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ESTIMATION OF THE GLOBAL TIME INTEGRATION ERROR IN LINEAR AND NONLINEAR STRUCTURAL DYNAMICS – COMPARING NEWMARK SCHEME AND GALERKIN METHOD

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Abstract. *In this paper two error estimators resp. indicators for time integration in structural dynamics are compared. Based on Wood's [10] observation of the equivalence between Newmark's scheme and a Galerkin formulation the corresponding test function $\mathbf{w}_h$ is given explicitely. This allows to develop a global error estimator for the time integration based on the dual problem. This error estimator is compared to an error indicator based on finite differences. Both are tested on linear and nonlinear problems; a particular focus is on the limits of the error estimator for almost instable nonlinear problems.*

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1   GENERAL PROBLEM

The kinetics of rigid bodies play a major role in the field of mechanics. This kind of equations can be derived also from the spatial discretization of the equation of motion in elastodynamics. The ordinary differential equations (ODE) in time are written in the following general form,

$$\mathbf{M\ddot{u}} + \mathbf{h}(\mathbf{u}, \dot{\mathbf{u}}, t) = \mathbf{0}, \quad \forall t > 0,\tag{1}$$

$$\text{with initial conditions: } \mathbf{u}(t = 0) = \mathbf{u}_0 \quad \text{and} \quad \dot{\mathbf{u}}(t = 0) = \dot{\mathbf{u}}_0.$$

$\mathbf{M} \in \mathbb{R}^{n \times n}$ is the mass matrix, which is positiv definite. $\mathbf{h} \in \mathbb{R}^n$ is a function, which may include some geometric nonlinearities. In the linear case $\mathbf{h}(\mathbf{u}, \dot{\mathbf{u}}, t)$ represents the loading, the constant damping and constant stiffness properties of the considered model. The solution $\mathbf{u}(t)$ can be determined analytically only in some special cases, e.g. the Two-Body-Problem and problems in linear dynamics.

In order to guarantee the solvability and uniqueness of the solution of eqn.(1) the basic inequality of $\mathbf{h}$ has to be checked, with some norm $\| \cdot \|$ in $\mathbb{R}^n$, see Stoer/Burlisch [9],

$$\|\mathbf{h}(\mathbf{u}_1, t) - \mathbf{h}(\mathbf{u}_2, t)\| \leq \mathcal{L}\|\mathbf{u}_1 - \mathbf{u}_2\|.\tag{2}$$

$\mathbf{u}_1$ and $\mathbf{u}_2$ are two different solutions of (1) with different initial conditions, $\mathcal{L}$ is some real constant, $\mathcal{L} > 0$. Secondly $\mathbf{h}$ has to be finite and continuous. This latter, so-called Lipschitz condition can be replaced by the more common condition on the Jacobian $\mathbf{K}$ of $\mathbf{h}$, which comes from the mean value theorem,

$$\mathbf{K} = \frac{\partial \mathbf{h}}{\partial \mathbf{u}}.$$

Furthermore, each element of $\mathbf{K}$ has to be continuous and bounded.

Then for every initial condition $(\mathbf{u}_0, \dot{\mathbf{u}}_0)$ we can find only one unique solution $\mathbf{u}(t)$, which is continuous and continuously differentiable in time.

2   Newmark's method as a Petrov-Galerkin formulation

In linear dynamics eqn.(1) reads:

$$\mathbf{M\ddot{u}} + \mathbf{h}(\mathbf{u}, \dot{\mathbf{u}}, t) = \mathbf{M\ddot{u}} + \mathbf{C\dot{u}} + \mathbf{Ku} - \mathbf{F} = \mathbf{0}.\tag{3}$$

The time domain is usually divided into N time intervals with states, $n = 0...N$, $\Delta t_n = t_{n+1} - t_n$.

Considering the change of velocity $\dot{\mathbf{u}}$ and displacement $\mathbf{u}$ between two time states t_n and t_{n+1}, based on Taylor's expansions, Newmark [7] proposed the following dependence for $\mathbf{u}$ and $\dot{\mathbf{u}}$:

$$\dot{\boldsymbol{u}}_{n+1} = \dot{\boldsymbol{u}}_n + \Delta t(1 - \gamma)\ddot{\boldsymbol{u}}_n + \Delta t \gamma \ddot{\boldsymbol{u}}_{n+1},\tag{4}$$

$$\boldsymbol{u}_{n+1} = \boldsymbol{u}_n + \Delta t \dot{\boldsymbol{u}}_n + \Delta t^2(1 - 2\beta)\ddot{\boldsymbol{u}}_n/2 + \Delta t^2 \beta \ddot{\boldsymbol{u}}_{n+1}.\tag{5}$$

Then the differential equation in time (3) is solved at the discrete time level t_{n+1}:

$$\mathbf{M}\,\ddot{u}_{n+1} \,+\, \mathbf{C}\,\dot{u}_{n+1} \,+\, \mathbf{K}u_{n+1} \,-\, \mathbf{F}_{n+1} \,=\, \mathbf{0}\,, \tag{6}$$

and the assumptions in eqns.(4,5) are introduced leading to an equation for the analysis at t_{n+1}. With the obtained accelerations the velocity and the displacements at t_{n+1} can be computed. This is a typical example of a Finite Difference method. In many papers and books the properties of this procedure w.r.t. the parameters β and γ are discussed. The properties are mostly analyzed using the amplification matrix $\mathbf{A}_{FD}$, which maps the state variables from the situation at $t = t_n$ to state $t = t_{n+1}$. Our focus is on the special values $\beta = 1/4$ and $\gamma = 1/2$. This combination guarantees the second order accuracy $\mathcal{O}(\Delta t^2)$ of this method and the A-stability, see Wood [10]. This means, the numerical solution is bounded in absence of an excitation. With other parameter configurations the accuracy of the method can be risen, but then the A-stability is lost, see Dahlquist [2].

Since 1970 the Finite Element method became also popular for time integration. The following considerations are based on a Petrov-Galerkin scheme applied to eqn. (3),

$$\int_0^T \mathbf{w} \,\cdot\, (\mathbf{M}\ddot{u} \,+\, \mathbf{C}\dot{u} \,+\, \mathbf{K}u \,-\, \mathbf{F})\, dt \,=\, 0\,, \forall \mathbf{w} \in V\,, \tag{7}$$

with $\mathbf{w} \in V$ as the test function and V as a inner product space. Wood [10] showed, there exists a Finite Element formulation, which is equivalent to the Finite Difference scheme (6) with $\beta = 1/4$, $\gamma = 1/2$. It is a separate task to find the correct test function $\mathbf{w}_h$ for the Finite Element method as a Petrov-Galerkin scheme. The ansatz function is then a 2-nd order polynomial,

$$\mathbf{u}_h \,=\, \mathbf{u}_n \,+\, (t - t_n)\dot{\mathbf{u}}_n \,+\, 1/2(t - t_n)^2 \ddot{\mathbf{u}}_n\,. \tag{8}$$

We solve a system of equations and find as the corresponding test functions,

$$\mathbf{w}_h \,=\, \mathbf{W}_h \left(1/5 - (t - t_n)/\Delta t + (t - t_n)^2/\Delta t^2\right)\,. \tag{9}$$

The discrete Petrov-Galerkin method can then be written as,

$$\int_0^T \mathbf{w}_h \,\cdot\, (\mathbf{M}\ddot{u}_h \,+\, \mathbf{C}\dot{u}_h \,+\, \mathbf{K}u_h \,-\, \mathbf{F})\, dt \,=\, 0\,, \forall \mathbf{w}_h \in V_h\,, \tag{10}$$

V_h is the finite subspace of V, $\mathbf{w}_h$ is the discrete element of $\mathbf{w}$. In contrast to the discrete time levels (used in eqns.(4,5), the time domain is split into N finite time intervals resp. time elements, in which the integration is performed,

$$\int_0^T \,=\, \sum_{n=0}^N \int_{t_n}^{t_{n+1}}\,, \qquad n = 0...N\,, \Delta t_n \,=\, t_{n+1} - t_n\,.$$

Despite the continuous ansatz function, the second integration scheme can also be cast in a form like a Finite Difference (FD) method,

$$\left(\begin{array}{c} \mathbf{u}_{n+1} \\ \dot{\mathbf{u}}_{n+1} \end{array} \right) = \mathbf{A}_{FE} \left(\begin{array}{c} \mathbf{u}_n \\ \dot{\mathbf{u}}_n \end{array} \right) . \tag{11}$$

Comparing the amplification matrices $\mathbf{A}_{FE}$ and $\mathbf{A}_{FD}$, their equivalence can be shown for the special case with $\gamma = 2\beta$, Wood [10]. Now Newmark's scheme with $\gamma = 2\beta$ can be looked upon and treated as a Finite Element method. It is not necessary to compute the initial acceleration $\ddot{\mathbf{u}}_0$, which in the Finite Difference scheme is found via,

$$\ddot{\mathbf{u}}_0 = \mathbf{M}^{-1} \left(\mathbf{F}(t=0) - \mathbf{C}\dot{\mathbf{u}}_0 - \mathbf{K}\mathbf{u}_0 \right) . \tag{12}$$

The major advantage of the Finite Element formulation is the consequence for the error analysis. It allows to use some well-established techniques from problems in elastostatics for the equations in structural dynamics. Obviously, the considerations concerning the equivalence of the FD and FE approach are valid in the linear regime. For nonlinear ordinary differential equations the Finite Element method and the Finite Difference scheme are not comparable.

3   Error indicator based on the Finite Difference Method

If a numerical technique is applied to an equation, the numerical solution has to be investigated w.r.t. errors, coupled to the used technique. Here the global time integration error at time $t = t_m$ is the goal:

$$e_g = e(t = t_m) = u(t = t_m) - u_m . \tag{13}$$

$u(t = t_m)$ is the value of the exact solution at $t = t_m$, u_m is the result of the numerical integration at $t = t_m$. In order to estimate e_g for the Newmark-scheme, we will use the error indicator proposed by Riccius [8]. It is based on the local error indicator $e_l(t_m)$ for displacements in the time interval $t \in [t_{m-1}, t_m]$,

$$e_l(t_m) = \Delta t^3 \left(1/6 - \beta \right) \dddot{u}_m = \Delta t^2 \left(1/6 - \beta \right) \left(\ddot{u}_{m-1} - \ddot{u}_m \right) . \tag{14}$$

Assuming that the local error $e_l(t_m)$ is constant in $t_m/\Delta t$ time intervals, the error indicator $\tilde{e}_g$ for the global time integration error at time $t = t_m$ can be computed in a very simple manner,

$$\tilde{e}_g(newm) = \frac{t_m}{\Delta t} e_l(t_m) . \tag{15}$$

4   Error estimator based on the Finite Element Method

An error estimator for the global time integration, based on the Petrov-Galerkin method, is developed for linear differential equations first. This results also in an error

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estimator for the Newmark-scheme. The starting point of the derivation is the variational form of the ODE and the corresponding discretized form,

$$\int_0^T \mathbf{w}_h \cdot (\mathbf{M}\ddot{\mathbf{u}} + \mathbf{C}\dot{\mathbf{u}} + \mathbf{K}\mathbf{u} - \mathbf{F})\, dt = 0\,, \forall \mathbf{w}_h \in V_h\,, \tag{16}$$

$$\int_0^T \mathbf{w}_h \cdot (\mathbf{M}\ddot{\mathbf{u}}_h + \mathbf{C}\dot{\mathbf{u}}_h + \mathbf{K}\mathbf{u}_h - \mathbf{F})\, dt = 0\,, \forall \mathbf{w}_h \in V_h\,, \tag{17}$$

with a division in N time intervals: $\displaystyle\int_0^T = \sum_{n=0}^N \int_{t_n}^{t_{n+1}}\,.$

If equations (16) and (17) are subtracted, the well known Galerkin-orthogonality of the residual $\mathbf{R}$ is found, which also leads directly to the differential equation for the error (19),

$$\int_0^T \mathbf{w}_h \cdot \mathcal{D}\mathbf{e}\, dt = 0\,, \quad \mathbf{e} = \mathbf{u} - \mathbf{u}_h\,, \tag{18}$$

$$\begin{aligned}
\text{with}:\quad \mathcal{D}\mathbf{e} &= \mathbf{M}\,(\ddot{\mathbf{u}} - \ddot{\mathbf{u}}_h) + \mathbf{C}(\dot{\mathbf{u}} - \dot{\mathbf{u}}_h) + \mathbf{K}(\mathbf{u} - \mathbf{u}_h) \\
&= \mathbf{M}\,\ddot{\mathbf{e}} \qquad + \mathbf{C}\dot{\mathbf{e}} \qquad + \mathbf{K}\mathbf{e} \\
&= \mathbf{F} - \mathbf{M}\ddot{\mathbf{u}}_h - \mathbf{C}\dot{\mathbf{u}}_h - \mathbf{K}\mathbf{u}_h = \mathbf{R}\,.
\end{aligned} \tag{19}$$

Next an additional equation is introduced, the so-called dual problem. Bangerth [1] showed this technique for 1-st order differential equations, Maute [5] used the dual problem for 2-nd order differential equations. The dual problem, also known as the adjoint problem, is derived from the primal problem (7) via partial integration, leading to a backward integration with $\mathbf{z}$, $\dot{\mathbf{z}}$ and $\ddot{\mathbf{z}}$ as the corresponding displacement, velocity and accelerations.

$$\mathbf{M}\ddot{\mathbf{z}} - \mathbf{C}\dot{\mathbf{z}} + \mathbf{K}\mathbf{z} = \mathbf{J}\,, \forall t < t_m \tag{20}$$

with the initial conditions at $t = t_m$: $\quad \mathbf{z}(t = t_m) = \mathbf{z}_m$ and $\dot{\mathbf{z}}(t = t_m) = \dot{\mathbf{z}}_m\,.$

$\mathbf{J}$ is a functional, the r.h.s. of the dual problem, which will be chosen later. Now the differential equation (20) is tested with the error $\mathbf{e}$ of the primal problem and the differential equation of the error, equation (19), is tested with the solution of the dual problem, equation (20),

$$\int_0^T \mathbf{e} \cdot (\mathbf{M}\ddot{\mathbf{z}} - \mathbf{C}\dot{\mathbf{z}} + \mathbf{K}\mathbf{z})\, dt = \int_0^T \mathbf{z} \cdot (\mathbf{M}\ddot{\mathbf{e}} + \mathbf{C}\dot{\mathbf{e}} + \mathbf{K}\mathbf{e})\, dt \equiv \int_0^T \mathbf{e} \cdot \mathbf{J}\, dt\,,$$

$$\rightarrow \int_0^T \mathbf{z} \cdot \mathcal{D}\mathbf{e}\, dt \equiv \int_0^T \mathbf{z} \cdot \mathbf{R}\, dt = \int_0^T \mathbf{e} \cdot \mathbf{J}\, dt\,. \tag{21}$$

This procedure is very similar to the principle of Betti, which is well known in linear elastostatics. The right hand side can be specified as the Dirac functional $\boldsymbol{\delta}$ at time $t = t_m$, as $\boldsymbol{\delta}$ posses the filter property,

$$\mathbf{J} = \boldsymbol{\delta}(t = t_m) \rightarrow \int_0^T \mathbf{e} \cdot \mathbf{J}\,dt = e_g(t = t_m)\,. \tag{22}$$

The basis for the computation of the necessary initial conditions for the dual problem is the linear momentum, eqn.(24). It is assumed, that the linear momentum at $t = t_m$ jumps from the value 0 at $t = t_m + \epsilon$, with $\epsilon > 0$, to the value 1 at $t = t_m$ for each degree of freedom. The initial displacement is set to 0, and it is known, that the velocity $\dot{\mathbf{z}}$ at $t_m + \epsilon$ is zero,

$$\mathbf{z}(t_m) = \mathbf{0}\,,$$
$$\dot{\mathbf{z}}(t_m + \epsilon) = \mathbf{0}\,,$$
$$\mathbf{M}\dot{\mathbf{z}}(t_m + \epsilon) - \mathbf{M}\dot{\mathbf{z}}(t_m) = \int_{t_m}^{t_m+\epsilon} \boldsymbol{\delta}\,dt = \mathbf{1}\,, \tag{23}$$
$$\dot{\mathbf{z}}(t_m) = -\mathbf{M}^{-1}\,\mathbf{1}\,. \tag{24}$$

Up to now linear ordinary equations have been considered and it is well known, that the duality principle is valid only for linear operators,

$$\int_0^T \mathbf{z} \cdot \mathcal{D}\mathbf{e}\,dt = \int_0^T \mathbf{e} \cdot \mathcal{D}^*\mathbf{z}\,dt \tag{25}$$
$$\text{with:}\ \mathcal{D}^*\mathbf{z} = \mathbf{M}\ddot{\mathbf{z}} - \mathbf{C}\dot{\mathbf{z}} + \mathbf{K}\mathbf{z}\,. \tag{26}$$

If the nonlinear equation reads,

$$\mathbf{M}\ddot{\mathbf{u}} + \mathbf{h}(\dot{\mathbf{u}}, \mathbf{u}, t) = \mathbf{0}\,, \forall t > 0\,, \quad \mathbf{u} \in \mathbb{R}^n\,, \tag{27}$$

the linearized differential operator of $\mathbf{h}$ can be computed as,

$$d\mathbf{h} = \frac{\partial \mathbf{h}}{\partial \dot{\mathbf{u}}}\,d\dot{\mathbf{u}} + \frac{\partial \mathbf{h}}{\partial \mathbf{u}}\,d\mathbf{u}$$

The linearized dual problem is then derived via partial integration as

$$\mathcal{D}^*\mathbf{z} = \mathbf{M}\ddot{\mathbf{z}} - \left(\frac{\partial \mathbf{h}}{\partial \dot{\mathbf{u}}}\right)^T \dot{\mathbf{z}} + \left(\frac{\partial \mathbf{h}}{\partial \mathbf{u}}\right)^T \mathbf{z} = \mathbf{J}\,. \tag{28}$$

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In real computations the solution of the dual problem (20,28) is determined numerically with the same integration scheme as the primal problem. E.g. the identity (21) is fulfilled only approximately. The right hand side of the dual problem **J** is chosen, e.g. as

$$\mathbf{J} = (\delta_1(t = t_m), ..., \delta_{neq}(t = t_m))^T \ . \tag{29}$$

neq is the number of degrees of freedom. Then the global error estimate of the time integration error for the proposed continuous Galerkin method (10) has the form,

$$\tilde{e}_g(cgp2) = |e_1(t = t_m) + ... + e_{neq}| \ . \tag{30}$$

In contrast to Maute [5], the Cauchy-Schwarz inequality and interpolation estimates for the dual problem are not applied, because then some interpolation constants would be needed, which are in generally unknown. However, from the a-priori estimates the order of error is known. This order coincides with the order of the a posteriori estimates, which is "proven" with numerical experiments, see section 5.

5 Examples

5.1 Single degree of freedom system

The simplest model in linear dynamics is a single degree of freedom, which is described with some given parameters and given initial conditions as:

$$0.25\ddot{u} + 0.9u = 0 \ , \ \forall t > 0 \ \text{with} \ u(t = 0) = 1.0 \ , \ \dot{u}(t = 0) = 0.0 \ . \tag{31}$$

Here, the error indicator ($\tilde{e}_g(newm)$) for Newmarks's method, the FD scheme, is compared with the error estimator ($\tilde{e}_g(cgp2)$)for the Petrov-Galerkin scheme, the FE method. The exact solution ($e_g(anal)$) is known for this simple problem, thus exact error and estimated errors for u can be easily computed, see table 1. In order to show the order for the estimated error $\tilde{e}_g(cgp2)$ and $\tilde{e}_g(newm)$, different time steps are chosen for the numerical solution, $\Delta t = 0.05/0.1/0.2$. The computation of the estimated error and the exact error is performed at time $t = 1$. The efficiency index $\eta = \frac{\tilde{e}_g}{e_g(anal)}$ is very close to 1.

Δt	$\tilde{e}_g(cgp2)$	$\tilde{e}_g(newm)$	e_g (anal)
0.05	1.3454e-3	1.3669e-3	1.3463e-3
0.1	5.3533e-3	5.5221e-3	5.3674e-3
0.2	2.0968e-2	2.2217e-2	2.1189e-2

Table 1: Comparison of estimated and exact displacement error for Newmark's scheme as a FD ($\tilde{e}_g(newm)$) and as a FE scheme ($\tilde{e}_g(cgp2)$)

It must be noted, that both estimated errors and exact error have the same global order $\mathcal{O}(\Delta t^2)$ of error. We also see, that the order reduction compared to the local error,

see Riccius [8], is two. This is caused by the algorithmic coupling of displacement error and velocity error and the transfer of the local errors to the global error, see Hairer et.al [4]. Also, the efficiency index $\eta = \frac{\tilde{e}_g}{e_g}$ is very close to 1.

5.2 TWO DEGREE of FREEDOM SYSTEM

Next, both error estimators are tested on the simplest multi degree of freedom system, the two degree of freedom system, see figure 5.2. The governing equations of motion are:
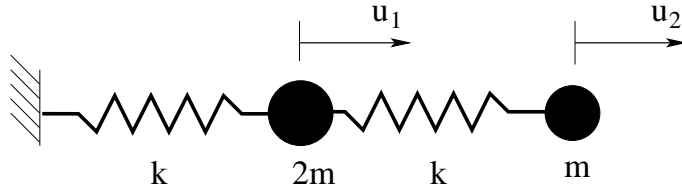

Figure 1: System of two degrees of freedom (2DOF)

$$\begin{bmatrix} 2m & 0 \\ 0 & m \end{bmatrix} \begin{bmatrix} \ddot{u}_1 \\ \ddot{u}_2 \end{bmatrix} + \begin{bmatrix} 2k & -k \\ -k & k \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \mathbf{0} \quad \text{for } t > 0\,,$$

with the initial conditions: $\begin{bmatrix} u_1 \\ u_2 \end{bmatrix}_{t=0} = \begin{bmatrix} u_1^0 \\ u_2^0 \end{bmatrix}$ and $\begin{bmatrix} \dot{u}_1 \\ \dot{u}_2 \end{bmatrix}_{t=0} = \begin{bmatrix} \dot{u}_1^0 \\ \dot{u}_2^0 \end{bmatrix}$ \hfill (32)

and the parameters: $m = 200$, $k = 100$,
$$u_1^0 = 0.5,\ u_2^0 = 1.0,\ \dot{u}_1^0 = 0.0,\ \dot{u}_2^0 = 0.0,\ \Delta t = 0.05\,.$$

In order to estimate the displacement error the corresponding initial conditions for the dual problem have to be chosen for the Galerkin scheme as:

$$\mathbf{z}(t = t_m) = \mathbf{0} \quad \text{and} \quad \dot{\mathbf{z}}(t = t_m) = -\mathbf{M}^{-1}\mathbf{1}\,.$$

The time step size for the dual solution is also chosen as $\Delta t = 0.05$.

Here the estimated displacement error $e_{g,h}$ consists of two components,

$$|e_g| = |e_{g,1} + e_{g,2}|\,. \hfill (33)$$

As numerical results the efficiency index of the error of the Petrov-Galerkin (FE) approach as well as both the exact and the error for the Newmark scheme (FD approach) based on the local error estimate are given. The efficiency index η for the Petrov-Galerkin scheme, see figure 2, is approximately 1 over the full time domain, thus it appears possible to use this as a reliable estimator in an adaptive time stepping scheme. Though representing the exact error a rather closely for a fairly long time with further growing time the estimated error $\tilde{e}_g(newm)$, based on the FD-idea, shows oscillations around the exact global error e_g. This is caused by the loss of some digits in the representation of numbers using numerical differentiation for the 3-rd derivative of u at time $t = t_m$ in equation (14).
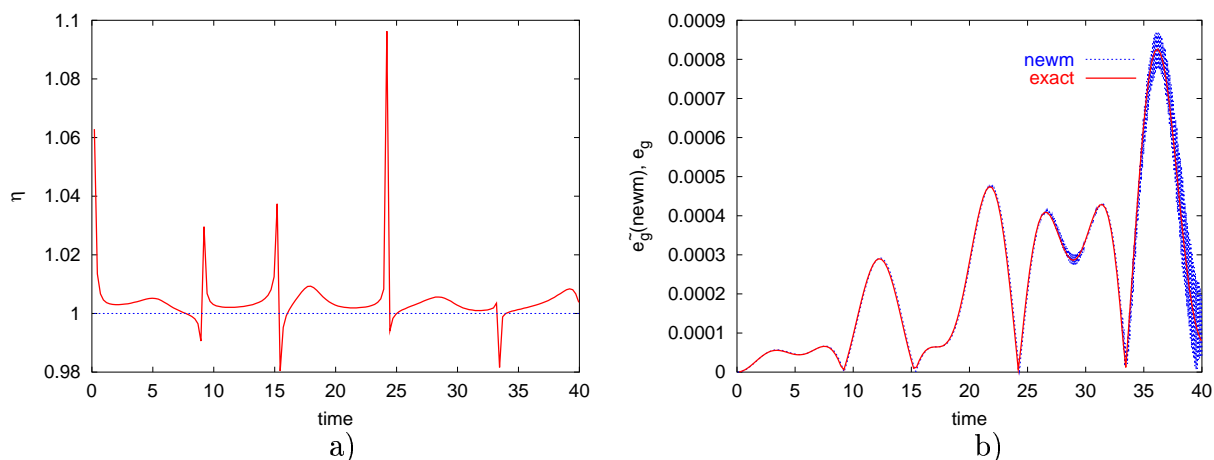
Figure 2: 2DOF-system, a) Efficiency index $\eta = \frac{\tilde{e}_g(cgp2)}{e_g}$ for Petrov-Galerkin (FE) scheme, b) Comparison of exact error and estimated error (FD) based on local error indicator (eqn.15)

5.3 Nonlinear Problems

Now, the Petrov-Galerkin method is applied to two nonlinear problems. First, the so-called spring pendulum is discussed, see figure 3. Due to 4 state variables, strong non-
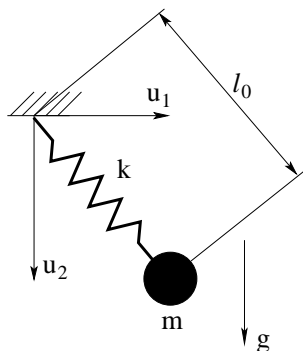

Figure 3: Nonlinear Spring pendulum with two degrees of freedom, $m = 1.4$, $k = 38.5$, $l_0 = 0.46$ (length of unstretched spring)

linearities and the requirement of conservation of energy deterministic chaos is possible. However, the focus of the following investigations is not on the kind of motion (chaos, quasi-periodicity, periodicity). Based on the Lagrangian equations the equation of motion

become,

$$
\begin{bmatrix}
m\ddot{u}_1 + ku_1 \dfrac{\sqrt{u_1^2 + u_2^2} - l_0}{\sqrt{u_1^2 + u_2^2}} = 0 \\[2ex]
m\ddot{u}_2 + ku_2 \dfrac{\sqrt{u_1^2 + u_2^2} - l_0}{\sqrt{u_1^2 + u_2^2}} = g
\end{bmatrix}
\quad \text{with} \quad
\begin{aligned}
u_1(t=0) &= u_1^0 \\
u_2(t=0) &= u_2^0 \\
\dot{u}_1(t=0) &= \dot{u}_1^0 \\
\dot{u}_2(t=0) &= \dot{u}_2^0
\end{aligned}
\quad \text{for } t > 0, \qquad (34)
$$

and in matrix representation,

$$
\mathbf{M\ddot{u}} + \mathbf{h(u)} = \mathbf{f}. \qquad (35)
$$

For this particular problem Mettler [6] showed with the regular, linear perturbation method, that the unperturbed solution $u_1^o = 0$, $u_2^o = U_2 \cos(\sqrt{k/m}t)$ becomes unstable for some special parameters g, k, m, l_0. Here the initial conditions are chosen as;

$$
u_1^0 = 1.0 \cdot 10^{-11}, \quad u_2^0 = 1.5, \quad \dot{u}_1^0 = \dot{u}_2^0 = 0.0. \qquad (36)
$$

The small horizontal perturbation u_1^0 is used to initiate the horizontal motion from the beginning. The time step for the numerical time integration is set to $\Delta t = 0.05$. A reference solution is computed with $\Delta t = 0.000625$ to determine the efficiency index η. The basic solution for the horizontal displacement and velocity is depicted in figure 4. It is obvious, that in regular time distances the horizontal motion of the spring pendulum is excited, which is identical to the unstable motion of the linear perturbed problem, see Mettler [6]. From the Poincare map for the horizontal motion we obtain, that with the prescribed initial conditions, eq. (36), the (numerical) solution has quasiperiodic behavior.

The displacement error e_g is estimated with the linearized dual problem from section 4. Despite Newmark's scheme is not applied to the spring pendulum, the formula for the local error indicator (eq. (15)) is used also in conjunction with the Petrov-Galerkin scheme. It is obvious, see figure 5b), that the local error becomes small, (in the limit zero) if the horizontal motion is excited. On the other hand, the global error is very large at these time points. Looking at the efficiency index, the estimator for the global error of the Petrov-Galerkin scheme, see figure 6, shows a mild overestimation up to the first horizontal excitation, $0 < \eta < 8$. Later, beyond $t > 150$, the exact error is overestimated dramatically. The reason is partially the linearized dual problem, e.g. the negligence of the nonlinear terms. By this we have to bear in mind, that the duality principle is only valid for linear operators. Secondly, the linearized dual problem is solved numerically. The time integration error of the dual problem itself plays an important rule too.

Finally we have to note, that numerical experiments with other initial conditions, $\mathcal{O}(u_1^0) \approx \mathcal{O}(u_2^0)$, thus a problem far from the perfect system [6], leads to considerably better results for the error estimation, e.g. w.r.t. the efficiency index η.
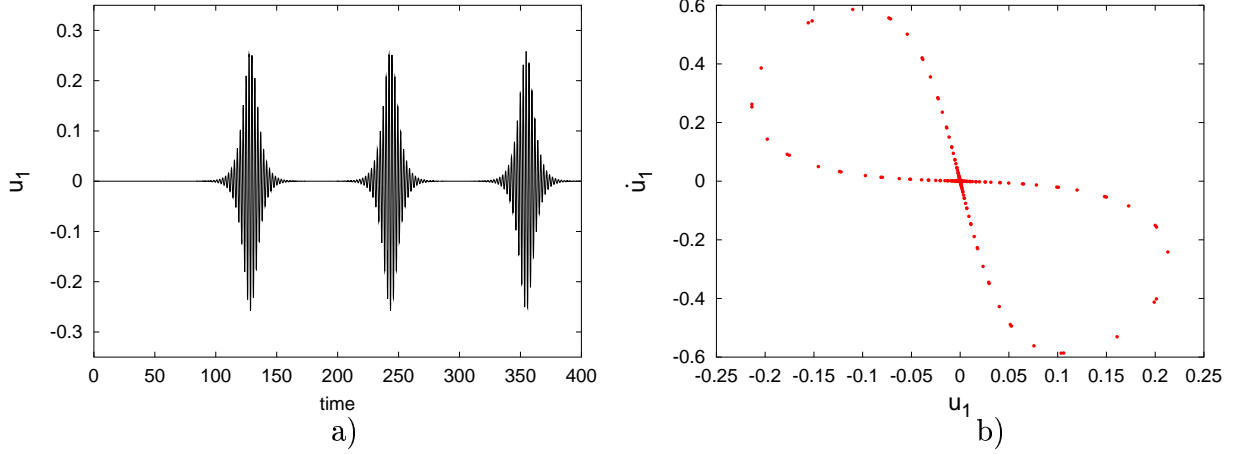
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Figure 4: Spring pendulum, a) horizontal displacement u_1 vs. time,   b) corresponding Poincare map
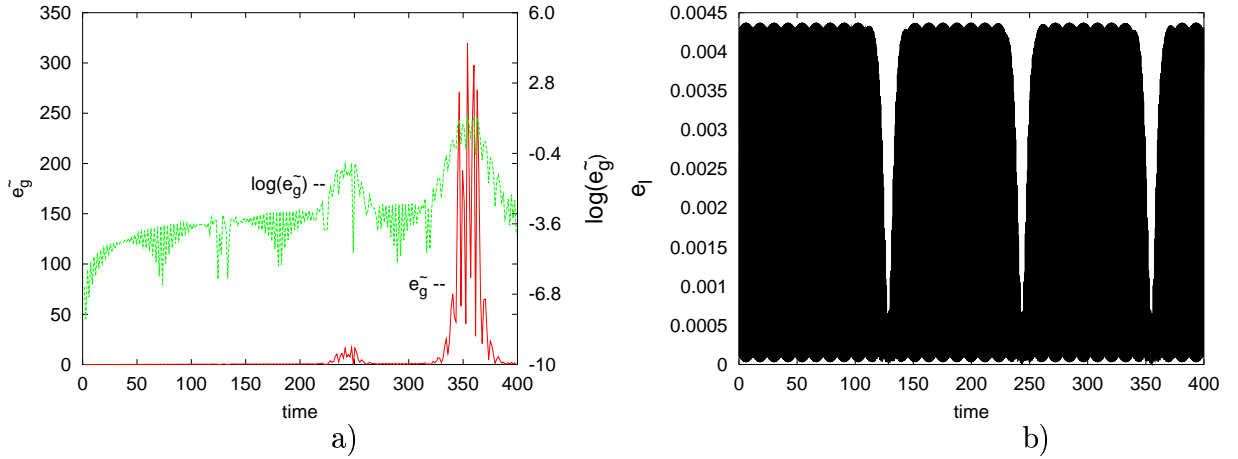

Figure 5: Spring pendulum, a) estimated global error $\tilde{e}_g(cgp2)$ - with standard and log-scale,   b) estimated local error e_l

The second nonlinear example is the so called two body problem, also a plane problem from rigid body dynamics in a gravitation field (γ), see figure 7. On the basis of the Lagrangian equations the equation of motion are obtained as;

$$\left[\begin{array}{l} m\ddot{u}_1 + \gamma\dfrac{u_1}{\left(u_1^2 + u_2^2\right)^{3/2}} = 0 \\[2ex] m\ddot{u}_2 + \gamma\dfrac{u_2}{\left(u_1^2 + u_2^2\right)^{3/2}} = 0 \end{array} \right] \text{ for } t > 0 \text{, with } \begin{array}{l} u_1(t=0) = 0.4 \\ u_2(t=0) = 0.0 \\ \dot{u}_1(t=0) = 0.0 \\ \dot{u}_2(t=0) = 2.0 \end{array} \tag{37}$$

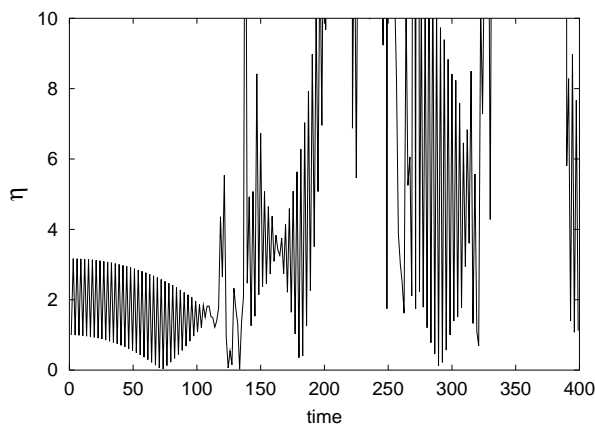This example with this particular initial conditions was extracted from a paper of Estep

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Figure 6: Spring pendulum, efficiency index η for the estimated error $\tilde{e}_g\,(cgp2)$
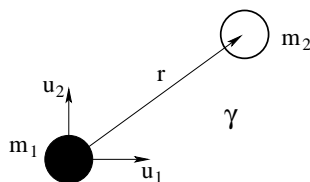

Figure 7: Two body problem, $\gamma = 1$, $|\mathbf{r}| = \sqrt{u_1^2 + u_2^2}$, $m = \dfrac{m_1\,m_2}{m_1 + m_2} = 1$

[3]. The exact analytic solution is known as:

$$u_1(t) \;=\; \cos(\tau) \,-\, 0.6\,, \quad u_2(t) \;=\; \sin(\tau)\,, \;\; \text{with:} \;\; t \;=\; \tau - 0.6\,\sin(\tau)\,.$$

Again the Petrov-Galerkin scheme is applied for the solution and the corresponding error estimation for the displacements is applied. The time step size is set to $\Delta t = 0.05$. From figure 8 the periodic character of the solution can be identified, there is only one point in the Poincare map. As before the local and global error based on eqn. (14) and (15) were also determined. For this fairly regularly behaving system the efficiency index η is rather close to 1 for the Petrov-Galerkin scheme, see figure 9b). Also the global error based on the FD scheme, see figure 10b), shows qualitatively almost the same behavior as the exact error.

6 Remarks concerning the velocity error estimation

Up to now the displacement error was analyzed. For the estimation of the velocity error $\dot{e}_g$ there are two possibilities. First, based on the estimation of the global displacement error e_g, the global velocity error $\dot{e}_g$ can be directly estimated via numerical differentiation,

$$\dot{e}_g \;=\; \frac{d\,e_g}{dt} \;\approx\; \dot{\tilde{e}}_g \;=\; \frac{-e_{t_{m-1}} + e_{t_{m+1}}}{2\Delta t}\,.$$
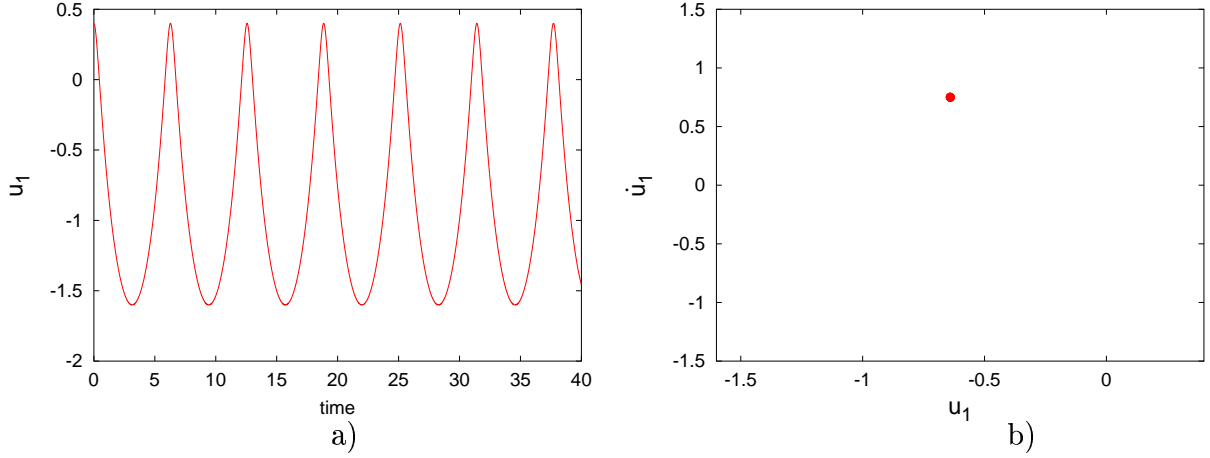
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Figure 8: Two body problem, a) Numerical solution u_1 vs. time,   b) corresponding Poincare map
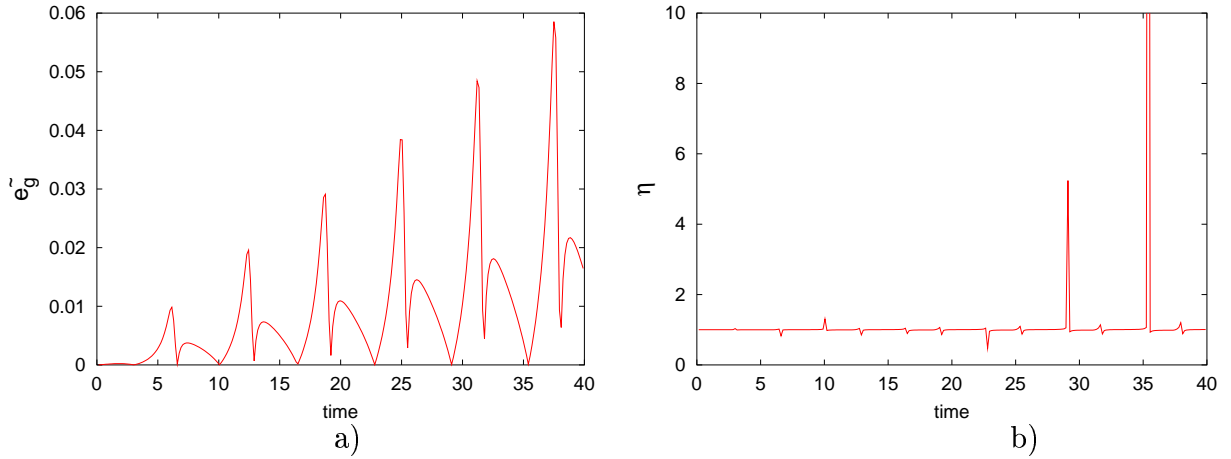

Figure 9: Two body problem, a) estimated global error $\tilde{e}_g(cgp2)$,   b) efficiency index η for Petrov-Galerkin scheme

The accuracy order of this difference quotient is two, so no order reduction compared to the displacement error estimate is expected. However, truncation and round-off errors in the numerical computation of the quotient some digits are often lost.

The second possibility to estimate the global velocity error $\dot{e}_g$ is similar to the procedure shown in section 4. In section 2 the primal problem was tested with $\mathbf{w}$ resp. $\mathbf{w}_h$. Now the primal problem is tested with $\dot{\mathbf{w}}$ resp. $\dot{\mathbf{w}}_h$. After some manipulations the corresponding error quantity, see eqn.(19) and eqn.(21) can be now formulated with $\dot{\mathbf{z}}$ and $\dot{\mathbf{e}}$,

$$\int_0^T \dot{\mathbf{e}} \cdot (\mathbf{M}\ddot{\mathbf{z}} - \mathbf{C}\dot{\mathbf{z}} + \mathbf{K}\mathbf{z})\, dt = \int_0^T \dot{\mathbf{z}} \cdot (\mathbf{M}\ddot{\mathbf{e}} + \mathbf{C}\dot{\mathbf{e}} + \mathbf{K}\mathbf{e})\, dt = \int_0^T \dot{\mathbf{e}} \cdot \mathbf{J}\, dt \,,$$
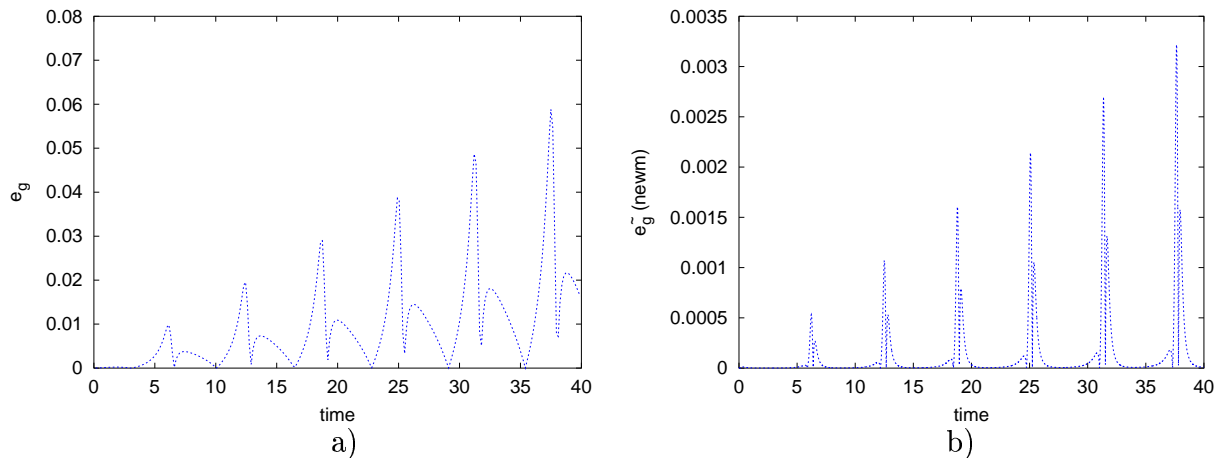
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Figure 10: Two body problem, a) exact global error e_g, b) estimated global error on FD basis $\tilde{e}_g(newm)$

$$\int\limits_0^T \dot{\mathbf{z}} \cdot \mathcal{D}\mathbf{e}dt \;=\; \int\limits_0^T \dot{\mathbf{z}} \cdot \mathbf{R}\, dt \;=\; \int\limits_0^T \dot{\mathbf{e}} \cdot \mathbf{J}\, dt \;=\; \dot{e}_g. \tag{38}$$

Thus it is possible to use the same dual problem for the error estimation of the global time integration error of the velocity as for the corresponding displacement error.

7 Conclusions

A Petrov Galerkin method was applied to linear and nonlinear equations of motions in structural dynamics. For a special test function $\mathbf{w}_h$ it can be shown [10], that this solution scheme is identical with Newmark' method for linear problems. This equivalence is lost in nonlinear dynamics.

Using the mentioned equivalence and the duality argument, a global estimator for displacement error e_g was derived.

Two different error estimators for the global time integration error were tested on some linear and nonlinear problems. The major criterion for the evaluation of the error estimator is the efficiency index η, which was computed on 4 examples. In linear examples η is approximately one, thus it is a very reliable tool. However for nonlinear problems the situation is different; e.g. the displacement error is overestimated dramatically for the spring pendulum. This is mainly caused by the linearization of the primal problem $\mathbf{h}(\mathbf{u})$ used also for the dual problem. Also the time integration error for the dual problem plays an important role as the time span is increasing. The global error indicator based on a Finite Difference scheme can be used only for linear problems. For such a class of problems this indicator is very efficient.

The disadvantage of the error estimator for the Petrov Galerkin is the large numerical effort necessary for the computation of the dual problem. For linear problems, primal and

dual problem can easily be transformed to an identical form, see Maute [5], thus the effort can be reduced somehow. This transformation, however, cannot be applied for nonlinear problems. Here, the full primal solution $\mathbf{u}_h$ has to be stored for the correct computation of the corresponding dual problem. In addition the numerical effort for the computation of dual problem has the same order as the effort for the primal problem, which makes such an error estimation rather questionable considering large nonlinear systems.

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