the solution process. The major drawback associated with this method is that there is yet no formal proof of the global convergence of the method, a task that remains to be approached in the future. While HHT-I3 has been implemented and tested on a large number of complex models in ADAMS (and all these results have indicated good robustness and convergence behavior), if one wants to stand on solid theoretical ground then the NSTIFF method is the next best alternative. Global convergence results are available for this second order method and, moreover, our experience indicates that NSTIFF is actually more efficient than HHT-I3. However, the method is plagued by a somewhat more intense numerical damping that cannot be controlled like in HHT-I3. For a slower, but numerically sound approach, one can select the second order HHT-SI2 or NSTIFF-SI2 methods. They are comparable in terms of efficiency, HHT-SI2 having an edge due to its ability to adjust the value of numerical damping introduced into the problem. Preliminary results presented in the paper indicate that satisfying both the position and velocity kinematic constraint equations come at a price of about a 30% increase in simulation time.

ACKNOWLEDGEMENTS

The authors would like to thank Radu Serban and Nick Schafer for reading the manuscript and providing suggestions for improvement.

REFERENCES

Abraham, R. and J. E. Marsden (1985). Foundations of Mechanics. Reading, MA, Addison-Wesley.

Alishenas, T. (1992). Zur numerischen Behandlungen, Stabilisierung durch Projection und Modellierung mechanischer Systeme mit Nebenbedingungen und Invarianten, PhD Thesis, Royal Institute of Technology, Stockholm.

Arnold, V. I. (1989). Mathematical Methods of Classical Mechanics. New York, NY, Springer.

Ascher, U. M., H. Chin, et al. (1995). " Stabilization of constrained mechanical systems with DAEs and invariant manifolds." Mechanics of Structures and Machines **23**(2): 135-157.
Ascher, U. M., H. Chin, et al. (1994). "Stabilization of DAEs and invariant manifolds." Numerische Mathematik **67**(2): 131-149.

Ascher, U. M. and L. R. Petzold (1993). "Stability of Computational Methods for Constrained Dynamics Systems." SIAM Journal on Scientific Computing **14**(1): 95-120.

Bauchau, O. A., C. L. Botasso, et al. (2003). " Robust integration schemes for flexible multibody systems." Computer Methods in Applied Mechanics and Engineering, **192**(3): 395-420.

Bottasso, C. L., O. A. Bauchau, et al. (2007). "Time-Step-Size-Independent Conditioning and Sensitivity to Perturbations in the Numerical Solution of Index Three Differential Algebraic Equations." SIAM Journal on Scientific Computing: accepted.

Brenan, K. and B. E. Engquist (1988). "Backward Differentiation Approximations of Nonlinear Differential/Algebraic Systems." Mathematics of Computation **51**(184)

Brenan, K. E., S. L. Campbell, et al. (1989). Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations. New York, North-Holland.

Cardona, A. and M. Geradin (1989). "Time Integration of the Equations of Motion in Mechanism Analysis." Computers and Structures **33**: 801-820.

Cardona, A. and M. Geradin (1994). Numerical Integration of Second Order Differential-Algebraic Systems in Flexible Mechanics Dynamics. Computer-Aided Analysis of Rigid and Flexible Mechanical Systems, Kluwer Academic Publishers

Chung, J. and G. M. Hulbert (1993). "A Time Integration Algorithm for Structural Dynamics with Improved Numerical Dissipation: the Generalized-a Method." Transactions of ASME, Journal of Applied Mechanics **60**(2): 371-375.

Führer, C. and B. J. Leimkuhler (1991). "Numerical solution of differential-algebraic equations for constrained mechanical motion." Numerische Mathematik **59**(1): 55-69.

Gear, C. W. (1971). Numerical Initial Value Problems of Ordinary Differential Equations. Englewood Cliffs, NJ, Prentice Hall.

Gear, C. W. (1971). "The Simultaneous Numerical Solution of Differential-Algebraic Equations." IEEE Trans. Circuit Theory **CT-18**: 89-95.

Gear, C. W., G. Gupta, et al. (1985). "Automatic integration of the eulerlagrange equations with constraints." J. Comp. Appl. Math. **12**: 77-90.

Geradin, M. and D. Rixen (1994). Mechanical Vibrations: Theory and Application to Structural Dynamics. New York, NY, Wiley.

Hairer, E., C. Lubich, et al. (1989). The Numerical Solution of Differential-Algebraic Equations by Runge-Kutta Methods. Berlin, Springer

Hairer, E. and G. Wanner (1996). Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems. Berlin, Springer.

Haug, E. J. (1989). Computer-Aided Kinematics and Dynamics of Mechanical Systems. Volume I:Basic Methods. Boston, MA, Allyn and Bacon.

Haug, E. J., D. Negrut, et al. (1997). "A State-Space Based Implicit Integration Algorithm for Differential-Algebraic Equations of Multibody Dynamics." Mechanics of Structures and Machines **25**(3): 311-334.

Hilber, H. M., T. J. R. Hughes, et al. (1977). "Improved Numerical Dissipation for Time Integration Algorithms in Structural Dynamics." Earthquake Eng. and Struct. Dynamics **5**: 283-292.

Hughes, T. J. R. (1987). The Finite Element Method - Linear Static and Dynamic Finite Element Analysis. Englewood Cliffs, New Jersey, Prentice-Hall.

Jay, L. O. and D. Negrut (2006). "Extensions of the HHT-α method to differential-algebraic equations in mechanics." Electronic Transactions on Numerical Analysis, accepted.

Jay, L. O. and D. Negrut (2007). A second order extension of the generalized-alpha method for constrained systems in mechanics. ECCOMAS, Milan, Italy.

Liang, C. D. and G. M. Lance (1987). "A Differentiable Null-Space Method for Constrained Dynamic Analysis." ASME Journal of Mechanism, Transmission, and Automation in Design **109**: 405–411.

Lötstedt, C. L. and L. R. Petzold (1986). "Numerical Solution of Nonlinear Differential Equations with Algebraic Constraints (I): Convergence Results for Backward Differentiation Formulas." Mathematics of Computation **46**: 491-516.

Lubich, C., U. Nowak, et al. (1995). "MEXX - Numerical Software for the Integration of Constrained Mechanical Multibody Systems." Mechanics of Structures and Machines **23**: 473-495

Mani, N., E. J. Haug, et al. (1985). "Singular Value Decomposition for Analysis of Mechanical System Dynamics." ASME Journal of Mechanisms, Transmissions, and Automation in Design **107**: 82-87.

Negrut, D., E. J. Haug, et al. (2003). "An implicit Runge-Kutta method for integration of Differential-Algebraic Equations of Multibody Dynamics." Multibody System Dynamics **9**(2): 121-142.

Negrut, D., R. Rampalli, et al. (2007). "On an Implementation of the HHT Method in the Context of Index 3 Differential Algebraic Equations of Multibody Dynamics." ASME Journal of Computational and Nonlinear Dynamics **2**(1): 73-85.

Newmark, N. M. (1959). "A method of computation for Structural Dynamics." Journal of the Engineering Mechanics Division, ASCE: 67-94

Orlandea, N., M. A. Chace, et al. (1977). "A Sparsity-Oriented Approach to the Dynamic Analysis and Design of Mechanical Systems: Part I and Part II." Journal of Engineering for Industry **99**: 773-784.

Potra, F. A. and W. C. Rheinboldt (1991). "On the numerical solution of Euler-Lagrange equations." Mechanics of structures and machines **19**(1): 1-18.

Rheinboldt, W. C. (1984). "Differential-algebraic systems as differential equations on manifolds " Mathematics of Computation **Vol. 43**: 473-482.

Schafer, N., R. Serban, et al. (2007). An investigation of new numerical methods for Molecular Dynamics simulation (DETC2007-35519). 6th ASME International Conference on Multibody Systems, Nonlinear Dynamics and Control, Las Vegas, NV, ASME.

Shabana, A. A. (2005). Dynamics of Multibody Systems. New York, NY, Cambridge University Press.

Wehage, R. A. and E. J. Haug (1982). "Generalized Coordinate Partitioning for Dimension Reduction in Analysis of Constrained Dynamic Systems." J. Mech. Design **104**: 247--255

Yen, J. (1993). "Constrained Equations of Motion in Multibody Dynamics as ODEs on Manifolds." SIAM Journal on Numerical Analysis **30**(2): 553-568.

Yen, J., L. R. Petzold, et al. (1998). "A Time Integration Algorithm for Flexible Mechanism Dynamics: The DAE a-method." Computer Methods in Applied Mechanics and Engineering **158**: 341-355.