Estimation of global time integration errors in rigid body dynamics

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ABSTRACT. *The popular Newmark time integration scheme is used in the standard finite difference form as well as in an equivalent Galerkin form for the time integration of rigid body dynamics problems. Estimators for local and global time integration errors are developed. In particular the evaluation of the dual problem for different goals of the error is discussed. A special focus is also on the comparison for linear and nonlinear problems. Finally an adaptive time integration scheme is presented for which both - the local and the global - error estimators are used. The merits and limits are shown for some particular numerical problems.*

RÉSUMÉ. *Pour la dynamique de corps rigides, le très populaire schéma d'intégration en temps de Newmark est utilisé soit sous sa forme classique de différences finies soit sous une forme de Galerkin équivalente. Des estimateurs des erreurs locale et globale d'intégration en temps sont développés. On discute plus particulièrement l'évaluation du problème dual orienté vers differents objectifs pour l'estimation d'erreur. Une attention particulière est portée à la comparaison des problèmes linéaires et non linéaires. Finalement un schéma adaptif d'intégration en temps est présenté pour lequel, les deux estimateurs des erreurs locale et globale sont utilisés. Les avantages et inconvénients sont montrés pour quelques problèmes numériques particuliers.*

KEYWORDS: *time integration, error estimation, adaptive methods, rigid bodies, dynamics.*

MOTS-CLÉS : *intégration en temps, estimation d'erreur, méthodes adaptatives, corps rigides, dynamique.*

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1. Introduction

The solution of coupled ordinary differential equation systems, resulting from e.g. rigid body dynamics or from a spatial FE discretization in structural dynamics, can be determined for rather general cases only numerically. For linear equations the modal decomposition method provides a very clear and comprehensible tool, however, the numerical effort is rather large for systems with many degrees of freedom. Nonlinear systems of equations can be treated only numerically. Up to now we know only few nonlinear equation systems from rigid body dynamics, where an exact solution is given.

In principle many numerical methods exist to solve the corresponding second order ordinary differential equations in rigid body dynamics, which can be e.g. separated into Finite Difference and Finite Element Methods. A very popular integration method in the engineering community is Newmark's time integration scheme. For this scheme Wood (Wood, 1990) proved, that an equivalent Galerkin formulation for linear equations with constant coefficients exists. Both variants of the Newmark method will be in the focus of this contribution.

The estimation of the global time integration error for Finite Difference Methods is a very difficult task. One proposal is to consider the accumulation of the local error to the global error using the amplification matrix A. However, the numerical effort for the computation of the amplification matrix is very high, in particular as the dimension of A is $2\mathcal{N}_{eq} \times 2\mathcal{N}_{eq}$. For nonlinear systems the use of the amplification matrix is not possible.

The mentioned equivalence between the Finite Difference and the Galerkin form of Newmark's scheme is the basis to apply an essential estimation technique, which is usually used for the error estimation of FE-solutions of elliptic problems, e.g. quasi-static problems. The duality principle is mapped to the global time error estimation, which allows us to estimate the global time integration error also for the Galerkin form of Newmark's scheme. For a general derivation concerning the duality principle in dynamics, we refer to Bangerth/Rannacher (Bangerth *et al.*, 1999) and for an extensive derivation of the discussed subject to Neumann (Neumann, 2004). The derived method is tested on four linear resp. nonlinear numerical problems. In order to solve the problems efficiently and with prescribed accuracy the time step size should be adapted based on the global error. Thus an adaptation scheme is developed, which is based on the local and global error estimation and applications to nonlinear problems are presented.

2. Class of problems

The basic equation system of rigid body dynamics or after a spatial FE discretization in structural dynamics is given as:

$$\boldsymbol{M}\ddot{\mathbf{d}} + \boldsymbol{n}(t, \mathbf{d}, \dot{\mathbf{d}}) = \mathbf{0} \quad \forall t(0, T]\,, \tag{1}$$

with initial conditions at $t = 0 : \mathbf{d}(t = 0) = \mathbf{d}_0\,, \quad \dot{\mathbf{d}}(t = 0) = \dot{\mathbf{d}}_0\,.$

The mass matrix $\boldsymbol{M} \in \mathbb{R}^{\mathcal{N}_{eq} \times \mathcal{N}_{eq}}$ is positive definite, the vector of nonlinearities $\boldsymbol{n} \in \mathbb{R}^{\mathcal{N}_{eq}}$ contains stiffness, damping and loading properties. The first derivative of $\boldsymbol{u}$ with respect to time is called velocity $\dot{\mathbf{d}} = \frac{d\mathbf{d}}{dt}$, the second derivation of the displacement $\mathbf{d}$ w.r.t. time is the acceleration $\ddot{\mathbf{d}} = \frac{d\dot{\mathbf{d}}}{dt}$. For the solution the equation system [1] has to be solved in the time domain $(0, T]$. To guarantee an unique solution $\mathbf{u}$ of Equation [1] the vector $\mathbf{n}(t, \mathbf{d}, \dot{\mathbf{d}} : (\mathbb{R}, \mathbb{R}^{\mathcal{N}_{eq}}, \mathbb{R}^{\mathcal{N}_{eq}}) \rightarrow \mathbb{R}^{\mathcal{N}_{eq}}$ must fulfill the Lipschitz condition, see Stoer/Burlisch (Stoer *et al.*, 1990);

$$||\mathbf{n}(t, \mathbf{d}_1, \dot{\mathbf{d}}_1) \; - \; \mathbf{n}(t, \boldsymbol{d}_2, \dot{\mathbf{d}}_2)|| \leq \mathcal{L}||\mathbf{d}_1 \; - \; \mathbf{d}_2|| \text{ mit } \mathcal{L} > 0\,. \qquad [2]$$

The solutions $\mathbf{d}_1$ and $\mathbf{d}_2$ belong to two different initial conditions, thus the general solution $\mathbf{d}$ depends continuously on the initial conditions. The Lipschitz conditions [2] can be substituted by the mean value theorem, which leads to conditions for the partial derivatives, the so-called Jacobian $D_{\mathbf{d}}\mathbf{n}$:

$$\begin{aligned} D_{\mathbf{d}}\mathbf{n} &= \frac{\partial \mathbf{n}_i}{\partial \mathbf{d}_j}\,(i,j = 1...\mathcal{N}_{eq}) \text{ continuous and bounded} \quad \text{and} \\ D_{\dot{\mathbf{d}}}\mathbf{n} &= \frac{\partial \mathbf{n}_i}{\partial \dot{\mathbf{d}}_j}\,(i,j = 1...\mathcal{N}_{eq}) \text{ continuous and bounded}\,. \end{aligned} \qquad [3]$$

If the Jacobian matrices $D_{\mathbf{d}}\mathbf{n}$ or $D_{\dot{\mathbf{d}}}\mathbf{n}$ exist, then the solution $\mathbf{d}$ can be differentiated continuously. The following equations of motion will fulfill the conditions [2] or [3].

3. Numerical time integration

The class of Equations [1] will be solved by two different schemes. First we write down the well known method of Newmark in difference form (FD) (Newmark, 1959):

$$\begin{aligned} &\mathbf{d}_{n+1} = \mathbf{d}_n + k\dot{\mathbf{d}}_n + (1-2\beta)k^2/2\ddot{\mathbf{d}}_n + \beta k^2 \ddot{\mathbf{d}}_{n+1}\,, \\ &\dot{\mathbf{d}}_{n+1} = \dot{\mathbf{d}}_n + (1-\gamma)k\ddot{\mathbf{d}}_n + \gamma k \ddot{\mathbf{d}}_{n+1}\,, \\ &\text{nonlinear case}: \mathbf{M}\ddot{\mathbf{d}}_{n+1} \; + \; \mathbf{n}(\mathbf{d}_{n+1}, \dot{\mathbf{d}}_{n+1}, t_{n+1}) \; = \; \mathbf{0}\,, \\ &\text{linear case}: \mathbf{M}\ddot{\mathbf{d}}_{n+1} \; + \; (c_M\mathbf{M} + c_K\mathbf{K})\,\dot{\mathbf{d}}_{n+1} \; + \; \mathbf{K}\mathbf{d}_{n+1} \; - \; \mathbf{F}_{n+1} \; = \; \mathbf{0}\,. \end{aligned} \qquad [4]$$

The exact solution $\mathbf{d}$ is substituted with discrete data $\mathbf{d}_n$; the parameters β and γ are taken to control the accuracy and numerical stability of the algorithm. $k = t_{n+1} - t_n$ is the time step size. For some special parameter combinations e.g. ($2\beta = \gamma = 0.5$) we can find an equivalent Galerkin formulation for linear second order differential equations. Wood (Wood, 1990) proved, that the following test- and ansatzfunctions lead to an equivalent so-called Continuous Galerkin form of Newmark's scheme:

$$\mathbf{d}^k(t) \;=\; \mathbf{d}_n \;+\; \dot{\mathbf{d}}_n(t-t_n) \;+\; \frac{1}{2}\,(t-t_n)^2\,\ddot{\mathbf{d}}_n \quad \forall t \in (t_n, t_{n+1}]\,,$$

$$\mathbf{g}^k(t) \;=\; \mathbf{G}_n \left(\frac{1}{5} - (t-t_n)/k + (t-t_n)^2/k^2 \right) \quad \forall t \in (t_n, t_{n+1}]\,,$$

with: $\mathbf{G}_n \in \mathbb{R}^{\mathcal{N}_{eq}} = const.$ as a vector of weighting coefficients,

$$\text{General nonlinear case: } \int_{t_n}^{t_{n+1}} \mathbf{g}^k \left(\mathbf{M}\ddot{\mathbf{d}}^k \;+\; \mathbf{n}\left(\mathbf{d}^k, \dot{\mathbf{d}}^k, t\right)\right) \;=\; 0\,\forall \mathbf{g}^k\,, \qquad [5]$$

$$\text{Linear case: } \int_{t_n}^{t_{n+1}} \mathbf{g}^k \left(\mathbf{M}\ddot{\mathbf{d}}^k \;+\; (c_M\mathbf{M} + c_K\mathbf{K})\dot{\mathbf{d}}^k \;+\; \mathbf{K}\mathbf{d}^k \;-\; \mathbf{F}\right) dt \;=\; 0\;\forall \mathbf{g}^k.$$

amplification matrices $\mathbf{A}_N$, $\mathbf{A}_C$ of both forms, the Finite Difference (N) [4] and the Continuous Galerkin (C) form [5]:

$$\begin{pmatrix} \mathbf{d}_{n+1} \\ \dot{\mathbf{d}}_{n+1} \end{pmatrix} \;=\; \mathbf{A}_N \begin{pmatrix} \mathbf{d}_n \\ \dot{\mathbf{d}}_n \end{pmatrix} \;=\; \mathbf{A}_C \begin{pmatrix} \mathbf{d}_n \\ \dot{\mathbf{d}}_n \end{pmatrix}. \qquad [6]$$

It must be noted, that this equivalence is of course only valid for linear second order differential equations without external loading thus without a particular solution. Furthermore both formulations for Newmark's method, *i.e.* Finite Difference form and Continuous Galerkin form, differ in the implementation. In the Finite Difference scheme $\ddot{\mathbf{d}}_n$ resp. $\ddot{\mathbf{d}}_{n+1}$ corresponds to the acceleration at time t_n resp. t_{n+1}. The vector $\ddot{\mathbf{d}}_n$ in the Continuous Galerkin scheme has to be interpreted as the average acceleration in the time step $k = t_{n+1} - t_n$. Here no *initial* acceleration has to be computed. This is in contrast to the Finite Difference scheme, where the *initial* acceleration $\ddot{d}_0 \;=\; -\mathbf{M}^{-1} \cdot \mathbf{n}(\mathbf{d}_0,\, \dot{\mathbf{d}}_0, t=0)$ is needed.

4. Local error *versus* global error

The local time integration error $\boldsymbol{e}_l(t_n)$ is defined as the difference between the numerical solution $\mathbf{d}_n$ and the exact solution $\mathbf{d}(t=t_n)$ in a certain time interval:

$$\boldsymbol{e}_l(t_n) \;=\; \mathbf{d}_n \;-\; \mathbf{d}(t=t_n)\,. \qquad [7]$$

E.g., then the error resulting from previous time steps, is neglected or is set to zero, thus $\mathbf{d}_{n-1} = \mathbf{d}(t=t_{n-1})$. The local velocity error is defined in the same way:

$$\dot{\boldsymbol{e}}_l(t_n) \;=\; \dot{\mathbf{d}}_n \;-\; \dot{\mathbf{d}}(t=t_n)\,. \qquad [8]$$

The global time integration error, however, $\boldsymbol{e}_t$ at $t = t_m$ is influenced by all previous local errors $\boldsymbol{e}_l(t_{m-1})$, thus $\mathbf{d}_{m-1} \neq \mathbf{d}(t_{m-1})$. The local errors are further filtered

and accumulated to the global error $\boldsymbol{e}_t(t_m)$, see Hairer *et al.* (Hairer *et al.*,1992), which can be written as:

$$\boldsymbol{e}_t(t_m) \;=\; \mathbf{d}_m \;-\; \mathbf{d}(t=t_m) \;=\; \sum_{i=1}^{m-1} \boldsymbol{e}_t(t_i) + \boldsymbol{e}_l(t_m)\,. \qquad [9]$$

The global velocity error is defined analogously:

$$\dot{\boldsymbol{e}}_t(t_m) \;=\; \dot{\mathbf{d}}_m \;-\; \dot{\mathbf{d}}(t=t_m) \;=\; \sum_{i=1}^{m-1} \dot{\boldsymbol{e}}_t(t_i) + \dot{\boldsymbol{e}}_l(t_m)\,. \qquad [10]$$

4.1. *Estimation of the local error*

Usually methods to estimate the local time integration error are simple to implement, because only the information of the last time step (t_{n-1}, t_n) is needed. Here a method proposed by Riccius *et al.* (Riccius *et al.*, 1996) based on a finite difference operation is applied for the local error estimation using Newmark's time integration scheme:

$$\begin{aligned} \tilde{\mathbf{e}}_l(t_n)_N &= \frac{k^2}{24}\left(\ddot{\mathbf{d}}_{n-2} + (2-24\beta)\ddot{\mathbf{d}}_{n-1} + (24\beta-3)\ddot{\mathbf{d}}_n\right) \approx \mathbf{e}_l(t_n)\,, \\ \tilde{\dot{\mathbf{e}}}_l(t_n)_N &= \frac{k}{12}\left(\ddot{\mathbf{d}}_{n-2} + (4-12\gamma)\ddot{\mathbf{d}}_{n-1} + (12\gamma-5)\ddot{\mathbf{d}}_n\right) \approx \dot{\mathbf{e}}_l(t_n)\,. \end{aligned} \qquad [11]$$

The local order of convergence for $\boldsymbol{e}_l(t_n)$ and $\dot{\boldsymbol{e}}_l(t_n)$ with $\gamma = 2\beta = 0.5$ can be established from Dahlquist (Dahlquist, 1963) as:

$$\mathbf{e}_l(t_n) = \mathcal{O}(k^3) \qquad \dot{\mathbf{e}}_l(t_n) = \mathcal{O}(k^2)\,. \qquad [12]$$

The single degree of freedom system:

$$\begin{aligned} &m\ddot{d} + \mu\dot{d} + cd \;=\; 0 \forall t \in (0,5] \\ &\text{with: } d(t=0) = 1.0\,, \quad \dot{d}(t=0) = 0.0 \text{ and } \; m = 1.0\,, \mu = 0.5\,, c = 1.0 \end{aligned} \qquad [13]$$

is the model problem to test the order of convergence for $\mathbf{e}_l(t_n)$ and $\dot{\mathbf{e}}_l(t_n)$.

The data from Table [1] give two essential informations:

i) the estimated local error has the exact order of convergence;

ii) the estimated error converges asymptotically to the exact error.

Table 1. *SDOF, see eq. [13]; order of convergence for estimated and exact local error at $t_n = 5.0$ for displacements and velocities using Newmark's scheme*

k	$\tilde{\mathbf{e}}_l(5)$	$\tilde{\dot{\mathbf{e}}}_l(5)$	$\mathbf{e}_l(5)$	$\dot{\mathbf{e}}_l(5)$
0.2	$1.635 \cdot 10^{-4}$	$1.302 \cdot 10^{-4}$	$1.585 \cdot 10^{-4}$	$1.517 \cdot 10^{-4}$
0.1	$1.999 \cdot 10^{-5}$	$1.790 \cdot 10^{-5}$	$1.985 \cdot 10^{-5}$	$1.907 \cdot 10^{-5}$
0.05	$2.480 \cdot 10^{-6}$	$2.319 \cdot 10^{-6}$	$2.482 \cdot 10^{-6}$	$2.388 \cdot 10^{-6}$
0.025	$3.105 \cdot 10^{-7}$	$2.943 \cdot 10^{-7}$	$3.103 \cdot 10^{-7}$	$2.987 \cdot 10^{-7}$

These results correspond well with *a priori* error estimates of Hairer/Norsett/Wanner (Hairer *et al.*, 1992):

$$\begin{aligned} &\|\mathbf{e}_l(t_m)\| \leq Ck^s\,, \\ &\text{with: } \mathbf{e}_l(t_m) \;=\; \mathbf{d}(t=t_m) - \mathbf{d}_m\,, \quad C>0\,. \end{aligned} \qquad [14]$$

$\|\cdot\|$ is some arbitrary norm, the accuracy order of the time integration scheme is $s-1$ with $s=3$ for the given parameter combination. The straightforward accumulation of all subsequent local errors – without a filtering – to the global error, however, yields to a substantial overestimation of the exact global error.

4.2. *Estimation of the global error*

To avoid this overestimation the transport of the local error from each time step has to be included in the consideration, see Figure 1. This filtering of the local error is formulated with the amplification matrix $\mathbf{A}$ of the considered time integrator:

$$\mathbf{e}_t(t_n) \;=\; \mathbf{A}\mathbf{e}_t(t_{n-1}) + \mathbf{e}_l(t_n)\,. \qquad [15]$$

A subsequent application of Equation [15] leads to the global error at $t = t_m$:

$$\mathbf{e}_t(t_m) \;=\; \mathbf{A}^0\mathbf{e}_t(t_0) + \sum_{i=1}^{m} \mathbf{A}^{m-i+1}\mathbf{e}_l(t_i)\,. \qquad [16]$$

With the assumption $\mathbf{e}_t(t_0) \;=\; \mathbf{0}$ the first term can be removed from Equation [16]. For verification the estimated global error has to be compared with *a priori* estimates. Hairer *et al.* (Hairer *et al.*, 1992) and Stoer/Burlisch (Stoer *et al.*, 1990) make an *a priori* statement for Finite Difference methods:

$$\begin{aligned} &\|\mathbf{e}_t(t_m)\| \leq k^{s-1}\frac{C}{L}\frac{e^{L(t_m-t_0)}-1}{L}\,, \\ &\text{with:}\quad L \text{ ... Lipschitz constant}\,,\; C>0. \end{aligned} \qquad [17]$$

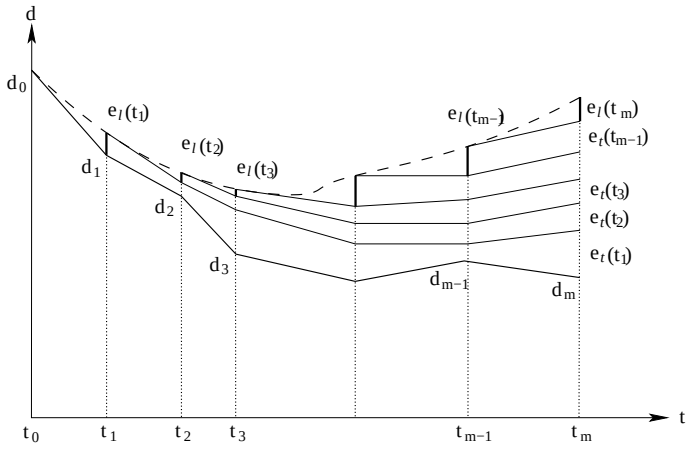

Figure 1. *Error propagation of the local time integration error $e_l(t_n)$ to the global time integration error $e_t(t_n)$, Hairer et al. (Hairer et al., 1992)*

There are also *a priori* error estimates for time-continuous and time-discontinuous Galerkin methods from Estep *et al.* (Estep *et al.*, 1994), (Estep, 1995):

$$|\mathbf{e}_t(t_m)|_{[0,t_m]} \leq C\left(1 + Lt_m e^{CLt_m}\right)^{1/2} \max_{i \leq m} k_i^{s-1} |\mathbf{d}^{(s-1)}|_{I_m} . \qquad [18]$$

Both estimates [17] and [18] for the global error show the loss of one order of convergence compared to the local estimate [14]. Based on the local error estimates [11] for Newmark's difference scheme (N) Riccius/Schweizerhof (Riccius *et al.*, 1996) proposed an alternative indicator for the global time integration error:

$$\tilde{\mathbf{e}}_t(t_m)_N \;=\; \frac{t_m}{k_m} \tilde{\mathbf{e}}_l(t_m)_N \,, \qquad [19]$$

$$\tilde{\dot{\mathbf{e}}}_t(t_m)_N \;=\; \frac{t_m}{k_m} \tilde{\dot{\mathbf{e}}}_l(t_m)_N \,. \qquad [20]$$

In difference to the simple accumulation of all local errors $\mathbf{e}_l(t_i)$ Riccius assumes that the local errors $\mathbf{e}_l(t_i)$ for $t < t_m$ are equally distributed with an average time step size of k_m up to $t = t_m$, when we estimate the corresponding global time integration error $\tilde{\mathbf{e}}_t(t_i)$ resp. $\tilde{\mathbf{e}}_t(t_m)$.

The equivalence between the FD form of Newmark's scheme and the continuous Galerkin formulation of Wood is used to apply the duality principle of Betti, see Cirak/Ramm (Cirak *et al.*, 1998), to the global error estimation. First the method is discussed for linear equations. The weak, discretized Galerkin formulation is written:

$$\sum_{n=0}^{m-1} \int_{t_n}^{t_{n+1}} \mathbf{g}^k \left(\mathbf{M}\ddot{\mathbf{d}}^k \,+\, \mathbf{C}\dot{\mathbf{d}}^k \,+\, \mathbf{K}\mathbf{d}^k \,-\, \mathbf{F} \right) dt \;=\; 0 \;\forall \mathbf{g}^k \in \mathcal{V}^k \subset \mathcal{V} \,. \qquad [21]$$

The corresponding weak Galerkin formulation:

$$\sum_{n=0}^{m-1} \int_{t_n}^{t_{n+1}} \mathbf{g}^k \left(\mathbf{M}\ddot{\mathbf{d}} + \mathbf{C}\dot{\mathbf{d}} + \mathbf{K}\mathbf{d} - \mathbf{F} \right) dt = 0 \; \forall \mathbf{g}^k \in \mathcal{V}^k \subset \mathcal{V} \qquad [22]$$

is subtracted from Equation [5] to get the Galerkin orthogonality of the residuum $\mathbf{R}$:

$$\begin{aligned} \int_0^{t_m} \boldsymbol{g}^k \cdot \mathcal{D}\mathbf{e}\, dt &= 0\,, \quad \mathbf{e} = \mathbf{d} - \mathbf{d}^k \\ \text{with}: \; \mathcal{D}\mathbf{e} &= \mathbf{M}\,(\ddot{\mathbf{d}} - \ddot{\mathbf{d}}^k) + \mathbf{C}(\dot{\mathbf{d}} - \dot{\mathbf{d}}^k) + \mathbf{K}(\mathbf{d} - \mathbf{d}^k) \\ &= \mathbf{M}\,\ddot{\mathbf{e}} \qquad + \mathbf{C}\dot{\mathbf{e}} \qquad + \mathbf{K}\mathbf{e} \\ &= -\left(\mathbf{M}\ddot{\mathbf{d}}^k + \mathbf{C}\dot{\mathbf{d}}^k + \boldsymbol{K}\mathbf{d}^k \right) + \mathbf{F} = \mathbf{R}\,. \end{aligned} \qquad [23]$$

With the principle of duality suggested by Bangerth *et al.* (Bangerth *et al.*, 1999) and used also by Maute (Maute, 2001) the corresponding dual equation in the dual variable $\mathbf{y}$ can be formulated,

$$\begin{aligned} &\mathcal{D}^*\mathbf{y} = \mathbf{M}\ddot{\mathbf{y}} - \mathbf{C}\dot{\mathbf{y}} + \mathbf{K}\mathbf{y} = \mathbf{0}\,, \forall t < t_m\,, \\ &\text{with the } \textit{initial} \text{ conditions at } t = t_m\text{: } \mathbf{y}_m = \mathbf{y}(t = t_m)\,,\; \dot{\mathbf{y}}_m = \dot{\mathbf{y}}(t = t_m)\,. \end{aligned} \qquad [24]$$

This backward problem results from partial integration of the primal problem with $\mathbf{y}$ as test function. The free *final* conditions or initial conditions of the backward problem $\mathbf{y}_m, \dot{\mathbf{y}}_m$ determine the kind of error norm, as will be shown later. The differential equation for the primal error [23] is tested with the solution $\mathbf{y}$ of the dual problem:

$$\int_0^{t_m} \mathbf{y}\mathbf{R}\, dt = -\dot{\mathbf{y}}\,\mathbf{M}\mathbf{e}_t \,|^{t_m}\,. \qquad [25]$$

Partial integration of Equation [25] gives the information for the choice of the *final* conditions:

$$\int_0^{t_m} \mathbf{y}\,\mathcal{D}\mathbf{e}\, dt = \int_0^{t_m} \mathbf{e}\,\mathcal{D}^*\mathbf{y}\, dt + \mathbf{y}\,\mathbf{M}\dot{\mathbf{e}} \,|_0^{t_m} - \dot{\mathbf{y}}\,\mathbf{M}\mathbf{e} \,|_0^{t_m} + \mathbf{y}\,\mathbf{C}\mathbf{e} \,|_0^{t_m}\,. \qquad [26]$$

The assumption for the primal problem concerning the initial conditions $\mathbf{e}(t = 0) = \mathbf{0}$ and $\dot{\mathbf{e}}(t = 0) = \mathbf{0}$ and the special choice $\mathbf{y}_m = \mathbf{y}(t_m) = \mathbf{0}$ leads to a removal of the rest of the boundary values at $t = 0$ and $t = t_m$:

$$\int_0^{t_m} \mathbf{y}\, \mathcal{D}\mathbf{e}\, dt \;=\; \int_0^{t_m} \mathbf{e}\, \mathcal{D}^*\mathbf{y}\, dt \;-\; \dot{\mathbf{y}}\, \mathbf{M}\mathbf{e}\, |^{t_m} \;.$$

As $\mathbf{y}$ is the solution of Equation [24] the *final* conditions for $\mathbf{y}_m = \mathbf{y}(t_m)$ can be found directly from:

$$\int_0^{t_m} \mathbf{y}\mathbf{R}\, dt \;=\; -\dot{\mathbf{y}}\, \mathbf{M}\mathbf{e}_t\, |^{t_m} \;. \qquad [27]$$

E.g., if we choose

$$\dot{\mathbf{y}}(t_m) \;=\; \frac{-\mathbf{M}^{-1}\mathbf{e}_t(t_m)}{|\mathbf{e}_t(t_m)|}\,. \qquad [28]$$

the global time integration error can be computed:

$$|\mathbf{e}_t(t = t_m)| \;=\; \int_0^{t_m} \mathbf{y}\mathbf{R}\, dt \;=\; -\dot{\mathbf{y}}\, \mathbf{M}\mathbf{e}_t\, |^{t_m}\,. \qquad [29]$$

The error distribution $\mathbf{e}_t(t_m)$ is not known, but at least a reasonable distribution of the error has to be given in the r.h.s. of Equation [28]. For this purpose the local time integration error $\mathbf{e}_l(t_m)$, Equation [11], can be estimated and is substituted for $\mathbf{e}_t(t_m)$ into the r.h.s of Equations [28] and [29],

$$\begin{aligned} \tilde{\mathbf{e}}_l(t_n)_N &= \frac{k^2}{24}\left(\ddot{\mathbf{d}}_{n-2} + (2 - 24\beta)\ddot{\mathbf{d}}_{n-1} + (24\beta - 3)\ddot{\mathbf{d}}_n\right) \approx \mathbf{e}_l(t_n)\,, \\ \tilde{\dot{\mathbf{e}}}_l(t_n)_N &= \frac{k}{12}\left(\ddot{\mathbf{d}}_{n-2} + (4 - 12\gamma)\ddot{\mathbf{d}}_{n-1} + (12\gamma - 5)\ddot{\mathbf{d}}_n\right) \approx \dot{\mathbf{e}}_l(t_n)\,. \end{aligned} \qquad [11]$$

If the global error is wanted only for one coordinate i it is not necessary to estimate the local error, as the right hand side of Equation [28] is reduced to:

$$\dot{\mathbf{y}}(t_m) \;=\; -\left(\mathbf{M}^{-1}\mathbf{I}\right)^T \;, \qquad [30]$$

with: $\mathbf{I} \in \mathbb{R}^{\mathcal{N}_{eq}}, \mathbf{I} = \mathbf{0}\,,$ excluding: $\mathbf{I}_i = 1$

$$\mathbf{e}_{t,i}(t = t_m) \;=\; \int_0^{t_m} \mathbf{y}\mathbf{R}\, dt \qquad [31]$$

In contrast to Equations [25] and [26], where $\mathbf{y}$ is used as test function, it would be alternatively possible to test Equation [23] with the velocities of the corresponding dual solution $\dot{\mathbf{y}}$,

$$\int_0^{t_m} \dot{\mathbf{y}}\, \mathcal{D}\mathbf{e}\, dt \;=\; \int_0^{t_m} \dot{\mathbf{y}}\, \mathbf{R}\, dt\,. \qquad [32]$$

If the *final* conditions $\mathbf{y}(t_m) \;=\; -\mathbf{M}^{-1}\mathbf{e}_t(t_m)$ and $\dot{\mathbf{y}}(t_m) \;=\; -\mathbf{M}^{-1}\dot{\mathbf{e}}_t(t_m)$ are chosen, then the global time integration error in the energy norm is computed for this alternative case:

$$\left(\|\mathbf{e}_t(t_m)\|_a^2 \;+\; \|\dot{\mathbf{e}}_t(t_m)\|_{L_2}^2\right)^{1/2} \;=\; \left(\int_0^{t_m} \dot{\mathbf{y}}\, \mathbf{R}\, dt\right)^{1/2}\,. \qquad [33]$$

In order to compute this alternative global error measure, also an approximation is necessary such as the estimated local error $\mathbf{e}_l(t_m)$ resp. $\dot{\mathbf{e}}_l(t_m)$.

In reality the exact or analytical solution $\mathbf{y}$ of the dual problem [24] is not available, thus $\mathbf{y}$ has to be replaced by $\mathbf{y}^k$. This numerical solution $\mathbf{y}^k$ is computed with the same Galerkin resp. Finite Difference method as the primal solution,

$$\sum_{n=m-1}^{0} \int_{t_{n+1}}^{t_n} \mathbf{g}^k \left(\mathbf{M}\ddot{\mathbf{y}}^k \;-\; \mathbf{C}\dot{\mathbf{y}}^k \;+\; \mathbf{K}\mathbf{y}^k\right) dt \;=\; 0\;\forall \mathbf{g}^k \in \mathcal{V}^k \subset \mathcal{V}\,. \qquad [34]$$

Thus $\mathbf{y}^k$ is the dual solution assuming the estimated global error $\tilde{\mathbf{e}}_t(t_m)$ as *final* conditions. The developed procedure for the estimation of the global time integration error can now be summarised:

a) solve the primal problem from $t = t_0$ to $t = t_m$, Equation [5], and compute the residuum $\mathbf{R}(t)$,

b) solve the dual problem from $t = t_m$ to $t = t_0$, Equation [34], using the time step size from the primal problem $k = k(t)$ and compute $\mathbf{y}^k$,

c) compute $\int_0^{t_m} \mathbf{y}_h\, \mathbf{R}\, dt$: $\rightarrow |\tilde{\mathbf{e}}_t(t_m)_C|$.

NOTE. – A numerical integration should be applied to compute this integral.

In order to show the convergence and the accuracy of the estimated global error $\tilde{\mathbf{e}}_t(t_m)$ as a **first test example** the following single degree of freedom system is used:

$$m\ddot{u} \;+\; \mu\dot{d} \;+\; cd \;=\; 0 \forall t \in (0, 2],$$
$$\text{with: } u(t=0) \;=\; 1.0\,,\; \dot{u}(t=0) \;=\; 0.0 \text{ and } m = 1.0\,,\; \mu = 0.5\,,\; c = 1.0\,. \qquad [35]$$

The global error is estimated at $t = 2$ and $t = 5$.

Table 2. *Single degree of freedom system,* $m = 1.0$, $\mu = 0.5$, $c = 1.0$*; convergence of the estimated global time integration error for both Finite Difference and Galerkin scheme* $\tilde{\mathbf{e}}_t(t_m)_N$ *[19] resp.* $\tilde{\mathbf{e}}_t(t_m)_C$ *[35] and exact global error of the numerical solution for displacement and velocity at* $t_m = 2.0$ *varying the time step size*

k	$\tilde{\mathbf{e}}_t(2)_N$	$\tilde{\dot{\mathbf{e}}}_t(2)_N$	$\tilde{\mathbf{e}}_t(2)_C$	$\tilde{\dot{\mathbf{e}}}_t(2)_C$	$\mathbf{e}_t(2)$	$\dot{\mathbf{e}}_t(2)$
0.2	$1.83 \cdot 10^{-2}$	$8.11 \cdot 10^{-2}$	$2.53 \cdot 10^{-2}$	$6.84 \cdot 10^{-2}$	$2.63 \cdot 10^{-2}$	$6.83 \cdot 10^{-2}$
0.1	$5.90 \cdot 10^{-3}$	$1.92 \cdot 10^{-2}$	$6.77 \cdot 10^{-3}$	$1.71 \cdot 10^{-2}$	$6.83 \cdot 10^{-3}$	$1.71 \cdot 10^{-2}$
0.05	$1.61 \cdot 10^{-3}$	$4.58 \cdot 10^{-3}$	$1.72 \cdot 10^{-3}$	$4.29 \cdot 10^{-3}$	$1.72 \cdot 10^{-3}$	$4.29 \cdot 10^{-3}$
0.025	$4.18 \cdot 10^{-4}$	$1.11 \cdot 10^{-3}$	$4.32 \cdot 10^{-4}$	$1.07 \cdot 10^{-3}$	$4.32 \cdot 10^{-4}$	$1.07 \cdot 10^{-3}$

Table 3. *Single degree of freedom system,* $m = 1.0$, $\mu = 0.5$, $c = 1.0$*; convergence of the estimated global time integration error for both Finite Difference and Galerkin scheme* $\tilde{\mathbf{e}}_t(t_m)_N$ *[19] resp.* $\tilde{\mathbf{e}}_t(t_m)_C$ *[35] and exact global error of the numerical solution for displacement and velocity at* $t_m = 5.0$ *varying the time step size*

k	$\tilde{\mathbf{e}}_t(5)_N$	$\tilde{\dot{\mathbf{e}}}_t(5)_N$	$\tilde{\mathbf{e}}_t(5)_C$	$\tilde{\dot{\mathbf{e}}}_t(5)_C$	$\mathbf{e}_t(5)$	$\dot{\mathbf{e}}_t(5)$
0.2	$4.41 \cdot 10^{-3}$	$3.25 \cdot 10^{-3}$	$4.04 \cdot 10^{-3}$	$3.78 \cdot 10^{-3}$	$4.00 \cdot 10^{-3}$	$3.80 \cdot 10^{-3}$
0.1	$1.04 \cdot 10^{-3}$	$8.95 \cdot 10^{-4}$	$9.97 \cdot 10^{-4}$	$9.53 \cdot 10^{-4}$	$9.95 \cdot 10^{-4}$	$9.54 \cdot 10^{-4}$
0.05	$2.54 \cdot 10^{-4}$	$2.32 \cdot 10^{-4}$	$2.49 \cdot 10^{-4}$	$2.39 \cdot 10^{-4}$	$2.48 \cdot 10^{-4}$	$2.39 \cdot 10^{-4}$
0.025	$6.28 \cdot 10^{-5}$	$5.89 \cdot 10^{-5}$	$6.20 \cdot 10^{-5}$	$5.96 \cdot 10^{-5}$	$6.21 \cdot 10^{-5}$	$5.97 \cdot 10^{-5}$

The results in Table 2, $\tilde{\mathbf{e}}_t(2)_C$, and Table 3, $\tilde{\mathbf{e}}_t(5)_C$, indicate, that the effectivity index:

$$\eta = \frac{\tilde{\mathbf{e}}_t}{\mathbf{e}_t} \text{ resp. } \frac{\tilde{\dot{\mathbf{e}}}_t}{\dot{\mathbf{e}}_t} \qquad [36]$$

is very close to 1 for the Galerkin formulation of Newmark's scheme. The results for the estimator of Riccius $\tilde{\mathbf{e}}_t(t_m)$ show, that the correct order of convergence $\mathcal{O}(k^2)$ can be observed for a sufficiently small time step size, see columns 2 and 3 in Table 2 and Table 3 .

As a **second test example** a linear system with two degrees of freedom is chosen,

$$\begin{bmatrix} 400 & 0 \\ 0 & 200 \end{bmatrix} \begin{bmatrix} \ddot{d}_1 \\ \ddot{d}_2 \end{bmatrix} + \begin{bmatrix} 200 & -100 \\ -100 & 100 \end{bmatrix} \begin{bmatrix} d_1 \\ d_2 \end{bmatrix} = \mathbf{0} \quad \text{for } 0 < t \leq 40\,, \qquad [37]$$

with the initial conditions: $\begin{bmatrix} d_1^0 \\ d_2^0 \end{bmatrix} = \begin{bmatrix} 0.5 \\ 1.0 \end{bmatrix}$ and $\begin{bmatrix} \dot{d}_1^0 \\ \dot{d}_2^0 \end{bmatrix} = \begin{bmatrix} 0.0 \\ 0.0 \end{bmatrix}$.

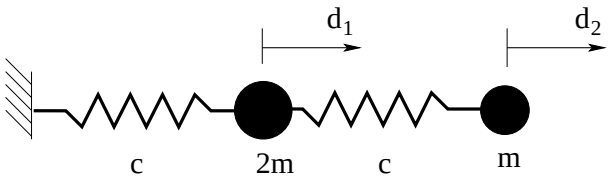

Figure 2. *Two degree of freedom system with* $c = 100$ *and* $m = 200$

The time step size is set to $k = 0.05 = const$. The exact solution d_1 and d_2 for system [37] is shown in Figure 3. Here the global time integration error in the Euclidean norm is estimated:

$$|\mathbf{e}_t| = \sqrt{e_{t,1}^2 + e_{t,2}^2}$$

Now the problem is to find the proper initial conditions for the dual problem. Because we do now know $e_{t,1}$ and $e_{t,2}$, the estimated local error $e_{l,1}(t_m)$, $e_{l,2}(t_m)$ at $t = t_m$ is substituted into Equation [28]:

$$\dot{\mathbf{y}}(t = t_m) = \frac{-\left(\mathbf{M}^{-T}\tilde{\mathbf{e}}_l(t_m)\right)^T}{|\tilde{\mathbf{e}}_l(t_m)|}\,.$$

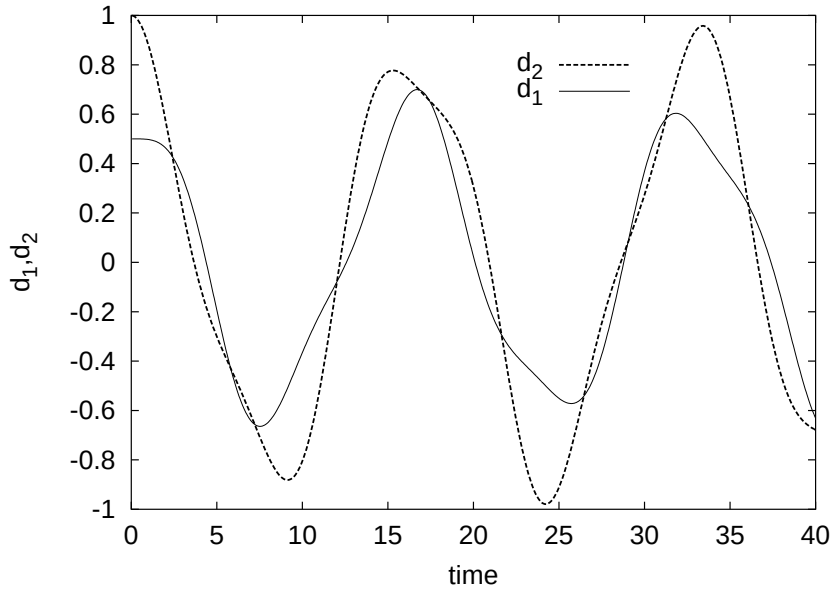

Figure 3. *Solutions* $d_1(t)$ *and* $d_2(t)$ *of two degree of freedom system with initial displacement conditions*

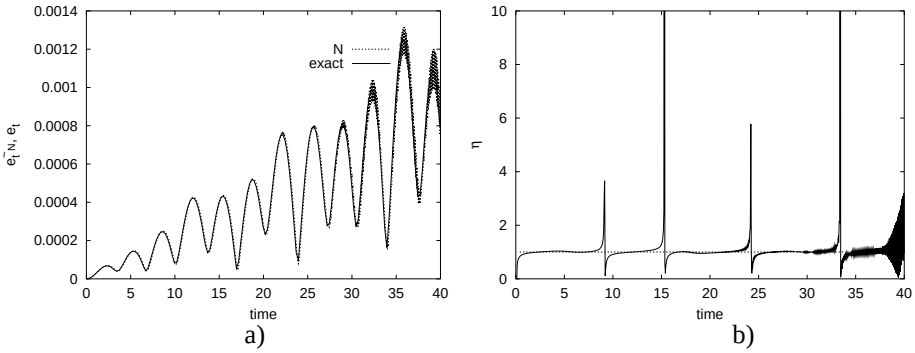

Figure 4. *Two degree of freedom system; a) comparison of estimated and exact global error of Newmark's scheme as difference scheme (N), measured in the Euclidean norm; b) efficiency index* η

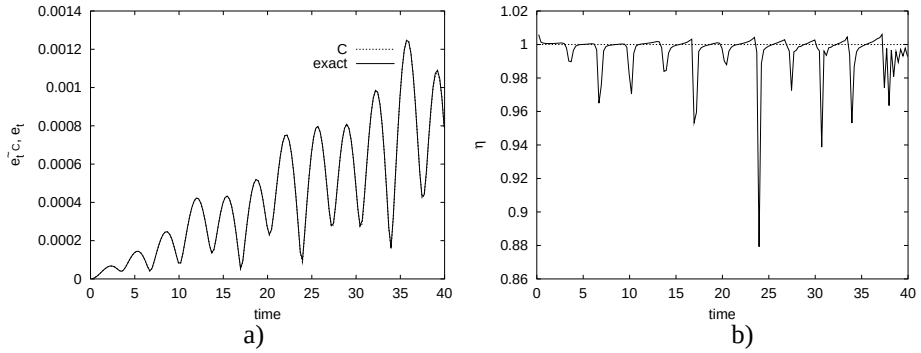

Figure 5. *Two degree of freedom system; a) comparison of estimated and exact global error of Newmark's scheme as continuous Galerkin scheme (C), measured in the Euclidean norm; b) efficiency index* η

The numerical results in Figures 4a) and 5a) show, that the estimated error corresponds rather well with the exact error. Visually there is almost no difference. The estimation, based on the extrapolation of the local error (Equation [19]), oscillates about the exact error with increasing time t, see Figure 4a). Beyond $t \approx 37$ the good efficiency index of about '1' also starts to deviate, see Figures 4b). The reason for this expected misbehaviour lies in the missing information about the error propagation, see Figure 1. In addition the numerical differentiation has some influence on the results due to the different difference formulas in the local error estimator [11]. However, for the Galerkin formulation of Newmark's scheme the chosen heuristics $\mathbf{e}_t(t_m) \rightarrow \tilde{\mathbf{e}}_l(t_m)$ for the initial conditions of the dual problem seem to be a fairly good choice, because the effectivity index η for $\mathbf{e}_{tC}$ is close to '1', see Figure 5b), though some problems appear to start at $t > 37$.

4.3. *Estimation of the global time integration error for nonlinear ordinary differential equations*

Here the estimators of the global time integration error [29, 19] will be applied to nonlinear problems of rigid body dynamics. The numerical solution $\mathbf{d}^k = \mathbf{d}^k(t)$ of the problem is given by Newmark's method resp. by the Continuous Galerkin formulation. In the numerical solution with the Continuous Galerkin method:

$$\int_{t_n}^{t_{n+1}} \mathbf{g}^k \cdot \mathbf{M}\ddot{\mathbf{d}}^k \, dt \, + \int_{t_n}^{t_{n+1}} \mathbf{g}^k \cdot \mathbf{n}(\mathbf{d}^k \, , \, \dot{\mathbf{d}}^k \, , \, t) \, dt \, = \, 0 \;\; \forall \, \mathbf{g}^k \in \mathcal{V}^k \qquad [38]$$

Newton's iteration method is embedded. The integral:

$$\int_{t_n}^{t_{n+1}} \mathbf{g}^k \cdot \mathbf{n}(\mathbf{d}^k \, , \, \dot{\mathbf{d}}^k \, , \, t) \, dt$$

is evaluated with the 4-point Gauss-Legendre integration rule.

As is well known, the principle of duality is valid only for linear operators $\mathcal{D} = \mathbf{n}$:

$$\int_0^{t_m} \mathbf{y} \cdot \mathcal{D}\mathbf{e} \, dt \, = \int_0^{t_m} \mathbf{e} \cdot \mathcal{D}^* \mathbf{y} \, dt \, ,$$

with the appropriate initial conditions for $\mathbf{e}$ and $\mathbf{y}$. Thus, if $\mathbf{n}$ is nonlinear, we have to use a linearization of $\mathbf{n}$ to define the dual problem. Thus the total differential of $\mathbf{n}$ is necessary:

$$d\mathbf{n} \, = \, \frac{\partial \mathbf{n}}{\partial \dot{\mathbf{d}}} d\dot{\mathbf{d}} \, + \, \frac{\partial \mathbf{n}}{\partial \mathbf{d}} d\mathbf{d} \, = \, \mathbf{C}(\dot{\mathbf{d}}, \mathbf{d}) d\dot{\mathbf{d}} \, + \, \mathbf{K}(\dot{\mathbf{d}}, \mathbf{d}) d\mathbf{d} \, . \qquad [39]$$

In addition we assume $\mathbf{K} \, = \, \mathbf{K}^T$, thus conservative problems. Now the procedure, see Equation [5], for linear differential equations can be mapped to the linearized primal problem. Thus, we multiply the linearized problem with the dual solution $\mathbf{y}$ and after partial integration we get:

$$\int_0^{t_m} \mathbf{y} \cdot \left(\mathbf{M} d\ddot{\mathbf{d}} + \mathbf{C}(\dot{\mathbf{d}}, \mathbf{d}) d\dot{\mathbf{d}} + \mathbf{K}(\dot{\mathbf{d}}, \mathbf{d}) d\mathbf{d} \right) dt$$
$$= \int_0^{t_m} d\mathbf{d} \cdot \left(\mathbf{M}\ddot{\mathbf{y}} - \mathbf{C}(\dot{\mathbf{d}}, \mathbf{d})\dot{\mathbf{y}} + \mathbf{K}(\dot{\mathbf{d}}, \mathbf{d})\mathbf{y} \right) dt \,. \quad [40]$$

For every primal solution $d\mathbf{d}$ the corresponding dual problem becomes then:

$$\mathbf{M}\mathbf{y} - \mathbf{C}(\dot{\mathbf{d}}, \mathbf{d})\dot{\mathbf{y}} + \mathbf{K}(\dot{\mathbf{d}}, \mathbf{d})\mathbf{y} = \mathbf{0} \,. \quad [41]$$

As a consequence we have either to store or to recompute $\mathbf{K}(\dot{\mathbf{d}}, \mathbf{d})$ and $\mathbf{C}(\dot{\mathbf{d}}, \mathbf{d})$ for the complete time range for which we intend to perform an error estimation.

Two rigid body problems will be used in the following to test both methods, Equations [19], [29], for global error estimation.

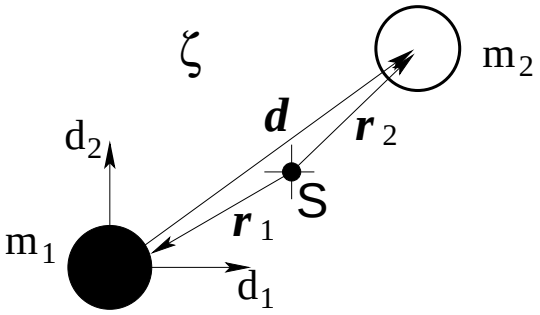

Figure 6. *Two-body problem*

The **two-body problem** (Estep *et al.*, 1994), Figure 6, consists of two mass points m_1 and m_2, which interact due to a gravity field. The motion of m_1 and m_2 with the coordinates $\mathbf{r}_1$ and $\mathbf{r}_2$ w.r.t. the center of gravity S is transformed to the motion of one mass with $m = \frac{m_1 m_2}{m_1 + m_2}$ with the coordinate $\mathbf{d} = (d_1, d_2)^T$. The gravity field is point symmetric with a gravity constant $\zeta = 1.0$:

$$\left[\begin{array}{l} m\ddot{d}_1 + \zeta \frac{d_1}{(d_1^2 + d_2^2)^{3/2}} = 0 \\ m\ddot{d}_2 + \zeta \frac{d_2}{(d_1^2 + d_2^2)^{3/2}} = 0 \end{array} \right] \text{ for } t > 0 \quad [42]$$

with initial conditions: $d_1^0 = 0.4$, $d_2^0 = 0.0$, $\dot{d}_1^0 = 0.0$, $\dot{d}_2^0 = 2.0$.

For $m = 1.0$ an analytical (classical) solution to the problem [42] can be given,

$$d_1(t) = \cos(\tau) - 0.6\,,\; d_2(t) = 0.8\sin(\tau) \;\text{ with: } t = \tau - 0.6\sin(\tau)\,.$$

The time step size for the numerical solution with the Continuous Galerkin (Newmark) scheme and the standard Newmark scheme (FD form) with $2\beta = \gamma = 0.5$ is set to $k = 0.005 = const.$. The solution of the two-body problem is given in Figure 7a) with the time t as the natural coordinate of the curve. The chosen initial conditions guarantee a periodic solution, see figure 7b) with the Poincaré map for $d_1 = 0$ and $\dot{d}_1 > 0$.

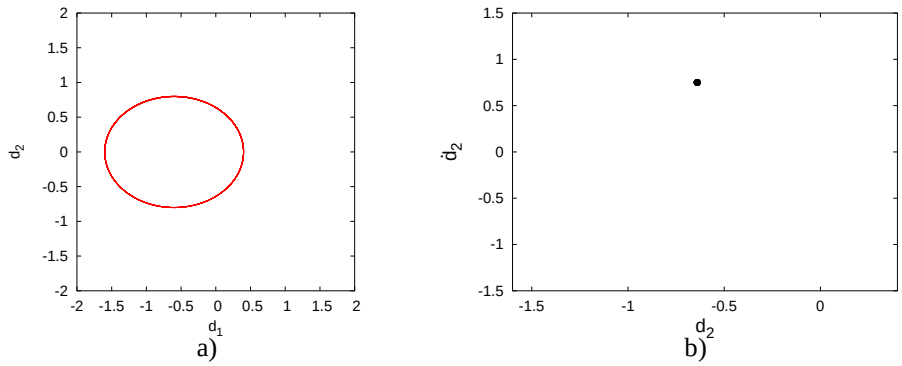

Figure 7. *Two-body problem; a) solution $d_2(t)$ over $d_1(t)$ and b) Poincaré map $\dot{d}_2(t) - d_2(t)$ for $d_1 = 0$ and $\dot{d}_1 > 0$*

Both global estimators, the local extrapolation error and the other one, based on the Galerkin formulation and dual problem are applied to the nonlinear problem of rigid body dynamics. First we estimate the global time integration error for the Continuous Galerkin method [5] with initial conditions for the dual solution based on the local error estimate of the standard (FD) Newmark scheme [5]. In Figure 8a) the estimated global error $\tilde{\mathbf{e}}_{tC}$ is depicted, the effectivity index η is evaluated in Figure 8b). Although η oscillates considerably the maximum and the minimum of the global error in the Euclidean norm are estimated rather well, η being fairly close to '1'. This undesirable effect is due to the approximation of the initial conditions $\mathbf{e}_{tC} \rightarrow \tilde{\mathbf{e}}_{lN}$ for the dual problem at $t = t_m$. As the exact solution is known and the exact error for this problem can be computed, we can confirm this presumption choosing the correct initial conditions $\dot{\mathbf{y}}^k(t = t_m) = -\left(\mathbf{M}^{-T}\mathbf{e}_t(t_m)\right)^T / |\mathbf{e}_t(t_m)|$ with the results displayed in Figure 9. There is no visible difference between the exact and the estimated global error which is also shown in the effectivity index. The latter grows – as expected – with increasing time. In Figure 10 the estimated global error [19] for Newmark's scheme based on the local error indicator [11] is displayed. The effectivity index η is very small, $\eta \ll 1$, a complete contrast to the corresponding linear problem. Interestingly, the maxima of the global error $\tilde{\mathbf{e}}_{tN}$ correspond qualitatively to the maxima

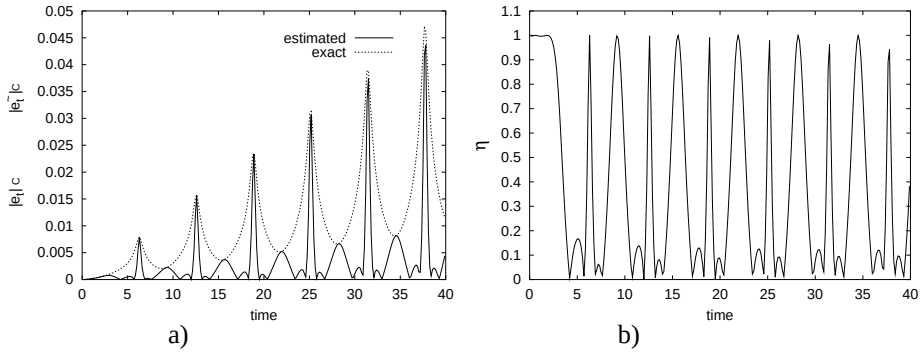

Figure 8. *Two-body problem; a) estimated error $\tilde{\mathbf{e}}_{tC}$ and exact error $\mathbf{e}_{tC}$, measured in Euclidean norm, and b) corresponding efficiency index η for Continuous Galerkin scheme with approximated initial conditions for the dual problem*

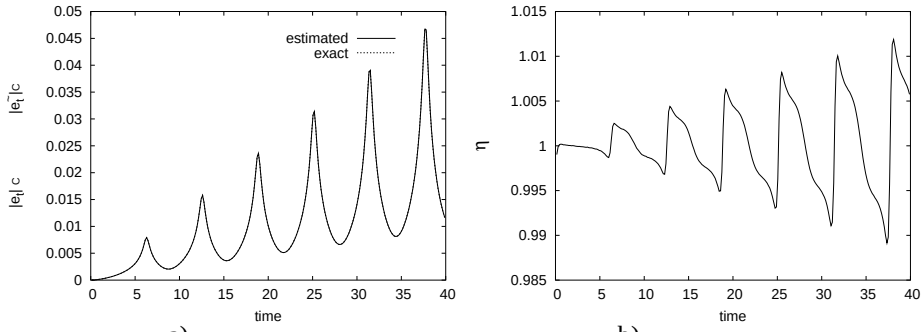

Figure 9. *Two body problem; a) estimated error $\tilde{\mathbf{e}}_{tC}$ and exact error $\mathbf{e}_{tC}$, measured in Euclidean norm, and b) corresponding efficiency index η for Continuous Galerkin scheme with the 'exact' initial conditions for the dual problem*

of the exact global error, however, the quantities of the estimated error are completely wrong.

Finally the global time integration error is estimated separately for the coordinates d_1 and d_2 with the Galerkin form using the dual approach. According to Equation [30] the *initial* conditions for the dual problem aiming at the global error e_1 or e_2 are applied:

$$\dot{\mathbf{y}}_i^k \;=\; -\left(\mathbf{M}^{-1}\mathbf{I}_i\right)^T \quad \text{with: } \mathbf{I}_1 = (1,0)^T \text{ resp. } \mathbf{I}_2 = (0,1)^T .$$

The corresponding global error estimates and the exact errors are depicted in Figures 11a) and 11b). It is obvious, that the initial conditions for the dual problem

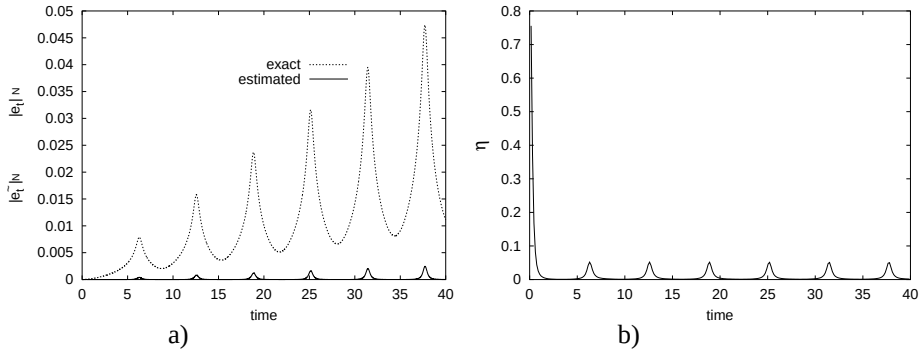

Figure 10. *Two body problem; a) estimated error $\tilde{\mathbf{e}}_{t\,N}$, measured in Euclidean norm and b) corresponding efficiency index η for Newmark's difference scheme*

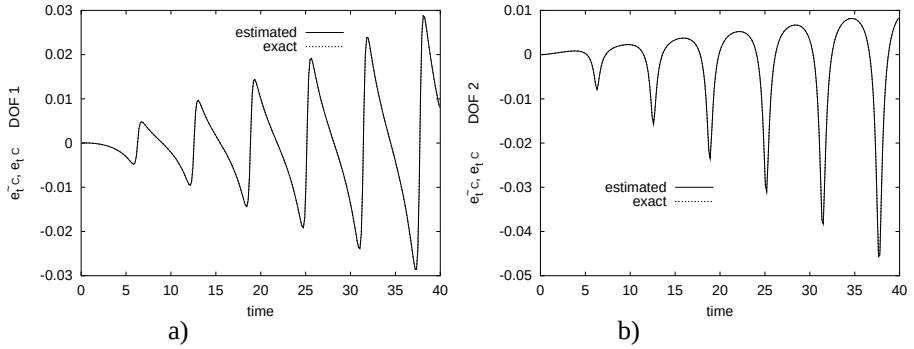

Figure 11. *Two-body problem; estimated error $\tilde{\mathbf{e}}_{tC}$ and exact error $\mathbf{e}_t$ of the continuous Galerkin scheme (C) for a) 1-st coordinate d_1 and for b) 2-nd coordinate d_1*

dominate the quality of the estimated global error. We also recognise that the error increases with increasing time.

In the second nonlinear example a **nonlinear spring pendulum** is discussed. Mettler (Mettler, 1959) uses this spring pendulum to model the instability behaviour of longitudinal motions in shaft constructions and on spring-supported foundations. The nonlinear spring pendulum, see Figure 12, has the following equation of motion:

$$\left[\begin{array}{l} m\ddot{d}_1 \,+\, cd_1 \dfrac{\sqrt{d_1^2+d_2^2}\,-\,l_0}{\sqrt{d_1^2+d_2^2}} \,=\, 0 \\[2ex] m\ddot{d}_2 \,+\, cd_2 \dfrac{\sqrt{d_1^2+d_2^2}\,-\,l_0}{\sqrt{d_1^2+d_2^2}} \,=\, mg \end{array}\right] \quad \forall\ t>0\,, \qquad [43]$$

with initial conditions: $d_1^0 = 10^{-1}$, $d_2^0 = 1.5$, $\dot{d}_1^0 = 0.0$, $\dot{d}_2^0 = 0.0$,

and parameters: $m = 1.4$, $l_0 = 1.0$ (length of unstretched spring) , $c = 38.5$.

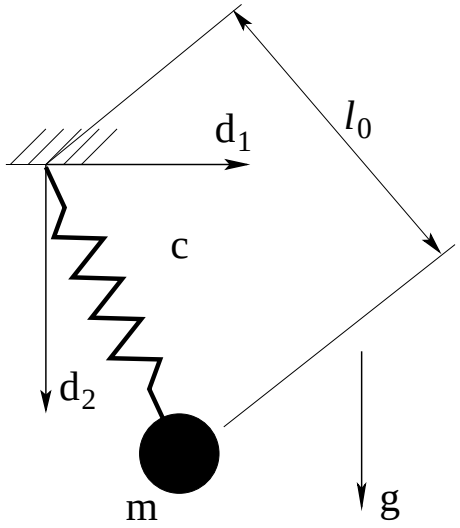

Figure 12. *Spring pendulum problem*

The numerical time integration is performed with the Galerkin scheme with quadratic test and ansatz functions $\mathbf{g}^k$ and $\mathbf{d}^k$. The Finite Difference form of Newmark's scheme is not used for the spring pendulum problem, because the estimation of the global time integration error failed due to a very small efficiency index, see Figure 10. The time step size is set to $k = 0.05 = const.$ As no solution of the differential Equation [43] is known, a reference solution with $k = 6.25 \cdot 10^{-4} = const.$ is determined.

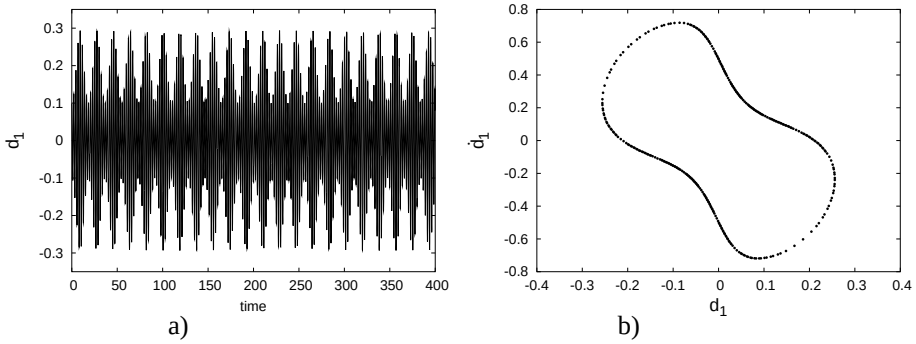

Figure 13. *Spring pendulum problem; a) solution $d_1(t)$ and b) Poincaré map $\dot{d}_1(t) - d_1(t)$ for $d_2 - (l_0 + mg/c) = 0$ and $\dot{d}_2 > 0$*

In Figure 13a) the horizontal motion $d_1(t)$ of the pendulum is shown, based on the initial perturbation d_1^0. In regular time intervals the fundamental solution of d_1 with

small amplitudes bifurcates into the *perturbed* solution with fairly large amplitudes. The solution with the chosen initial conditions is quasiperiodic, because the Poincaré map is a closed line, see Figure 13b). The estimated error $\tilde{\mathbf{e}}_{tC}$ for the displacement d_1 is of the same order as the exact error up to $t \approx 150$, see figure 14a). Then the estimated error deviates strongly from the exact error. This can be seen more clearly in the curve for the effectivity index, Figure 14b).

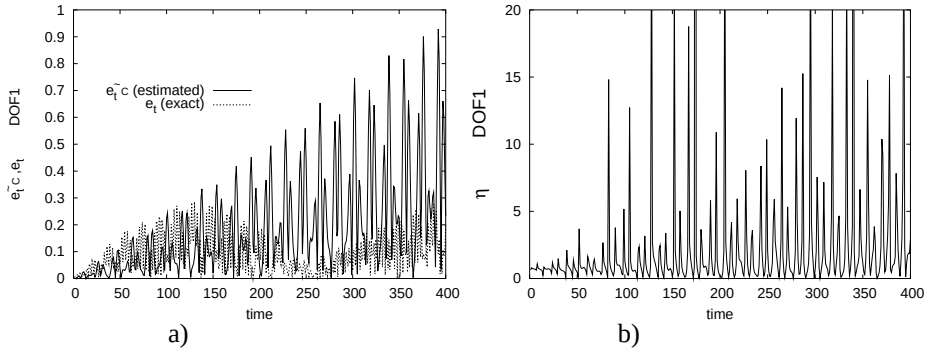

Figure 14. *Spring pendulum problem; estimated global error $\tilde{\mathbf{e}}_{tC}$ and exact error $\mathbf{e}_t$ for Continuous Galerkin scheme (C) a) 1-st coordinate d_1 and b) corresponding efficiency index η*

As in the two-body problem we discuss also the influence of the initial conditions for the dual problem. Now the time integration errors for the coordinates d_1, d_2 and the Euclidean norm are estimated separately. The initial conditions for the Euclidean norm are chosen according to Equation [30]. In contrast to the two-body problem the global time integration error for both coordinates d_1 and d_2 as well as the Euclidean norm is overestimated, see Figure 15. Up to $t \approx 150$ the estimated and the exact errors

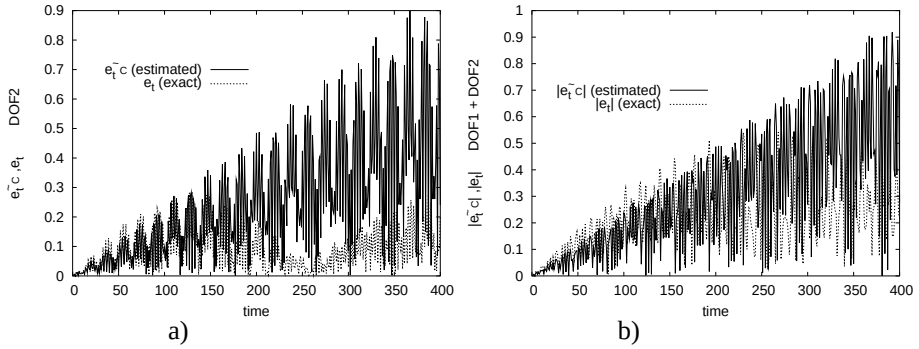

Figure 15. *Spring pendulum problem; estimated global error $\tilde{\mathbf{e}}_{tC}$ and exact error $\mathbf{e}_t$ for a) 2-nd coordinate d_2 and b) global time integration error, measured in Euclidean norm*

look fairly similar. Later the errors differ very much. Further we note that the error estimation in the Euclidean norm appears to behave better than the corresponding error estimation for the single coordinates, though there is only an estimation of the initial conditions of the dual problem.

In order to explain the deviation of the estimated error $\tilde{\mathbf{e}}_{tC}$ from the exact error $\mathbf{e}_t$ we compare the numerical solution with $k = 0.05 = const.$ with the reference solution for the first coordinate $\mathbf{d}_1$. It is obvious, that the estimated global error $\tilde{\mathbf{e}}_{tC}$

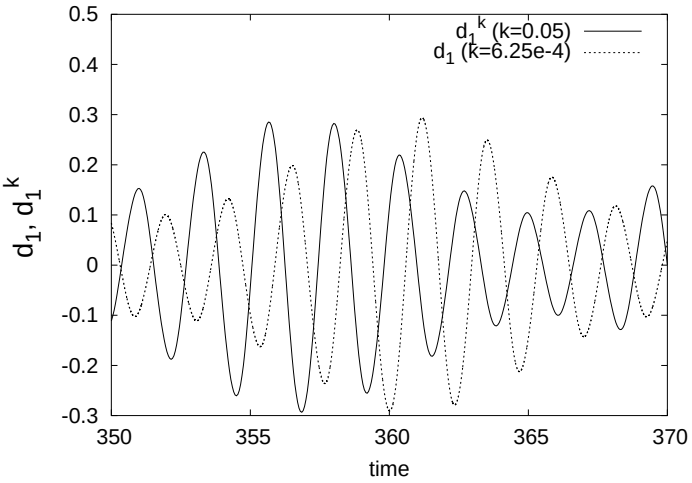

Figure 16. *Spring pendulum problem; comparison of numerical solution* $\mathbf{d}_1^k$ *for* $k = 0.05 = const.$ *and reference solution* $\mathbf{d}_1$ *with* $k = 6.25 \cdot 10^{-4} = const.$ *using the Continuous Galerkin method (C); showing a dominant effect of the phase error*

depends strongly on the primal solution $\mathbf{d}^k$ which shows a considerable phase difference for the two different time steps. This is a strong indication of the numerical sensitivity of the solution to the time step size and in particular of the dependency of the error estimation on the quality of the dual solution. The estimated error is for a long time as large as the amplitude of the controlled quantity and is even growing. As a consequence of this observation it appears to be less useful to perform a serious error estimation once the estimated error reaches the size of the controlled quantity and then the time step size should be reduced considerably to reach an error quantity of e.g. 10 % of the controlled value.

4.4. *Adaptive time stepping scheme*

To improve the efficiency of the numerical time stepping algorithm a procedure to automatically adapt the time step size is proposed. Here a combination of local and global error estimation is used to control the time step size. For the global error estimation we apply the estimator based on the duality principle, see Equation [26].

The local error estimator is based on the standard Newmark method, the FD form. However, it must be noted, that in general a local refinement of the time step size will not guarantee a reduction of the global time integration error. Thus in the combined adaptive time stepping scheme three bounds are introduced to control the local/global error:

i) upper bound for the global time integration error $gtol$;

ii) upper bound for the local time integration error $ltol_{up}$;
e.g. $ltol_{up} = gtol/C_{up}$, $C_{up} >> 1$,

iii) lower bound for the local time time integration error $ltol_{lo}$;
e.g. $ltol_{lo} = ltol_{up}/C_{lo}$, $C_{lo} = 2...10$.

With the estimated local error $\tilde{\mathbf{e}}_l$ the local time step size is controlled which limits consequently the local residuum $\mathbf{R}$ of the differential equation. The residuum itself has some influence on the global error $\tilde{\mathbf{e}}_t$ *via* the dual problem [29]. The local control of the time step size k is based on the proportionality between local error $\mathbf{e}_l$ and time step size. For Galerkin's method with quadratic test and ansatz functions for linear second order ordinary differential equations the local error is of order $\mathbf{O}(k^3)$:

$$\mathbf{e}_l \propto k^s\,, \quad s = 3. \qquad [44]$$

The maximum of the global error $emax = \max_{t\in[0,T]} \tilde{\mathbf{e}}_t(t_m)$ can be determined at the final time $t = T$. If the upper bound $emax > gtol$ is violated, then the numerical simulation starts at $t = 0$ with modified error bounds, $ltol_{up}(new)$, $ltol_{lo}(new)$. This iteration stops, if the inequality $emax < gtol$ is fulfilled over the complete time domain $0 < t \leq T$.

For the adaptation of the error bounds the knowledge about loosing one order of accuracy in the error computation going from local to global error is used,

$$gtol \propto k^{s-1}(new)\,, \;\; emax \propto k^{s-1}\,,$$
$$ltol_{up}(new) \propto k^s(new)\,, \, ltol_{up} \propto k^s\,,$$
$$\Rightarrow ltol_{up}(new) = \left(\frac{gtol}{emax}\right)^{s/(s-1)} ltol_{up}(old)\,,$$
$$\Rightarrow ltol_{lo}(new) = \left(\frac{gtol}{emax}\right)^{s/(s-1)} ltol_{lo}(old)\,.$$

In Figure 17 the algorithm to control the global time integration error is shown.

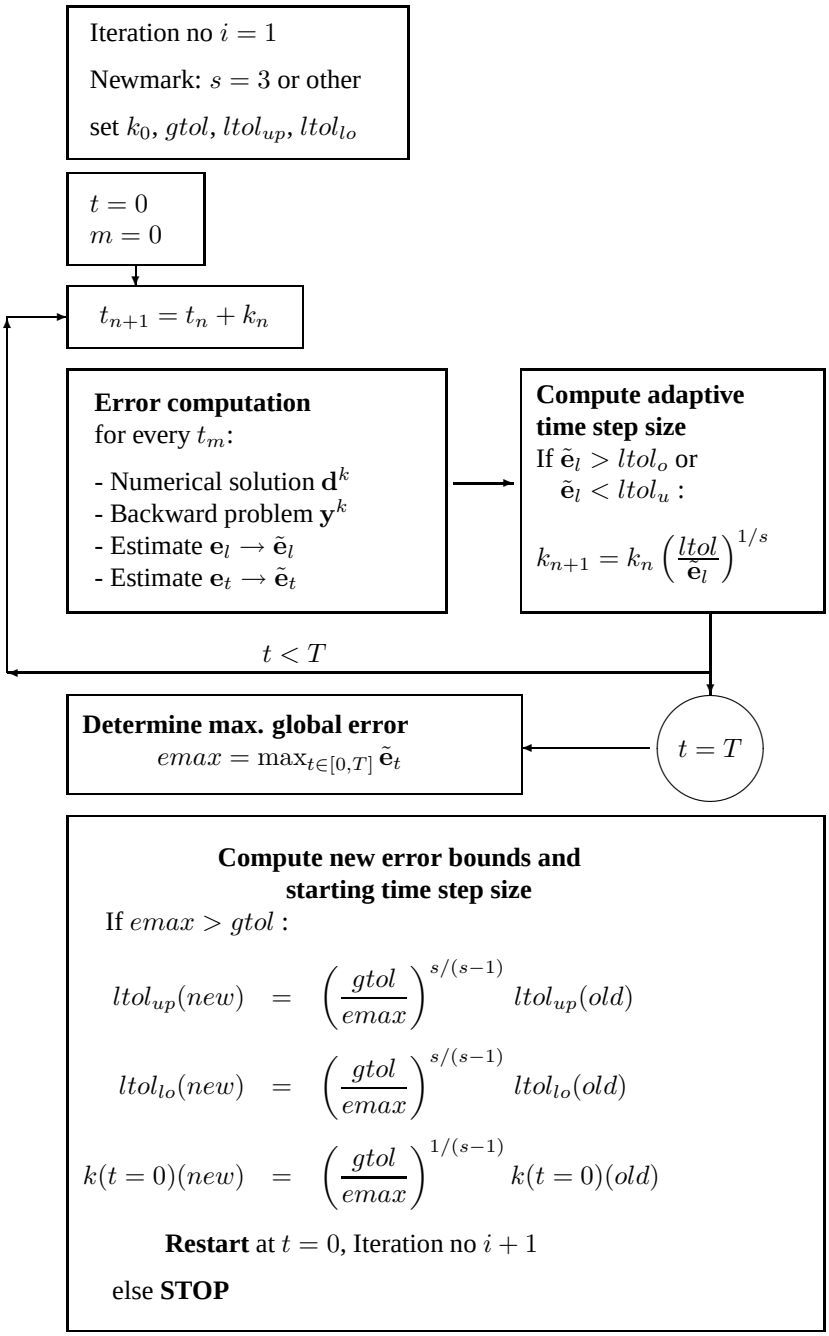

Figure 17. *Adaptive algorithm to control the time step size*

This adaptive time stepping scheme is tested now on two examples. For the **two-body problem** , Figure 6, the estimated and the exact global time integration error are computed for $k = const.$. To control the local and global time integration error the following error bounds are applied,

$$gtol = 1.5 \cdot 10^{-2} \, , \, ltol_{lo} = 1 \cdot 10^{-5} \, , \, ltol_{up} = 5 \cdot 10^{-5} \, .$$

Here the time integration is controlled in the Euclidean norm. The numerical results show, that 4 complete analysis, *i.e.* 4 iterations, are necessary to fulfill to upper bound $gtol$ of the global time integration error. In total the maximum time step size is reduced by a factor of 0.6 of the maximum in the first time interval of the first iteration. It is remarkable, that the estimated error in the 1-st iteration deviates barely from the estimated error in the 4-th iteration before $t = 30$, see Figure 18a).

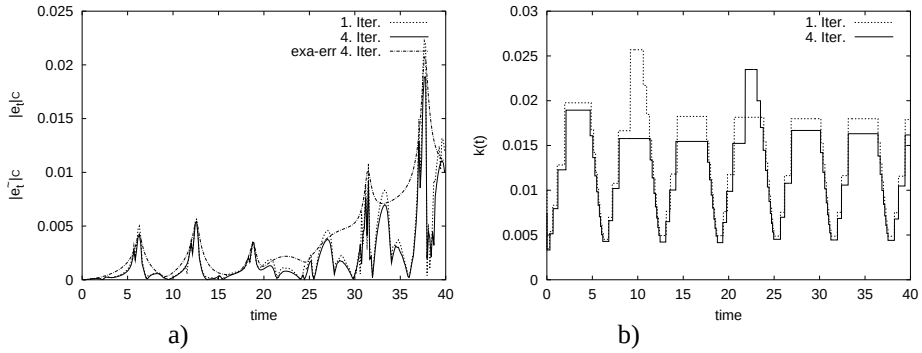

Figure 18. *Two-body problem, adaptation of the time step size; a) estimated global time integration error for 1-st iteration and for 4-th iteration, comparison with exact error of 4-th iteration, b) adapted time step size for 1-st iteration loop and 4-th iteration loop*

The same time stepping scheme is applied to the **spring pendulum problem**, see Figure 12. Here the following starting error bounds were used,

$$gtol = 0.05 \, , \, ltol_u = 1 \cdot 10^{-5} \, , \, ltol_o = 1 \cdot 10^{-4} \, .$$

As in the previous simulation of this problem with uniform time step size the global time integration error is controlled for the first dof $\mathbf{d}_1^k$ for $t \in (0, 400]$.

Because of the connection with the local error, which oscillates strongly, also the time step size oscillates, see Figure 19b). However, the adaptation procedure shows its qualities, the global error is considerably reduced below $0,02$ and does not show an increase up to $t = 400$, see Figure 20a). The comparison with the reference value (*exact* error), see Figure 20b) shows that the error is very well estimated after the second iteration. The final time history diagram for the analysis, see Figure 21 reveals the effectivity of the proposed procedure, as amplitude and phase of this highly nonlinear problem could be well captured.

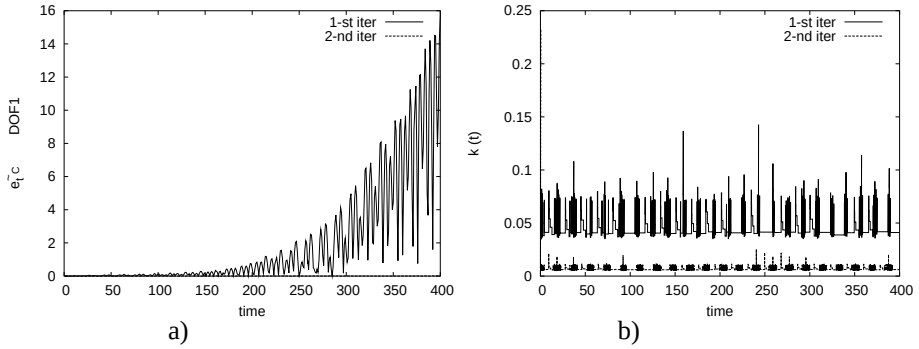

Figure 19. *Spring pendulum problem, adaptation of time step size; control of error for the 1-st dof* $\mathbf{d}_1$ *a) estimated global time integration error for 1-st iteration and for 2-nd iteration in logscale , b) adapted time step size for 1-st and 2-nd iteration loop*

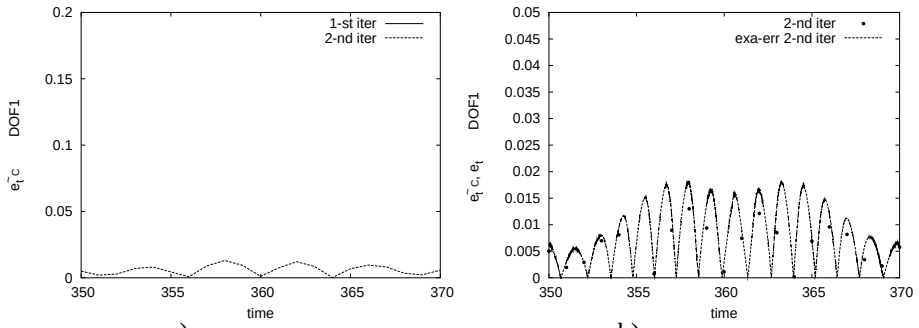

Figure 20. *Spring pendulum problem; adaptation of time step size; cutout range from* $t = 350 - 370$*; a) estimated global time integration error* $\tilde{\mathbf{e}}_{tC}$ *in logscale for 1-st and 2-nd iteration; b) comparison of estimated error with exact error* $\mathbf{e}_t$

5. Conclusions

The developed algorithms for error estimation of local and global errors for rigid body dynamics problems were explained and discussed on some linear and nonlinear, small size numerical problems. For the Newmark scheme in the finite difference form as well as in the Galerkin form the merits and the limits were presented. The effectivity of the local estimator as well as of the global estimator were demonstrated. It is clear that the dual concept with the Galerkin scheme leads to well defined global error quantity, however, somehow restricted to single coordinates. For a mixture of coordinates approximations for the initial or *final* conditions of the dual problem are necessary, which can be found e.g. by the local estimator, though this has some limitations.

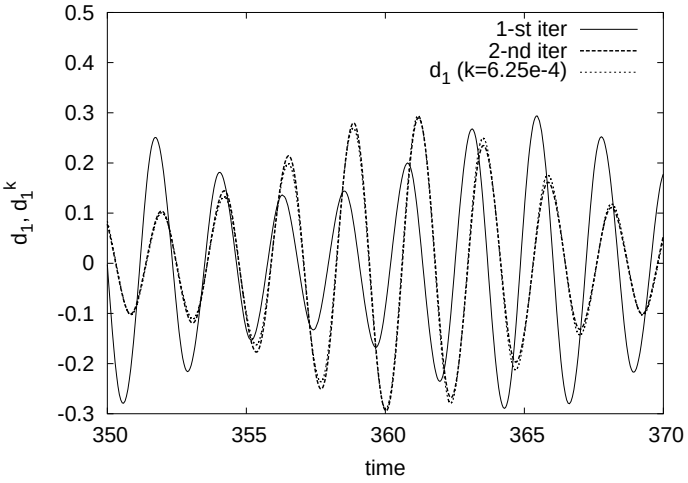

Figure 21. *Spring pendulum problem; adaptation of the time step size; numerical solution $d_1^k(t)$ for 1-st and 2-nd iteration, comparison with reference solution; main effect: reduction of the phase error*

For nonlinear problems the developed procedure for global error estimation based on the Galerkin scheme with a dual problem proves to work rather well. However, the quality of the error estimation strongly depends strongly on the primal solution, as not only the residuum for the error integral is needed, but also the linearized quantities at each time integration step for the dual solution, the backward problem. It was shown, that for large time steps due to the latter effect which is associated with an inaccurate dual solution the error estimator may fail completely.

The numerical effort for the dual problem involves a complete storage of the results of the primal problem to allow the evaluation of the integral, plus at least one backward analysis has to be performed. In addition, it is necessary to compute the dual solution with at least the same accuracy as the primal solution. In the nonlinear case the effort for storage of quantities needed to compute the linearized matrices is increasing considerably, making this duality based procedure rather questionable for large size problems.

However, the proposed adaptive time integration scheme based on a global as well as on a local error estimation has proven to be very effective and is capable to reduce the achieved error to the desired level. This can be well extended to standard FE discretized nonlinear problems, though the required overall numerical effort appears to be prohibitive.

The current use of duality based error estimation and related procedures appears to be on using the information from a duality based scheme to reduce the effort to compute a certain quantity needed for design, such as fatigue or long term response, see Meyer/Mathies (Meyer *et al.*, 2002 and 2003) or a maximum displacement, see

Kizio *et al.* (Kizio *et al.*, 2005). For alternative, fairly simple procedures for error analysis of dynamically loaded plate and shell structures discretized by finite elements we refer to Neumann, Schweizerhof (Neumann *et al.*, 1999), (Schweizerhof *et al.*, 2000 and 2001). Our future work is on combining the procedures for efficient tools applicable to large scale structures.

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