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On time integration error estimation and adaptive time stepping in structural dynamics

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In this paper we present two error estimators resp. indicators for the time integration in structural dynamics. Based on the equivalence between the standard Newmark scheme and a Galerkin formulation in time [1] for linear problems a global time integration error estimator based on duality [3] can also be derived for the Newmark scheme. This error estimator is compared to an error indicator based on a finite difference approach in time [2]. Finally an adaptive time stepping scheme using the global estimator and the local indicator is presented.

1 Introduction

The spatial discretization of the equation of motion in elastodynamics yields a system of coupled ordinary differential equations of the general form:

$$\mathbf{M}\ddot{\mathbf{u}} + \mathbf{h}(\mathbf{u}, \dot{\mathbf{u}}, t) = \mathbf{0}\,, \quad \forall t > 0\,, \tag{1}$$
$$\text{with initial conditions: } \mathbf{u}(t=0) = \mathbf{u_0} \quad \text{and } \dot{\mathbf{u}}(t=0) = \dot{\mathbf{u}}_0\,.$$

$\mathbf{M}$ is the (nth order) mass matrix, $\ddot{\mathbf{u}}$ is the vector of nodal accelerations. In the linear case $\mathbf{h}(\dot{\mathbf{u}}, \mathbf{u}, t)$ represents the external loading, the constant damping and the constant stiffness properties of the considered model:

$$\mathbf{M}\ddot{\mathbf{u}} + \mathbf{h}(\mathbf{u}, \dot{\mathbf{u}}, t) = \mathbf{M}\ddot{\mathbf{u}} + \mathbf{C}\dot{\mathbf{u}} + \mathbf{K}\mathbf{u} - \mathbf{F} = \mathbf{0} \tag{2}$$

The same type of equations also occurs in the kinetics of rigid bodies. In general a numerical time integration scheme is applied for the solution of (1). A very popular time integration scheme is the Newmark method which -in its original formulation - is based on a finite difference approach. For a special combination of the Newmark parameters the Newmark scheme is equivalent to a continuous Petrov-Galerkin formulation in time, see Wood [1].

2 Equivalence of the Newmark scheme and a Petrov-Galerkin formulation in time

The assumptions of the Newmark scheme concerning displacements and velocities in each time step are:

$$\dot{\mathbf{u}}_{\mathbf{n+1}} = \dot{\mathbf{u}}_{\mathbf{n}} + \Delta t(1-\gamma)\ddot{\mathbf{u}}_{\mathbf{n}} + \Delta t\gamma\ddot{\mathbf{u}}_{\mathbf{n+1}} \text{ and} \tag{3}$$
$$\mathbf{u}_{\mathbf{n+1}} = \mathbf{u}_{\mathbf{n}} + \Delta t\dot{\mathbf{u}}_{\mathbf{n}} + \Delta t^2(1-2\beta)\ddot{\mathbf{u}}_{\mathbf{n}}/2 + \Delta t^2\beta\ddot{\mathbf{u}}_{\mathbf{n+1}},$$

where $\mathbf{u_n}$, $\dot{\mathbf{u}}_{\mathbf{n}}$ and $\ddot{\mathbf{u}}_{\mathbf{n}}$ are the nodal displacement, velocity and acceleration vectors at time $t = n\Delta t$ and β and γ are the well known Newmark parameters. Here only the special case $2\beta = \gamma = 0.5$ which indicates constant accelerations in each time step is considered. There are many different formulations of the standard Newmark scheme, see [1], the most suitable for our considerations is the formulation as a single-step algorithm of the form:

$$\begin{pmatrix} \mathbf{u}_{\mathbf{n+1}} \\ \dot{\mathbf{u}}_{\mathbf{n+1}} \end{pmatrix} = \mathbf{A}_{FD} \begin{pmatrix} \mathbf{u}_{\mathbf{n}} \\ \dot{\mathbf{u}}_{\mathbf{n}} \end{pmatrix} + \mathbf{F}_{FD} \tag{4}$$

$\mathbf{A}_{FD}$ is the amplification matrix of the Finite Difference (FD) scheme which maps the state variables from the state t_n to t_{n+1}, $\mathbf{F}_{FD}$ is the corresponding forcing function. The equivalent Petrov-Galerkin formulation must result in the same equation as (4), i.e. the amplification matrix $\mathbf{A}_{FE}$ of the scheme, referred to as Finite Element (FE) formulation in time, should be identical. The Petrov-Galerkin approach for equation (2) reads, see [1]:

$$\int_0^T \mathbf{w} \cdot (\mathbf{M}\ddot{\mathbf{u}} + \mathbf{C}\dot{\mathbf{u}} + \mathbf{K}\mathbf{u} - \mathbf{F})\, dt = 0, \ \forall\, \mathbf{w} \in V \tag{5}$$

Dividing the time domain into N finite time intervals resp. time elements and using the ansatz function

$$\mathbf{u}_h = \mathbf{u}_n + (t - t_n)\dot{\mathbf{u}}_n + 1/2(t - t_n)^2\ddot{\mathbf{u}}_n, \ \forall t \in [t_n, t_{n+1}] \tag{6}$$

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for each time element leads to the discrete Galerkin formulation:

$$\sum_{n=0}^{n=N+1} \int_{t_n}^{t_{n+1}} \mathbf{w}_h \cdot (\mathbf{M}\ddot{\mathbf{u}}_h + \mathbf{C}\dot{\mathbf{u}}_h + \mathbf{K}\mathbf{u}_h - \mathbf{F}_h)\, dt = 0, \ \forall\, \mathbf{w}_h \in V_h \tag{7}$$

with the discrete test function $\mathbf{w}_h$. The Finite Element approach can also be transformed into the single-step form of eqn. (4). A separate task is to find the discrete test function $\mathbf{w}_h$ such that $\mathbf{A}_{FE} = \mathbf{A}_{FD}$. Comparing the amplification matrices one finds:

$$\mathbf{w}_h = \mathbf{W}_h[1/5 - (t - t_n)/\Delta t + (t - t_n)^2/\Delta t^2] \tag{8}$$

Hence the Newmark scheme with the Newmark parameters $2\beta = \gamma = 0.5$ can be treated as a Finite Element scheme in time. We will use this interpretation to derive an error estimator using well established techniques of finite element error estimation.

3 Error estimation

First an error estimator for the global time integration error, based on the Petrov-Galerkin method, is developed for linear differential equations. This results also in an error estimator for the Newmark scheme. The starting point of the derivation is the variational form (5) and the corresponding discrete form (7). Subtracting equations (5) and (7) yields the well known Galerkin orthogonality of the residual $\mathbf{R}$ which leads directly to the differential equation for the error $\mathbf{e} = \mathbf{u} - \mathbf{u}_h$:

$$\mathbf{M}\ddot{\mathbf{e}} + \mathbf{C}\dot{\mathbf{e}} + \mathbf{K}\mathbf{e} = \mathbf{F} - \mathbf{M}\ddot{\mathbf{u}}_h - \mathbf{C}\dot{\mathbf{u}}_h - \mathbf{K}\mathbf{u}_h = \mathbf{R} \tag{9}$$

Now the weak form of (9) is derived, using the solution $\mathbf{z}$ of the dual problem as test function. Bangerth [3] applied this technique to 1-st order differential equation, Maute [4] used the dual problem for the error estimation of 2-nd order differential equations. The weak form of (9) then reads:

$$\int_0^{t_m} \mathbf{z} \cdot \mathbf{R} dt = \int_0^{t_m} \mathbf{e} \cdot (\mathbf{M}\ddot{\mathbf{z}} - \mathbf{C}\dot{\mathbf{z}} + \mathbf{K}\mathbf{z}) dt - [\mathbf{e} \cdot \mathbf{M}\dot{\mathbf{z}}]_0^{t_m} + [\dot{\mathbf{e}} \cdot \mathbf{M}\mathbf{z}]_0^{t_m} + [\mathbf{e} \cdot \mathbf{C}\mathbf{z}]_0^{t_m} \tag{10}$$

The dual problem, also known as adjoint problem, follows from the primal problem (5) via partial integration, leading to a backward integration in time with initial conditions at $t = t_m$. Choosing $\mathbf{z}$ such that

$$\mathbf{M}\ddot{\mathbf{z}} - \mathbf{C}\dot{\mathbf{z}} + \mathbf{K}\mathbf{z} = \mathbf{0} \ \forall t \in [0, t_m] \ \text{ and } \ \mathbf{z}(t = t_m) = \mathbf{0} \tag{11}$$

and taking into account that $\mathbf{e}(t = 0) = \dot{\mathbf{e}}(t = 0) = \mathbf{0}$, equation (10) can be rewritten:

$$\int_0^{t_m} \mathbf{z} \cdot \mathbf{R} dt = -[\mathbf{e} \cdot \mathbf{M}\dot{\mathbf{z}}]^{t_m} \tag{12}$$

The initial conditions $\mathbf{z}(t = t_m)$ of the dual problem specify the error quantity to be computed. The required initial conditions for determining the Euclidean norm of the error $|\mathbf{e}| = \sqrt{\mathbf{e} \cdot \mathbf{e}}$ are:

$$\dot{\mathbf{z}}(t_m) = -\mathbf{M}^{-1}\mathbf{e}/|\mathbf{e}| \implies \int_0^{t_m} \mathbf{z} \cdot \mathbf{R} dt = \mathbf{e} \cdot \mathbf{e}/|\mathbf{e}| = |\mathbf{e}| \tag{13}$$

That means that the error $\mathbf{e}$ must be known a-priori. To overcome this obstacle the error representation (12) can for example be limited to one particular degree of freedom d. Then the required initial condition can be simplified:

$$\dot{\mathbf{z}}(t_m) = -\mathbf{M}^{-1}\mathbf{1} \implies \int_0^{t_m} \mathbf{z} \cdot \mathbf{R} dt = \mathbf{e} \cdot \mathbf{M}\mathbf{M}^{-1}\mathbf{1} = e_d = u_d - u_{d,h} \tag{14}$$

with $\mathbf{1}$ being a unity vector with $\mathbf{1}(i) = 1$ for $i = d$ and $\mathbf{1}(i) = 0$ for $i \neq d$. In (14) u_d is the exact displacement, whereas $u_{d,h}$ is the value determined with the time integration scheme.
In contrast to [4] we do not use Cauchy-Schwarz inequality but solve (12) directly. In general the solution of the dual problem is determined using the same time integration scheme as for the primal problem. Hence eqn. (12) is solved only approximately. Numerical tests have shown that the initial conditions of the dual problem for the estimation of the Euclidean norm $|\mathbf{e}|$ can also be determined approximately using the local error indicator for the Newmark scheme presented by Riccius [2] since in (13) only the correct spatial distribution of the error has to be known.

The error indicator for the global time integration error proposed by Riccius is based on a local error indicator $\tilde{\mathbf{e}}_l(t_m)$ for the displacements in the time interval $t \in [t_{m-1}, t_m]$:

$$\tilde{\mathbf{e}}_l(t_m) = \Delta t^3(1/6 - \beta)\dddot{\tilde{\mathbf{u}}}_m = \Delta t^2(1/6 - \beta)(\ddot{\mathbf{u}}_{m-1} - \ddot{\mathbf{u}}_m) \tag{15}$$

Obviously eqn. (15) is only reasonable for the choice $\beta \neq 1/6$. Assuming that the local error $\tilde{\mathbf{e}}_l(t_m)$ is constant in all $t_m/\Delta t$ time intervals, a global error indicator $\tilde{\mathbf{e}}_g$ - called here the global FD based indicator - can be computed in a very simple fashion:

$$\tilde{\mathbf{e}}_g(t_m) = (t_m/\Delta t)\, \tilde{\mathbf{e}}_l(t_m) \tag{16}$$

3.1 Numerical examples

Now the error estimation will be tested on two rather simple numerical examples. The first is the simplest linear multiple

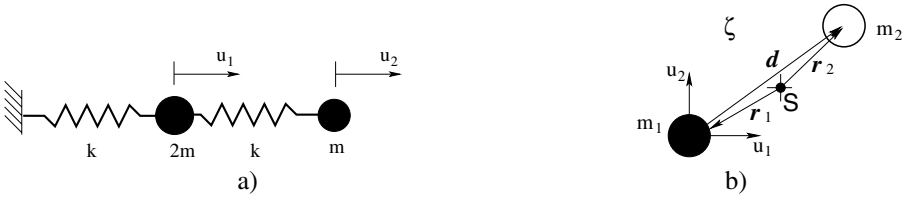

Fig. 1 Numerical examples: a) linear two degree of freedom system b) Two body problem

degree of freedom system, the 2 dof system, see fig. 1 a). The governing equations of motion are:

$$\begin{bmatrix} 2m & 0 \\ 0 & m \end{bmatrix} \begin{bmatrix} \ddot{u}_1 \\ \ddot{u}_2 \end{bmatrix} + \begin{bmatrix} 2k & -k \\ -k & k \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \mathbf{0} \text{ with } m = 200, k = 100 \tag{17}$$

$$\text{and initial conditions: } \mathbf{u_0}^T = [0.5, 1.0]^T \text{ and } \dot{\mathbf{u}}_\mathbf{0}^T = [0, 0]^T$$

Eqn. (17) is solved using the Newmark scheme with $2\beta = \gamma = 0.5$ and the constant time step size $\Delta t = 0.05$. The aim is the estimation of the Euclidean norm $|\mathbf{e}|$ of the global error. The required initial conditions of the dual problem are determined using the local error estimator $\tilde{\mathbf{e}}_l$ in the last time step:

$$\dot{\mathbf{z}}(t_m) = -\mathbf{M}^{-1}/\tilde{\mathbf{e}}_l(t_m)/|\tilde{\mathbf{e}}_l(t_m)| \tag{18}$$

Fig. 2 shows the effectivity indices $\eta = |\mathbf{e}_{est}|/|\mathbf{e}_{ex}|$ of the two global error estimators/indicators, which in both cases is close to one. Thus both estimations yield suitable results and the estimation (18) of the initial conditions of the dual problem seems to be feasible.

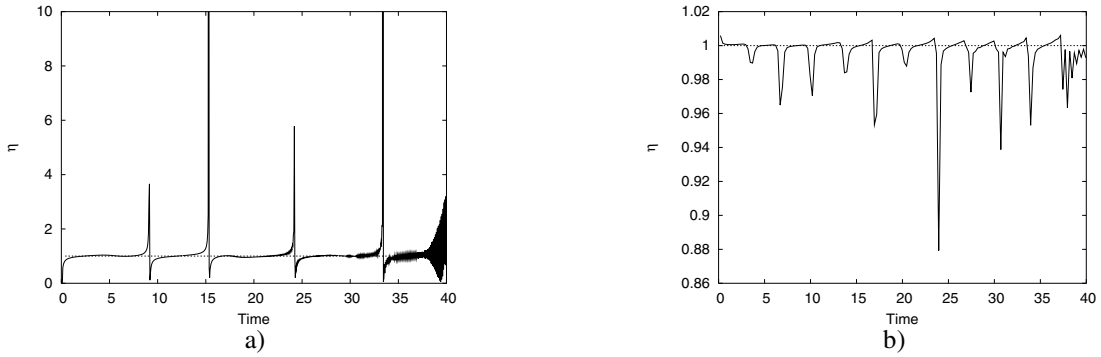

Fig. 2 Effectivity indices for the estimation of $|\mathbf{e}|$ for the 2 dof system a) Error indicator based on FD b) Error estimator based on FE

Though the duality principle in the strict sense is only valid for linear differential equations, we will now test the dual error estimator on a nonlinear problem. For nonlinear differential equations the standard Newmark scheme and the shown Galerkin method can not be matched, so a continuous Galerkin approximation based on equations (6) and (8) is applied for the solution of the nonlinear equation of motion (1). In order to adopt the duality principle eqn. (1) has to be linearized. Multiplication with the dual solution $\mathbf{z}$ and integration by parts yields the linearized dual problem

$$\mathbf{M}\ddot{\mathbf{z}} - \mathbf{C}(\dot{\mathbf{u}}, \mathbf{u})\dot{\mathbf{z}} + \mathbf{K}(\dot{\mathbf{u}}, \mathbf{u})\mathbf{z} = \mathbf{0}, \tag{19}$$

i.e. the dual problem depends on the solution of the primal problem. Hence $\mathbf{z}$ can not be computed independently as in the linear case. This results in a much higher effort for the error estimation. As nonlinear example we choose a problem of celestial mechanics, the two body problem see fig.1 b), for which the exact solution can be given explicitely, see Estep [5] . The two body problem consist of two mass points m_1 and m_2 in a gravitation field ζ. The equation of motion for the relative displacements u_1 and u_2 reads:

$$\begin{bmatrix} m\ddot{u}_1 + \zeta\frac{u_1}{(u_1^2+u_2^2)^{3/2}} = 0 \\ m\ddot{u}_2 + \zeta\frac{u_2}{(u_1^2+u_2^2)^{3/2}} = 0 \end{bmatrix} \text{ with initial conditions: } \mathbf{u_0}^T = [0.4, 0]^T \text{ and } \dot{\mathbf{u}}_\mathbf{0}^T = [0, 2]^T \tag{20}$$

For $\zeta = 1$ and $m = 1.0$ the exact solution of (20) is:

$$u_1(t) = \cos(\tau) - 0.6 \text{ and } u_2(t) = 0.8\sin(\tau) \text{ with } t = \tau - \sin(\tau) \tag{21}$$

The initial conditions of the dual problem are determined according to eqn. (14) since the global time integration errors at both degrees of freedom shall be estimated separately. The time step size is $\Delta t = 0.005$. The error estimation yields efficiency indices close to one, see Fig. (3), but the high effort and computing time for the analysis of the dual problem makes the practical application of the error estimator on larger nonlinear problems questionable.

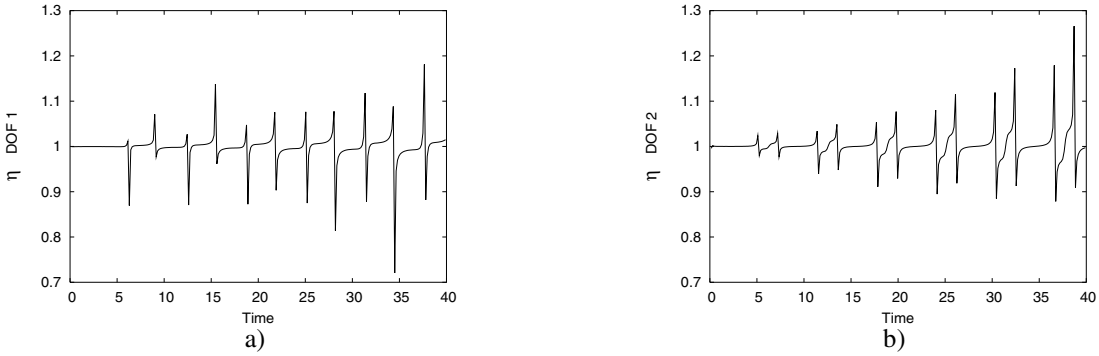

Fig. 3 Effectivity indices for global time integration error estimation of the two body problem a) DOF 1 b) DOF 2

4 Adaptive time stepping

The afore mentioned error estimators resp. indicators for the global and local time integration error can be used as the basis of an adaptive time stepping scheme. The aim is a computation with adaptively determined time step sizes, such that the global time integration error within the time interval $[0, T]$ does not exceed a prescribed limit. For this purpose it is suitable to adapt the time step size using a combination of local and global time integration error estimation. For the proposed adaptive algorithm three bounds have to be prescribed:

1. The upper bound for the global time integration error $gtol$. For example $gtol$ can be chosen proportional to the maximum displacement of the solution (e.q. based an a first coarse analysis): $gtol = c_g d_{i,max}$ with $c_g > 0$.
2. The upper bound for the local time integration error $ltol_{up}$. For example : $ltol_{up} = gtol/c_{up}$ with $c_{up} \gg 1$.
3. The lower bound for the local time integration error $ltol_{lo}$. For example: $ltol_{lo} = ltol_{up}/c_{lo}$ with $c_{lo} = 2..10$.

The local time step control is based on the relationship between the local error e_l and the time step size Δt which for the standard Newmark scheme and the corresponding continuous Galerkin method reads:

$$e_l \propto \Delta t^s \text{ with } s = 3 \tag{22}$$

In every time step the local error e_l is estimated. If the estimated local error exceeds $ltol_{up}$ or falls below $ltol_{lo}$ the time step size is adapted locally based on eqn. (22):

$$\text{if } e_l < ltol_{lo} \text{ then } \Delta t_{new} = \Delta t_{old} \cdot \left(\frac{ltol_{lo}}{e_l}\right)^{1/s} \text{ or if } e_l > ltol_{up} \text{ then } \Delta t_{new} = \Delta t_{old} \cdot \left(\frac{ltol_{up}}{e_l}\right)^{1/s} \tag{23}$$

If the largest global time integration error $e_{g,max} = \max_{t_m \in [0,t_n]} e_g(t_m)$ up to the current time step exceeds the limit value $gtol$ the computation is started again at time $t = 0$ with new values for $ltol_{lo}$ and $ltol_{up}$. Taking into account that $e_g \propto \Delta t^{(s-1)}$ one can determine the new values $ltol_{up,new}$ and $ltol_{lo,new}$ for the next iteration step:

$$ltol_{up,new} = ltol_{up,old} \cdot \left(\frac{gtol}{e_{g,max}}\right)^{s/(s-1)} \text{ and } ltol_{lo,new} = ltol_{lo,old} \cdot \left(\frac{gtol}{e_{g,max}}\right)^{s/(s-1)} \tag{24}$$

This proposed procedure yields a recurrence scheme that is terminated when $e_{g,max} = \max_{t_m \in [0,T]} e_g(t_m) \leq gtol$.

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