Estimation of the time integration error in structural dynamics
A comparison of two strategies

Karl Schweizerhof, Jens Neumann
Institut für Mechanik
Universität Karlsruhe

- Motivation
- General problem
- Newmark's method as
  - Finite Difference method
  - Finite Element formulation
- Estimation of global time integration error – displacements
- Examples – linear and non-linear dynamics
- Time step adaptation
  - A strategy for practical problems
  - Numerical examples
- Conclusions

Motivation

Goal: - strategy for time step adaptation using time stepping schemes in structural dynamics
- rigid body dynamics (no effect of spatial discretization)
- flexible bodies, FE discretized structures

- local + global error estimation needed

- error estimator should work for linear and nonlinear problems
$\rightarrow$ numerical tests

- time step adaptation,
how to use error estimation efficiently

General Problem

System of **O**rdinary **D**ifferential **E**quations in structural dynamics:

here rigid body dynamics: $\boldsymbol{M}\ddot{\boldsymbol{u}} + \boldsymbol{h}(\boldsymbol{u}, \dot{\boldsymbol{u}}, t) = \boldsymbol{0}\,, \forall t > 0\,,$ (1)

$\boldsymbol{u} \in \mathbb{R}^n\,, \boldsymbol{M}$ ... positive definite

initial conditions: $\boldsymbol{u}(t=0) = \boldsymbol{u}_0$ and $\dot{\boldsymbol{u}}(t=0) = \dot{\boldsymbol{u}}_0$

uniqueness of solution of equation (1)

$\boldsymbol{h}(\boldsymbol{u}, \dot{\boldsymbol{u}}, t)$ must satisfy [e.g. Burlisch/Stör]:

$$\|\boldsymbol{h}(\boldsymbol{u}_1, \dot{\boldsymbol{u}}_1, t) - \boldsymbol{h}(\boldsymbol{u}_2, \dot{\boldsymbol{u}}_2, t)\| \leq \mathcal{L}\|\boldsymbol{u}_1 - \boldsymbol{u}_2\|\,, \quad \text{with: } \mathcal{L} > 0,$$

$\boldsymbol{h}$ ... continuous, finite

or using mean value theorem:

$$\boldsymbol{K} = \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{u}} \text{ ...continuous, finite,} \quad \boldsymbol{K} \text{ ...Jacobian of } \boldsymbol{h}$$

General:
- Modal decomposition → numerically high effort required for linear coupled ODE-systems
- analytical solution for nonlinear ODE's unknown → Numerical time integration

Semidiscretized equations for structural dynamics (linear case):

$$\boldsymbol{M}\ddot{\boldsymbol{u}} + \boldsymbol{C}\dot{\boldsymbol{u}} + \boldsymbol{K}\boldsymbol{u} = \boldsymbol{0}\,, \forall t > 0\,, \quad \boldsymbol{u} \in \mathbb{R}^n\,, \tag{2}$$

initial conditions: $\boldsymbol{u}(t=0) = \boldsymbol{u}_0$, $\dot{\boldsymbol{u}}(t=0) = \dot{\boldsymbol{u}}_0$

Newmark's method derived from Finite Differences

(FD-Newm)

Numerical solution of (2) with Finite Differences
$\rightarrow$ split time domain $[0, T]$ into finite number N
of time intervals $\Delta t_n = t_{n+1} - t_n$, $n = 1...N$

Equilibrium at state t_{n+1}:

$$\boldsymbol{M}\ddot{\boldsymbol{u}}_{n+1} + \boldsymbol{C}\dot{\boldsymbol{u}}_{n+1} + \boldsymbol{K}\boldsymbol{u}_{n+1} = \boldsymbol{0}\,,$$

Newmark's scheme - derived from FD - with $\Delta t_n = \Delta t$:

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

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

Parameters: $\gamma = 1/2$, controls accuracy – $\mathcal{O}(\Delta t^2)$,
$\beta = 1/4$, A-stable, not L-stable

A-stable general numerical stability of algorithm
L-stable $\approx$ damping of 'fast transient' in stiff problems

Newmark's method as Finite Element formulation

(CG2-Newm)

CG2 – continuous Galerkin formulation with quadratic interpolation for eqn. (1)

- Divide time domain $[0, T]$ into N time intervals $\Delta t_n = t_{n+1} - t_n$:

$$\sum_{n=0}^{N} \int_{t_n}^{t_{n+1}} \boldsymbol{w} \cdot (\boldsymbol{M}\ddot{\boldsymbol{u}} + \boldsymbol{C}\dot{\boldsymbol{u}} + \boldsymbol{K}\boldsymbol{u}) dt = 0 \,, \quad \forall \boldsymbol{w} \in V$$

V ... function space with inner product,

discrete variational formulation: $V \to V_h$ (finite)

- Wood [1990]: Equivalent CG2-formulation for Newmark's method with $\gamma = 2\beta$

Interpolation function:

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

Special weighting function $\boldsymbol{w}_h$ (for equivalence):

$$\boldsymbol{w}_h = \boldsymbol{W}_h \left[1/5 - (t - t_n)/\Delta t + (t - t_n)^2/\Delta t^2 \right] \quad \forall t \in [t_n, t_{n+1}]$$

$$\sum_{n=0}^{N} \int_{t_n}^{t_{n+1}} \boldsymbol{w}_h \cdot (\boldsymbol{M}\ddot{\boldsymbol{u}}_h + \boldsymbol{C}\dot{\boldsymbol{u}}_h + \boldsymbol{K}\boldsymbol{u}_h) dt = 0 \,, \quad \forall \boldsymbol{w}_h \in V_h.$$

.... as
Finite Element formulation

(CG2-Newm)

$$\left(4\boldsymbol{M} + 2\Delta t_n \boldsymbol{C} + \Delta t_n^2 \boldsymbol{K}\right)\ \ddot{\boldsymbol{u}}_n = -2\left(\Delta t_n \boldsymbol{K}\dot{\boldsymbol{u}}_n + 2\boldsymbol{C}\dot{\boldsymbol{u}}_n + 2\boldsymbol{K}\boldsymbol{u}_n\right)$$

$\rightarrow$ Equivalence between schemes - Comparison of Amplification matrix:

$$\begin{pmatrix} \boldsymbol{u}_{n+1} \\ \dot{\boldsymbol{u}}_{n+1} \end{pmatrix} = \boldsymbol{A}_{FD-newm} \begin{pmatrix} \boldsymbol{u}_n \\ \dot{\boldsymbol{u}}_n \end{pmatrix} = \boldsymbol{A}_{CG2-newm} \begin{pmatrix} \boldsymbol{u}_n \\ \dot{\boldsymbol{u}}_n \end{pmatrix}$$

$\rightarrow$ in general only valid for linear ODE's,
$\rightarrow$ techniques for error estimation for Finite Element method can be used

Advantage: no computation of 'initial' acceleration for $\ddot{\boldsymbol{u}}_0$ necessary as with Finite Difference scheme: $\ddot{\boldsymbol{u}}_0 = \boldsymbol{M}^{-1}\left(-\boldsymbol{C}\dot{\boldsymbol{u}}_0 - \boldsymbol{K}\boldsymbol{u}_0\right)$

Global and local time integration error

Global error: Error at time t_n ,

$$e_g(t = t_m) = e(t = t_m) \; = \; u(t = t_m) \; - \; u_m$$

Local Error: Error in time step Δt_n,

$$e_l(\Delta t_n) \; = \; u(t = t_m) \; - \; u_m$$

with: $u(t = t_{m-1}) \; - \; u_{m-1} \; = \; 0$

u_m in general different for both methods ($\gamma \neq 2\beta$)

Error indicator for global time integration error based on Finite Difference scheme and local error indicator

Local error indicator for displacements [Riccius 1998] for $t \in [t_{m-1}, t_m]$:

$$e_l(t_m) \; = \; \Delta t_m^3 \left(\tfrac{1}{6} - \beta\right) \dddot{u}_m \; \approx \; \Delta t_m^2 \left(\tfrac{1}{6} - \beta\right) \left(\ddot{u}_{m-1} - \ddot{u}_m\right)$$

$\rightarrow$ based on difference between Taylor expansion and Newmark solution

Assumption: $e_l(t_m)$ constant in $t_m / \Delta t_m$ time intervals

Use for global error indicator (FD-based error indicator):

$$e_{gh}(FD - newm) \; = \; \frac{t_m}{\Delta t_m} \, e_l(t_m)$$

$\equiv$ Multiple of local error $e_l(\Delta t_m)$ in last time step

Error estimator for CG2-newm method

Def.: $e_g(t = t_m) = u(t = t_m) - u_m$

Basis: Finite Element formulation of ODE:

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

Variational form of ODE:

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

→ Galerkin orthogonality of residual

$$\int_0^T \boldsymbol{w}_h \cdot \mathcal{D}\boldsymbol{e}\, dt = 0\,,$$

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

Idea: Use adjoint ODE to equation (2), Bangerth[1997], Maute[2001]

$$\mathcal{D}^*\boldsymbol{z} = \boldsymbol{M}\ddot{\boldsymbol{z}} - \boldsymbol{C}\dot{\boldsymbol{z}} + \boldsymbol{K}\boldsymbol{z} = \boldsymbol{J}\,, \forall t < t_m \qquad \text{(Backward analysis)}$$

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

$\boldsymbol{J}$ ... functional, specified later (used to select error quantity)

J. Neumann, K. Schweizerhof
Mechanik, Universität Karlsruhe

use $\boldsymbol{e}$ as test function for adjoint ODE:

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

by partial integration:

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

$\widehat{=}$ using $\boldsymbol{z}$ as test function for $\mathcal{D}\boldsymbol{e} = \boldsymbol{R}$:

$$\int_0^T \boldsymbol{z}\cdot\mathcal{D}\boldsymbol{e}\,dt = \int_0^T \boldsymbol{z}\,\boldsymbol{R}\,dt = \int_0^T \boldsymbol{e}\,\boldsymbol{J}\,dt$$

$\rightarrow$ analogy to Betti's Principle from structural mechanics – here in time

Choice for $\boldsymbol{J}$:

$\boldsymbol{J}$ ... Dirac-Distribution – select quantity of interest for error:

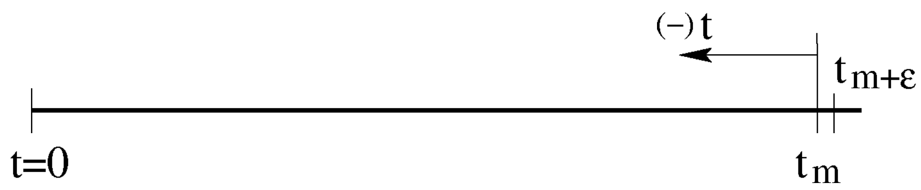
$$\boldsymbol{J} = \delta(t = t_m)\frac{\boldsymbol{e}(t = t_m)}{|\boldsymbol{e}(t = t_m)|} \rightarrow \int_0^T \boldsymbol{e}\cdot\boldsymbol{J}\,dt = |\boldsymbol{e}(t = t_m)| = e_g(t = t_m)$$

Corresponding initial conditions of adjoint ODE using linear momentum:

$$\boldsymbol{M}\dot{\boldsymbol{z}}(t_m + \epsilon) - \boldsymbol{M}\dot{\boldsymbol{z}}(t_m) = \int_{t_m}^{t_m+\epsilon} \boldsymbol{J}\,dt = \frac{\boldsymbol{e}(t = t_m)}{|\boldsymbol{e}(t = t_m)|},$$

Approximation for $\boldsymbol{e}$: $\boldsymbol{e}(t = t_m) \approx \boldsymbol{e}_l(t = t_m)$, (from numerical tests) ,

$$\boldsymbol{z}(t_m) = \boldsymbol{0}, \quad \dot{\boldsymbol{z}}(t_m + \epsilon) = \boldsymbol{0}, \quad \rightarrow \quad \dot{\boldsymbol{z}}(t_m) = -\boldsymbol{M}^{-1}\frac{\boldsymbol{e}_l(t_m)}{|\boldsymbol{e}_l(t_m)|}.$$



$\rightarrow$ all quantities in $\boldsymbol{z}$ selected ,

Alternative: one single dof with linear momentum

... global Error estimator CG2-newm (contd.)

Numerical effort:

a) same numerical effort required for computation of $\boldsymbol{z}_h$
as for computation of $\boldsymbol{u}_h$ in linear case

$\rightarrow$ numerical solution of adjoint ODE,
e.g. with same FE method

b) Computation of estimated error for $e_g(t = t_m)$: $$e_{gh} = \int_0^{t_m} \boldsymbol{R}\,\boldsymbol{z}_h\,dt$$

Requires:
- storage of $\boldsymbol{u}_h$, $\dot{\boldsymbol{u}}_h$ $\ddot{\boldsymbol{u}}_h$ at each time step,
- evaluation of $\boldsymbol{R}(\boldsymbol{u}_h, \dot{\boldsymbol{u}}_h, \ddot{\boldsymbol{u}}_h)$ and $\boldsymbol{z}_h$ at integration points, e.g. 3 Gauß points

... global Error estimator CG2-newm (contd.)

Same estimator for nonlinear problems?

Nonlinear ODE:

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

e.g. solution with CG2-method and Newton-Raphson scheme

→ linearization in each time step – iterative solution

→ Forward nonlinear analysis

Problem: duality principle only valid for linear operators:

$$\int_0^T \boldsymbol{z} \cdot \mathcal{D}\boldsymbol{e}\, dt = \int_0^T \boldsymbol{e} \cdot \mathcal{D}^*\boldsymbol{z}\, dt$$

For $\mathcal{D}^*\boldsymbol{z}$ linearized differential operator of primal equation used
→ total differential:

$$d\boldsymbol{h} = \frac{\partial \boldsymbol{h}}{\partial \dot{\boldsymbol{u}}} d\dot{\boldsymbol{u}} + \frac{\partial \boldsymbol{h}}{\partial \boldsymbol{u}} d\boldsymbol{u} = \boldsymbol{C}(\dot{\boldsymbol{u}}, \boldsymbol{u}) d\dot{\boldsymbol{u}} + \boldsymbol{K}(\dot{\boldsymbol{u}}, \boldsymbol{u}) d\boldsymbol{u}$$

Corresponding linearized adjoint ODE:

$$\boldsymbol{M}\ddot{\boldsymbol{z}} - \left(\frac{\partial \boldsymbol{h}}{\partial \dot{\boldsymbol{u}}}\right)^T \dot{\boldsymbol{z}} + \left(\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{u}}\right)^T \boldsymbol{z} = \boldsymbol{J}$$

Thus: backward linear analysis with operators linearized at current time of primal solution

... global Error estimator CG2-newm (contd.)

Algorithm to compute $e_{gh}(CG2-newm)$ at t_m for nonl. problems:

i) compute numerical solution $\boldsymbol{u}_h$ at discrete time states $t_0, ..., t_m$
$\rightarrow \boldsymbol{u}_h, \dot{\boldsymbol{u}}_h, \ddot{\boldsymbol{u}}_h$

ii) compute $\boldsymbol{z}_h$ with linearized adjoint ODE
with $\boldsymbol{K} = \boldsymbol{K}(t)$ and $\boldsymbol{C} = \boldsymbol{C}(t)$

iii) compute time integral $\int_0^{t_m} \boldsymbol{R} \cdot \boldsymbol{z}_h \, dt$,
- $\boldsymbol{z}_h$ with quadratic interpolation
- Gauß integration with e.g. 4 points due to nonlinearity

Numerical Examples

→ investigation of error estimators and indicators

Single degree of freedom: linear problem

$0.25\ddot{u} + 0.9u = 0$, $\forall t > 0$ with initial conditions: $u_0 = 1.0$, $\dot{u}_0 = 0.0$

- Numerical integration using CG2,
- Variation of $\Delta t = 0.05/0.1/0.2$

→ Global time integration error- e_g at $t_m = 1.0$:

Δt	$e_{gh}(CG2 - newm)$	$e_{gh}(FD - newm)$	e_g (exact)	$e_l(t = 1.0)$
0.05	1.3454e-3	1.3669e-3	1.3463e-3	6.834e-5
0.1	5.3533e-3	5.5221e-3	5.3674e-3	5.552e-4
0.2	2.0968e-2	2.2217e-2	2.1189e-2	4.443e-3

Results: - efficiency index $\eta = \frac{e_{gh}}{e_g(exact)} \approx 1$,

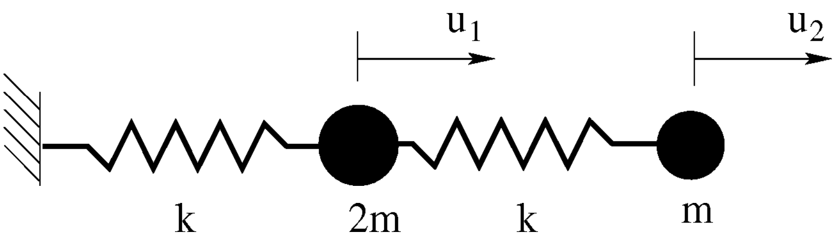
- order of local error: $e_l = C_l \Delta t^3$,

- order of global error: $e_g(t = t_m) = C_g \Delta t^2$

Reason: order reduction due to transport of local error

Hairer, Norsett, Wanner [1991]: min. order reduction $\mathcal{O}(\Delta t)$

Two degree of freedom system: linear problem



$$\begin{bmatrix} 400 & 0 \\ 0 & 200 \end{bmatrix} \begin{bmatrix} \ddot{u}_1 \\ \ddot{u}_2 \end{bmatrix} + \begin{bmatrix} 200 & -100 \\ -100 & 100 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} = \mathbf{0} \quad \text{for } t > 0\,,$$

with: $\boldsymbol{M}\ddot{\boldsymbol{u}} + \boldsymbol{K}\boldsymbol{u} = \mathbf{0}$

Initial conditions: $\begin{bmatrix} u_1^0 \\ u_2^0 \end{bmatrix} = \begin{bmatrix} 0.5 \\ 1.0 \end{bmatrix}$ and $\begin{bmatrix} \dot{u}_1^0 \\ \dot{u}_2^0 \end{bmatrix} = \begin{bmatrix} 0.0 \\ 0.0 \end{bmatrix}$

- Numerical integration - Newmark, Time step size: $\Delta t = 0.05$

Goal: • global displacement error:

$$e_g(t = t_m) = \left[(u_1 - u_{h,1})^2_{t=t_m} + (u_2 - u_{h,2})^2_{t=t_m} \right]^{1/2}$$

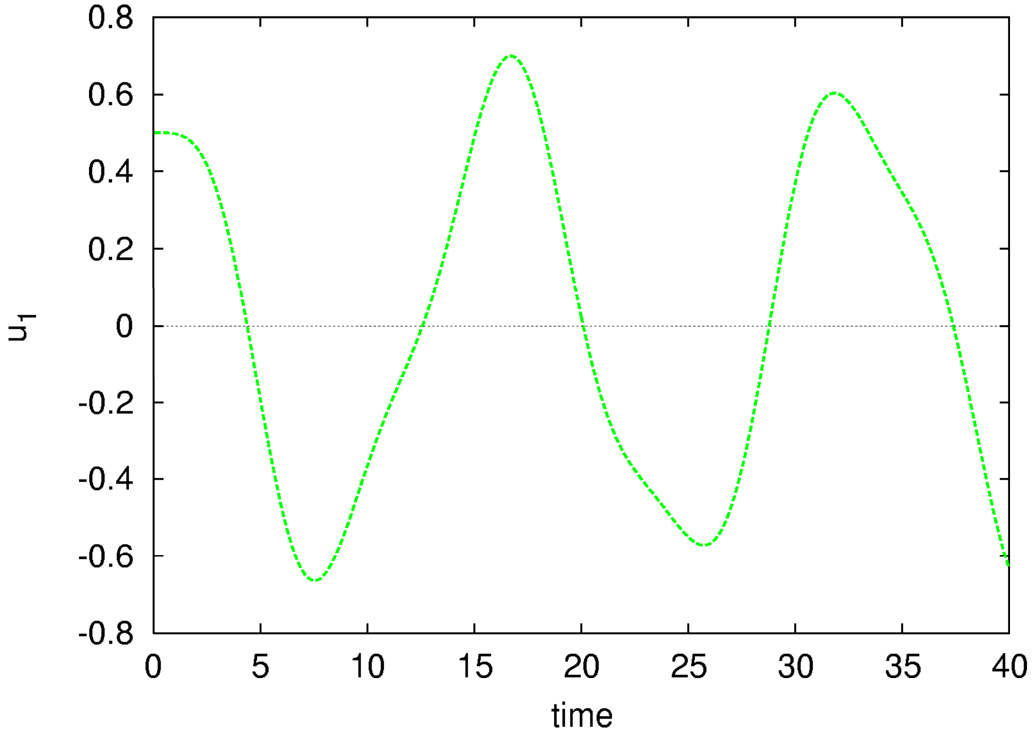
- Initial conditions – adjoint problem:

$$\boldsymbol{z}(t = t_m) = \mathbf{0}\,, \quad \dot{\boldsymbol{z}}(t = t_m) = -\boldsymbol{M}^{-1} \frac{\boldsymbol{e}_l(t_m)}{|\boldsymbol{e}_l(t_m)|}$$

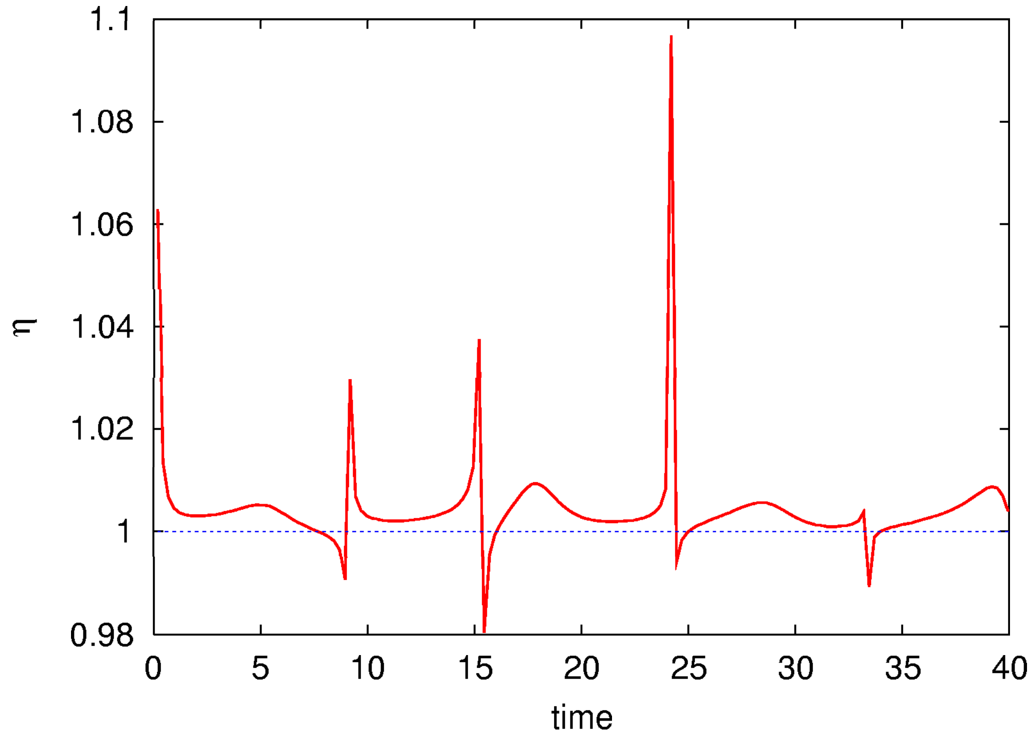
J. Neumann, K. Schweizerhof
Mechanik, Universität Karlsruhe

Two degree of freedom system:

Results: • $u_1(t)$ - displacement



• efficiency index $\eta(t)$ for $e_{gh}(CG2 - newm)$

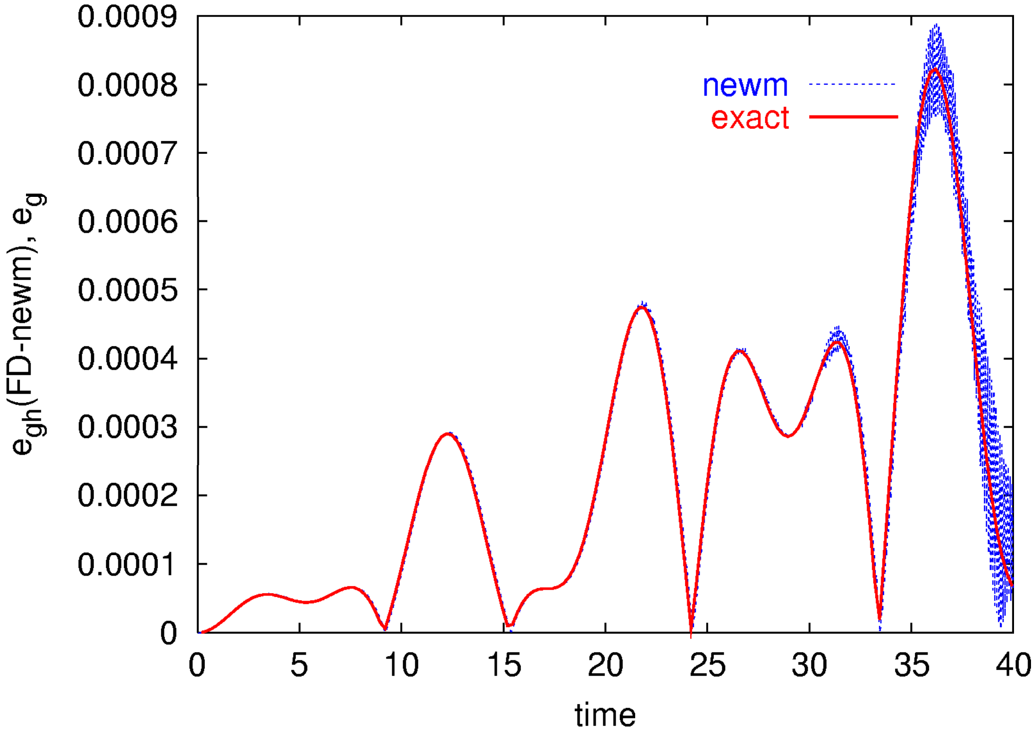


$$\eta = \frac{e_{gh}}{e_g}, \approx 1$$

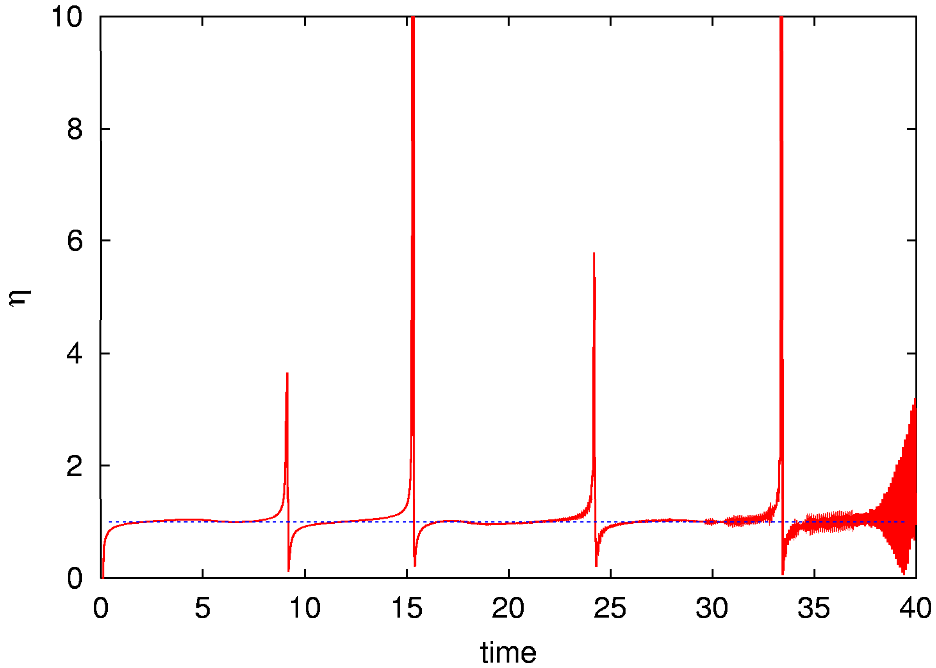
J. Neumann, K. Schweizerhof
Mechanik, Universität Karlsruhe

Two degree of freedom system: contd.

Results: • Estimated error $e_{gh}(FD - newm)$ compared to exact error



• efficiency index $\eta(t)$ for $e_{gh}(FD - newm)$

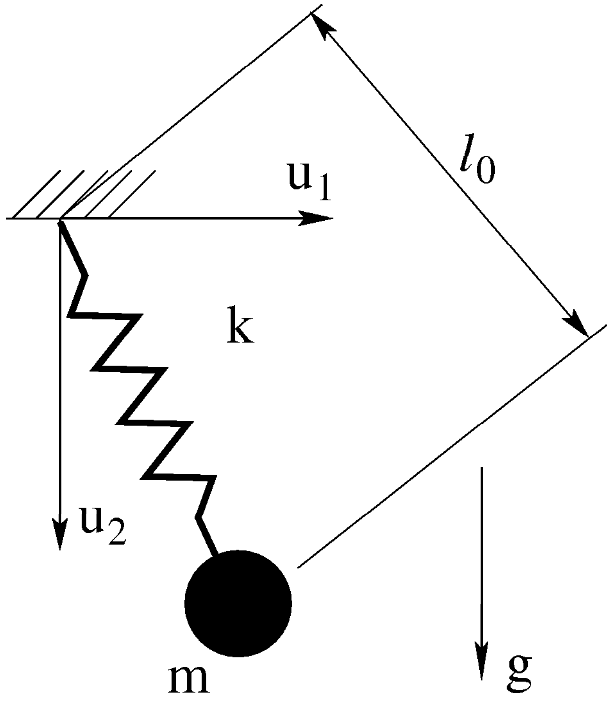


growing oscillations of $\eta = \dfrac{e_{gh}}{e_g}$,

→ higher efficiency index at lower values

→ appears usable for wide region

Spring pendulum – nonlinear problem



$$\left[\begin{array}{l} m\ddot{u}_1 + ku_1\dfrac{\sqrt{u_1^2+u_2^2} - l_0}{\sqrt{u_1^2+u_2^2}} = 0 \\ m\ddot{u}_2 + ku_2\dfrac{\sqrt{u_1^2+u_2^2} - l_0}{\sqrt{u_1^2+u_2^2}} = mg \end{array}\right] \quad \text{for } t > 0$$

initial conditions:

$$u_1^0 = 10^{-11}$$
$$u_2^0 = 1.5$$
$$\dot{u}_1^0 = 0.0$$
$$\dot{u}_2^0 = 0.0$$

$\rightarrow$ dominant vertical initial condition, minimal horizontal initial deflection

Parameters: $k = 38.5$, $m = 1.4$, $l_0 = 1.0$

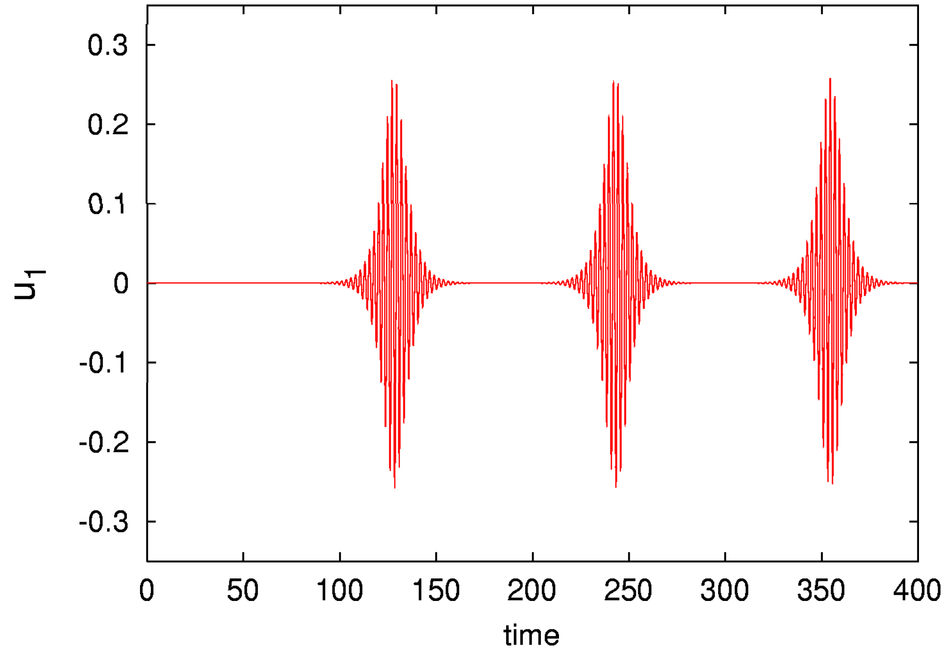
Numerical time integration CG2, $\Delta t = 0.05$,

Reference ('exact') solution with $\Delta t(ref) = 0.000625$

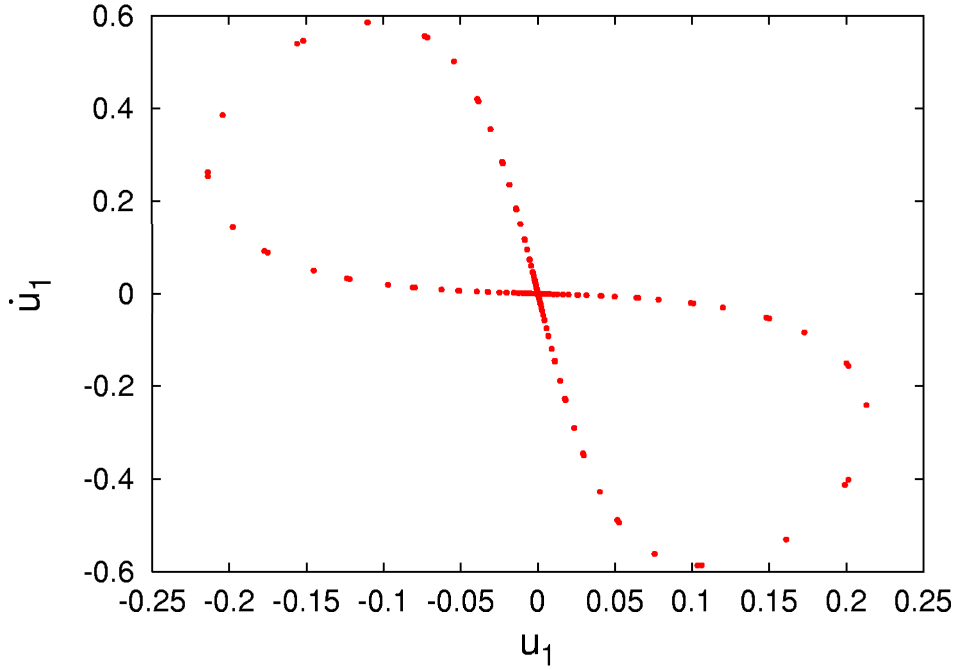
J. Neumann, K. Schweizerhof
Mechanik, Universität Karlsruhe

Spring pendulum – contd.

Results: • $u_1(t)$ horizontal displacement



• Poincaré map u_1-$\dot{u}_1$ for $u_2 - (l_0 + mg/k) = 0$, $\dot{u}_2 > 0$

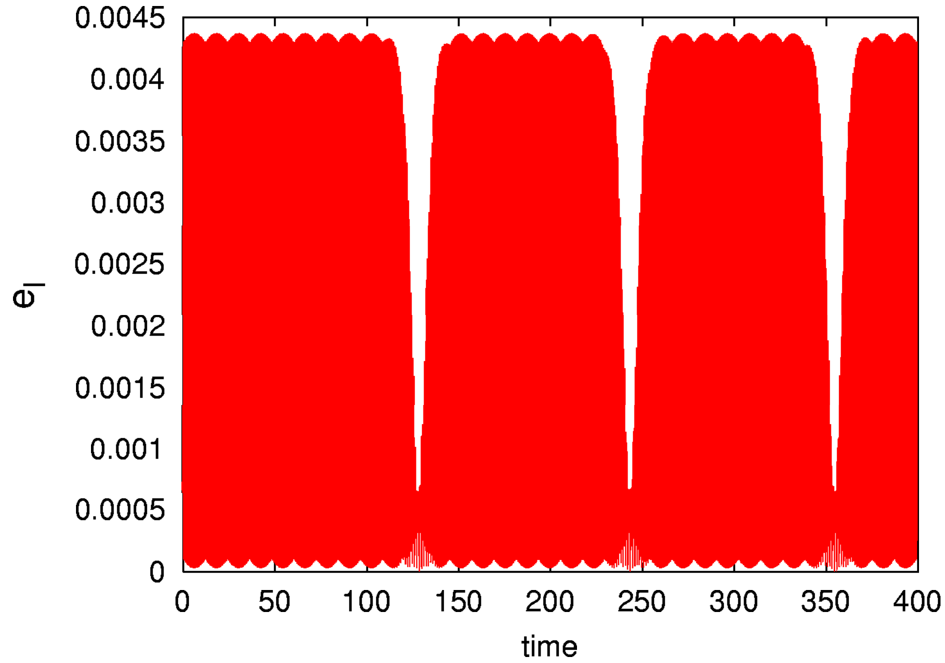


→ Poincaré map shows quasi-periodic solution,
Behaviour: perturbation of primal vibration in vertical direction with and $u_1 = \dot{u}_1 = 0$

J. Neumann, K. Schweizerhof
Mechanik, Universität Karlsruhe

Spring pendulum – contd.

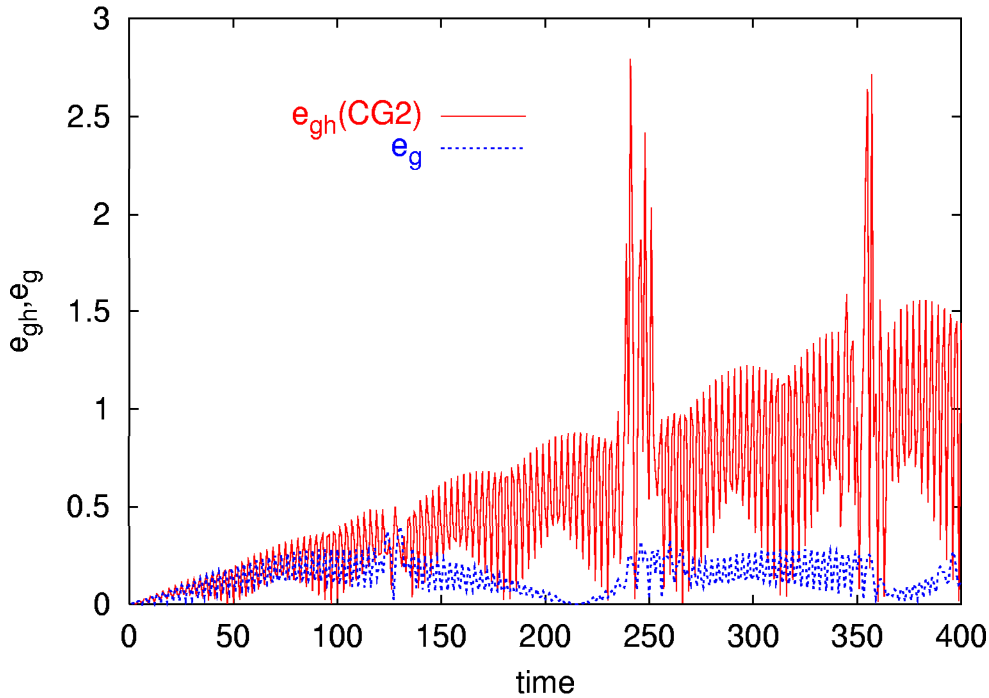
Results: • Estimated local time integration error e_l (from FD considerations)



Minima of estimated local error at $t \approx 125/240/360$

$\rightarrow$ not usable for global error estimation

• Estimated global time integration error $e_{gh}(cg2)$ and exact error e_g

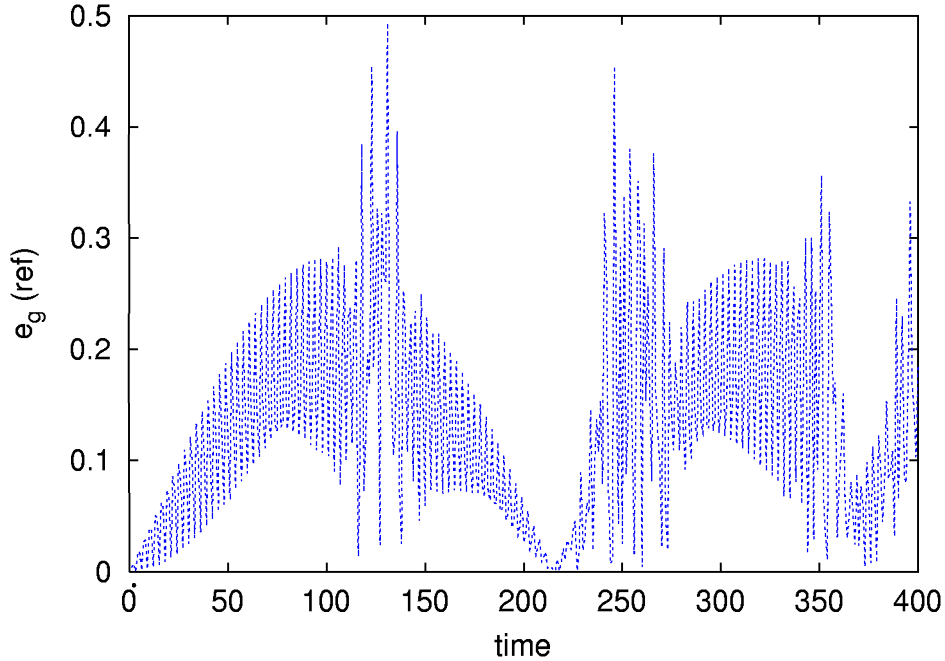


'Bifurcation' from longitudinal motion to horizontal motion at $t \approx 125/240/360$,

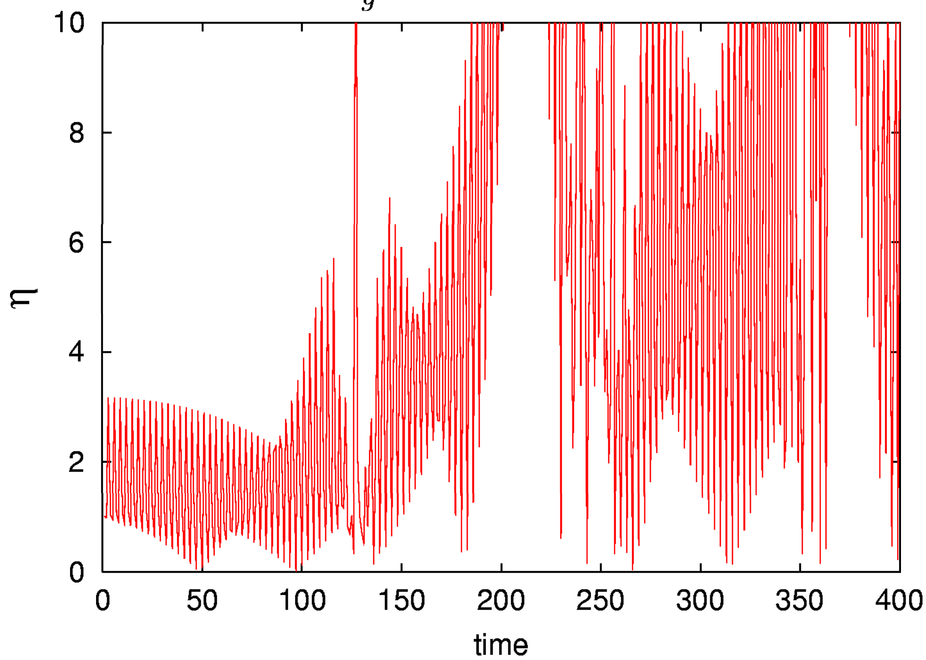
$\rightarrow$ Maxima of estimated global error at $t \approx 125/240/360$,

Spring pendulum – contd.

Results: • Global time integration error using reference solution, $\Delta t(ref) = 0.000625 \rightarrow$ 'exact' error



• Efficiency index $\eta = \dfrac{e_{gh}}{e_g}$



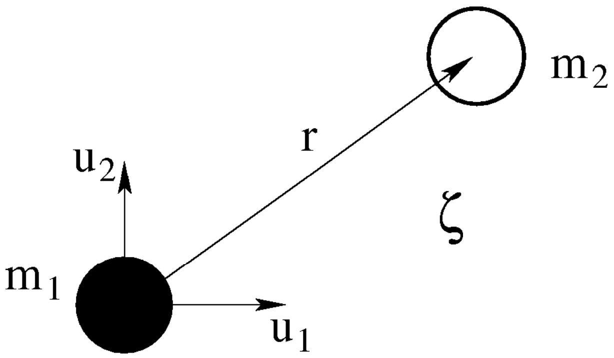
- Maxima of 'exact' global time integration error at $t \approx 125/240/360$,
- error somehow captured by error estimator only up to first 'bifurcation'

But: $t > 100$: $\eta \gg 1 \rightarrow$ huge overestimation of global time integration error

J. Neumann, K. Schweizerhof
Mechanik, Universität Karlsruhe

Two body interaction nonlinear problem

e.g. celestial mechanics



initial conditions:

$$\begin{bmatrix} m\ddot{u}_1 + \zeta\frac{u_1}{(u_1^2+u_2^2)^{3/2}} = 0 \\ m\ddot{u}_2 + \zeta\frac{u_2}{(u_1^2+u_2^2)^{3/2}} = 0 \end{bmatrix} \quad \text{for } t > 0$$

$$u_1^0 = 0.4$$
$$u_2^0 = 0.0$$
$$\dot{u}_1^0 = 0.0$$
$$\dot{u}_2^0 = 2.0$$

Parameters: $\zeta = 1.0$ (gravitational constant), $m = \frac{m_1 m_2}{m_1 + m_2} = 1$

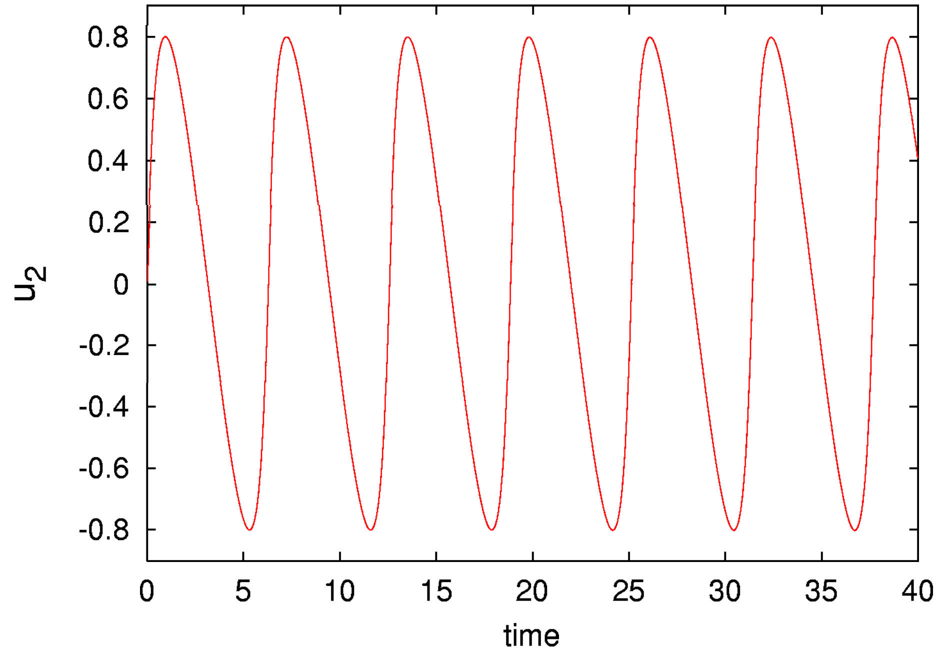
- Numerical time integration CG2-newm, $\Delta t = 0.05$,
- Exact solution: $u_1(t) = \cos(\tau) - 0.6$,

$$u_2(t) = 0.8\sin(\tau), \qquad \text{with: } t = \tau - 0.6\sin(\tau)$$

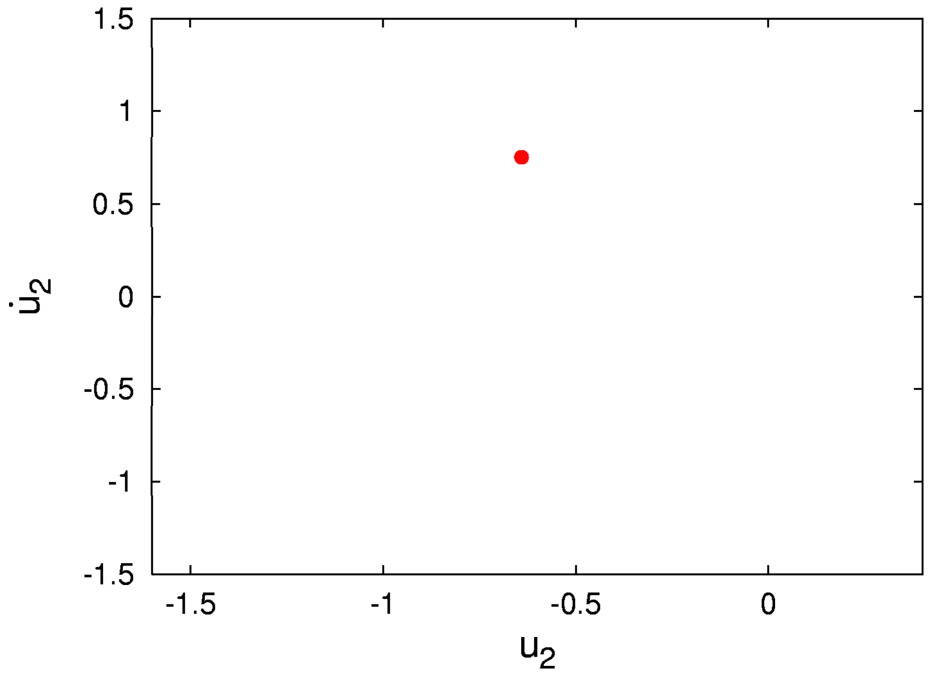
J. Neumann, K. Schweizerhof
Mechanik, Universität Karlsruhe

Two body interaction – contd.

Results: • $u_2(t)$ – vertical displacement



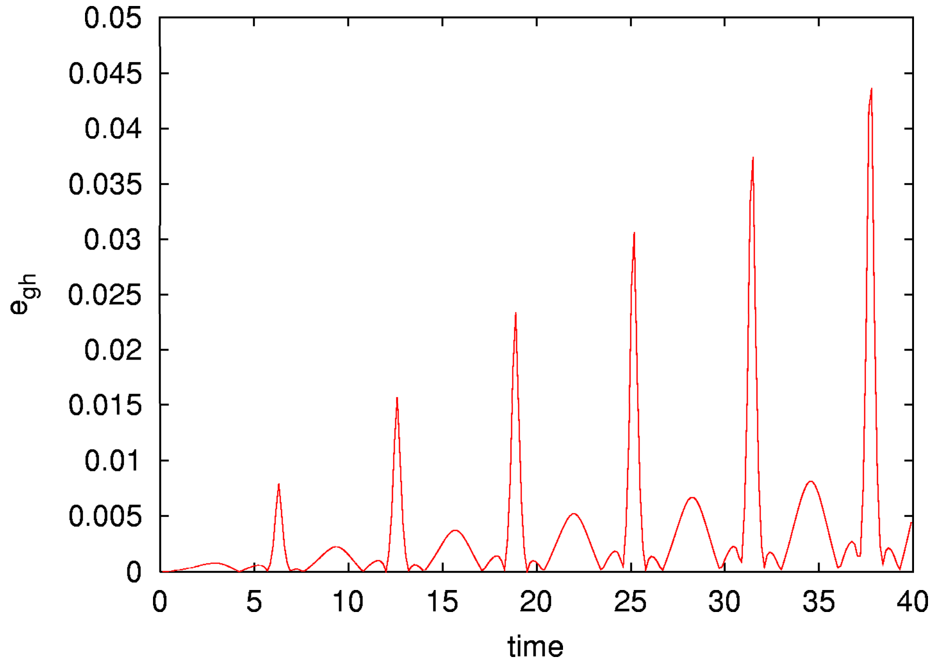
• Poincaré map u_2-$\dot{u}_2$ at $u_1 = 0$, $\dot{u}_1 > 0$



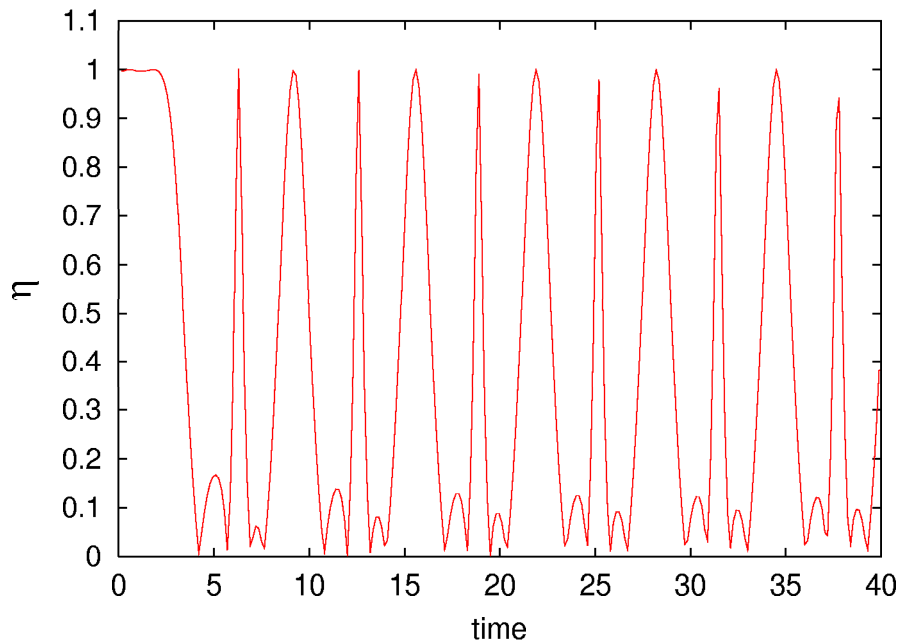
→ periodic solution

Two body interaction – contd.

Results: • Estimated global time integration error $e_{gh}(cg2 - newm)$ based on adjoint problem



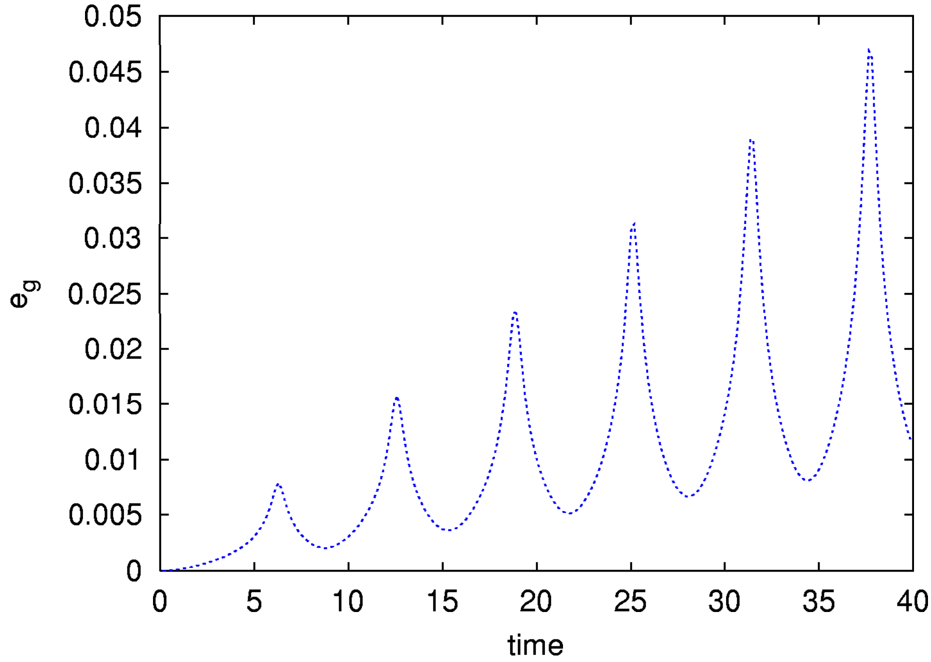
• Efficiency index $\eta = \frac{e_{gh}}{e_g}$



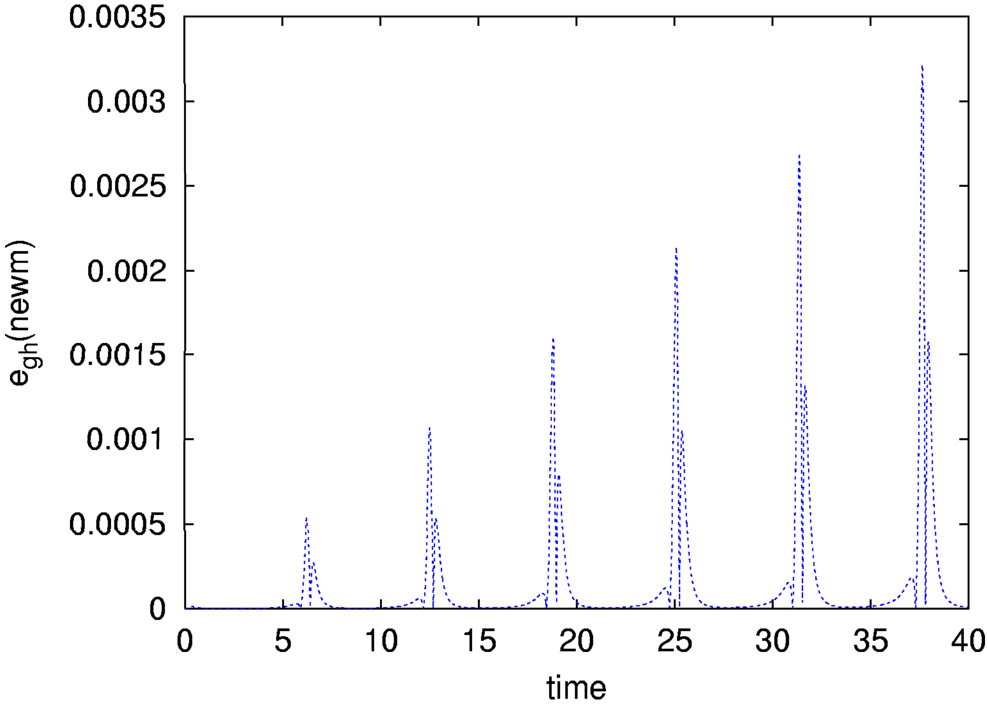
$\rightarrow$ 'smooth' periodic solution $\rightarrow \eta \approx 1$ at maxima of error ,

Two body interaction – contd.

Results:
- Exact global time integration error e_g for Finite Element scheme (CG2-newm)



- Estimated global time integration error based on FD-version of Newmark $e_{gh}(FD - newm)$

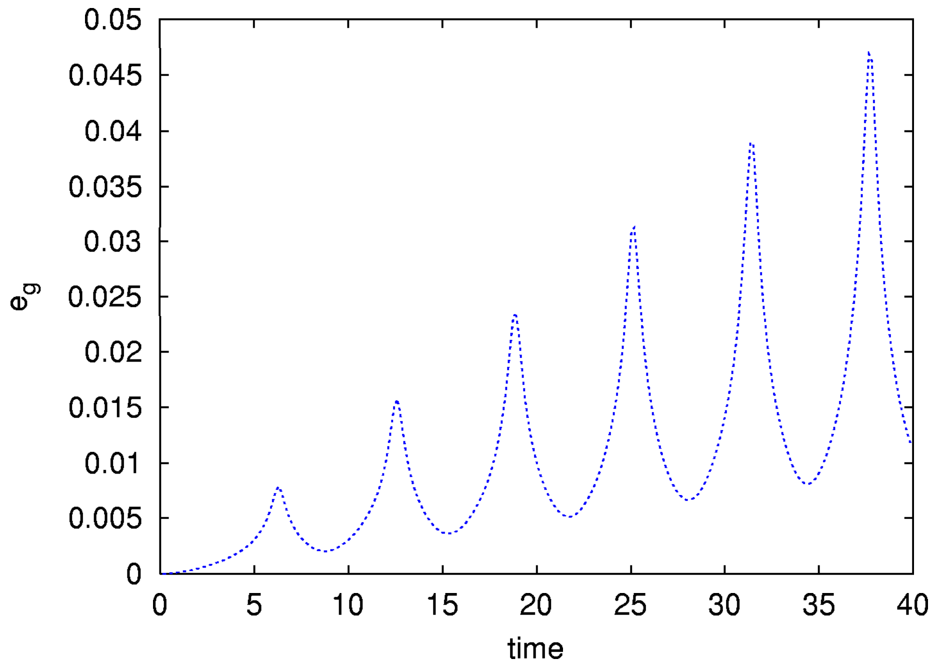


→ times of maxima of $e_{gh}(FD - newm)$ correspond to times of maxima in e_g and $e_{gh}(cg2)$

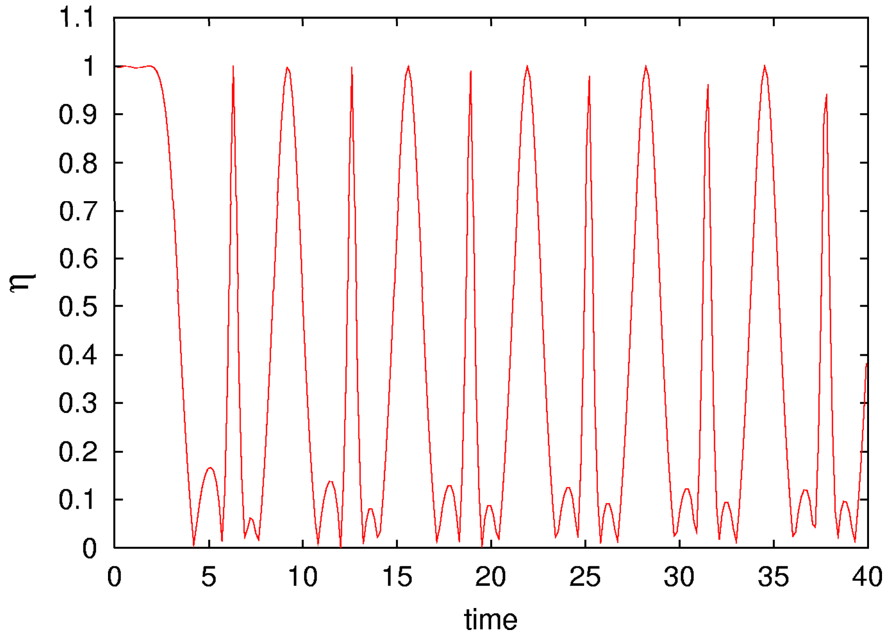
J. Neumann, K. Schweizerhof
Mechanik, Universität Karlsruhe

Two body interaction – contd.

Results: • Exact global time integration error e_g for Finite Element scheme (CG2-newm)



• Efficiency index $\eta = \frac{e_{gh}}{e_g}$



Time step adaptation scheme

Based on combination of estimator for global and local time integration error

Global estimator: $e_{gh}(CG2 - newm) = \int_0^{t_m} \boldsymbol{R}\, \boldsymbol{z}_h \, dt$, Local indicator: e_l

Idea
- perform multiple analysis
- assume upper/lower tolerance for time step (local tolerance)
- adjust local time step size
- compute global error, check maximum of analysis

Basis analysis
- compute with constant time step, determine max. displ.
- set global tolerance $gtol$ = fraction of max. displacement

$\rightarrow$ local tolerances $upper\, ltol = \frac{gtol}{N}$, $lower\, ltol = \frac{upper\, ltol}{1...10}$

Adaptive error control procedure

a) check local error e_l

modify Δt_m, if

$e_l < lower\ ltol$ or

$e_l > upper\ ltol$ then $\rightarrow \Delta t_m(new) = \Delta t_m \sqrt[3]{\frac{ltol}{e_l}}$

b) check global error, compute $emax = \max_{t \in (0,T)} e_{gh}$

modify $lower\ ltol$ and $upper\ ltol$ if

$emax > gtol$ then

$$upper\ ltol(new) = \left(\frac{gtol}{emax}\right)^{3/2} upper\ ltol(old)\ ,$$

$$lower\ ltol(new) = \left(\frac{gtol}{emax}\right)^{3/2} lower\ ltol(old)\ ,$$

$$\rightarrow \Delta t_0(new) = \left(\frac{gtol}{emax}\right)^{1/2} \Delta t_0(old)$$

Idea: global error is reduced quadratically, order of local error is $\mathcal{O}(\Delta t)^3$ if $\Delta t(new) = 0.5\, \Delta t(old)$

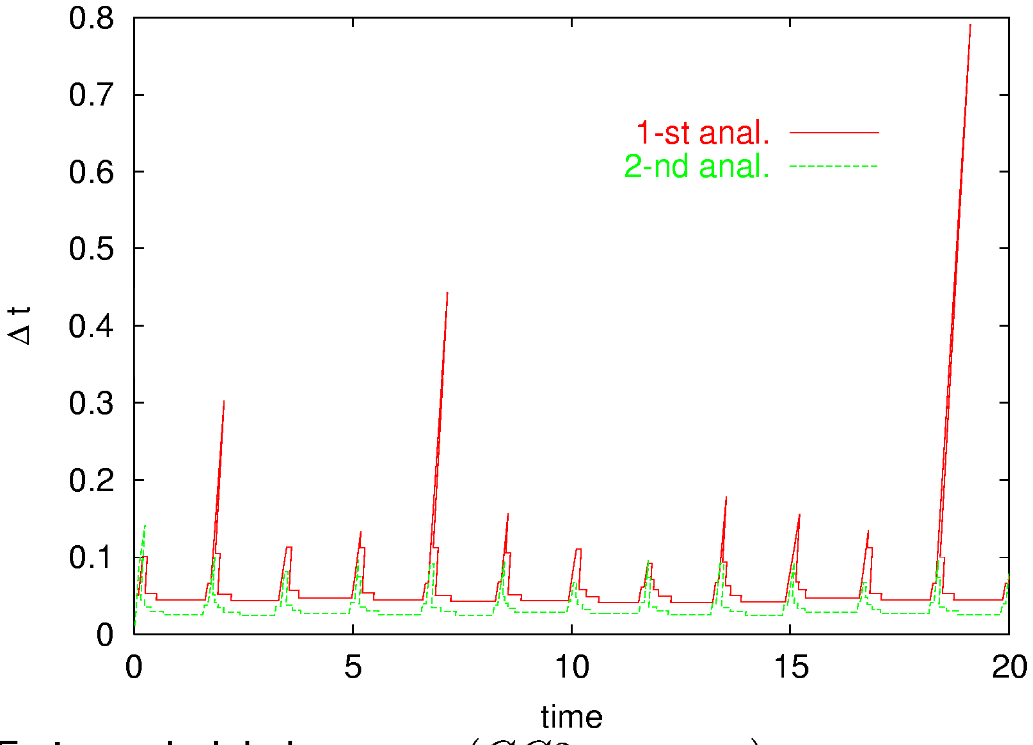
$\rightarrow$ Restart at $t = 0$ if $emax > gtol$

Time step adaptation

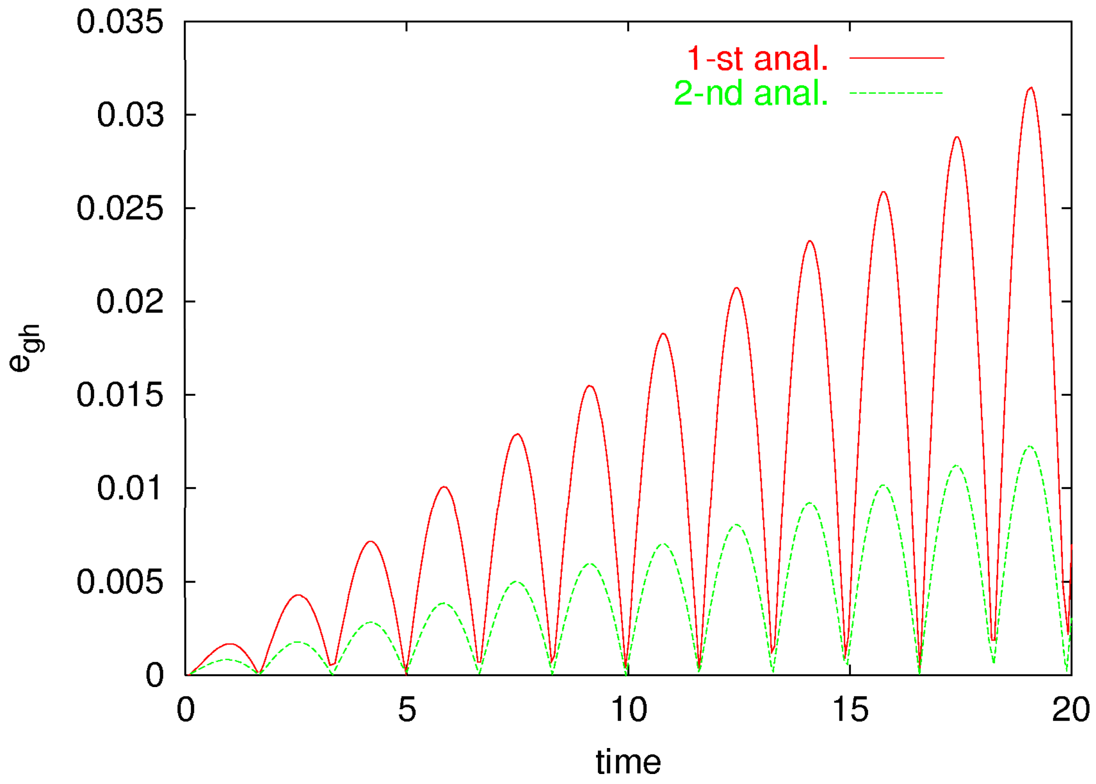
SDOF as before, starting tolerances:

$$lower\ ltol = 1.0 \cdot 10^{-5},\ upper\ ltol = 5.0 \cdot 10^{-5},\ gtol = 0.015$$

Results: • $\Delta t(t)$ - time step size



• Estimated global error $e_{gh}(CG2 - newm)$



→ in 2-nd analysis $emax < gtol$

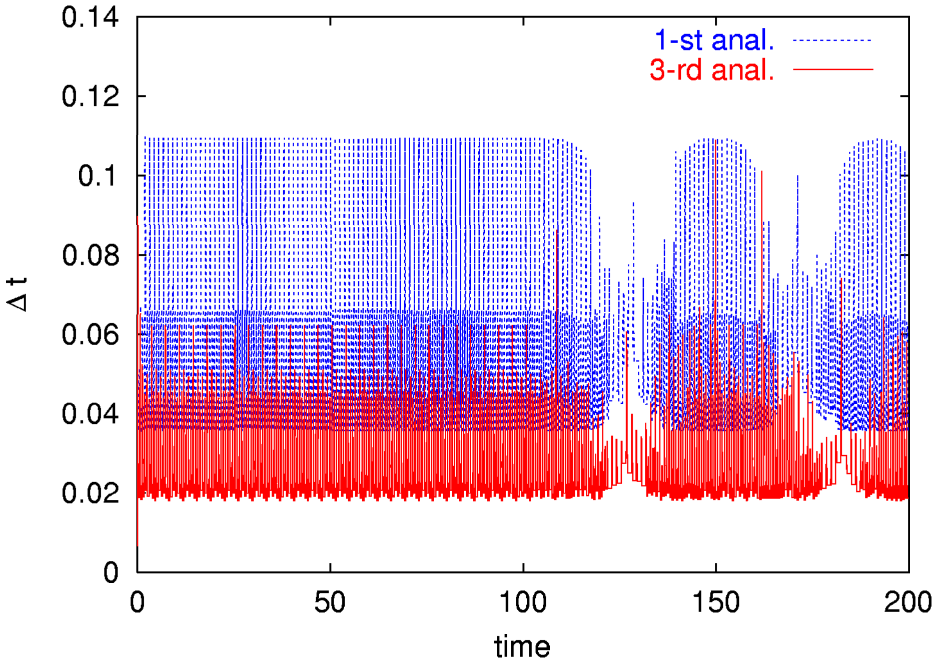
J. Neumann, K. Schweizerhof
Mechanik, Universität Karlsruhe

Time step adaptation

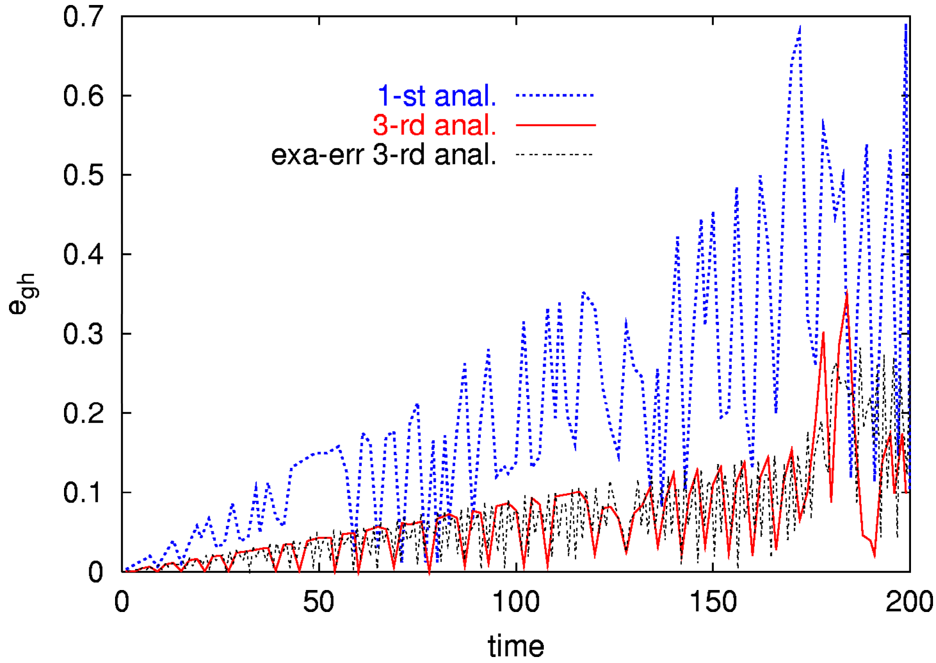
Spring pendulum: starting tolerances:

$$lower\ tol = 2.0 \cdot 10^{-5},\ upper\ tol = 1.0 \cdot 10^{-4},\ gtol = 0.6$$

Results: • $\Delta t(t)$ - time step size



• Estimated global error $e_{gh}(CG2 - newm)$; Exact error (exa-err)



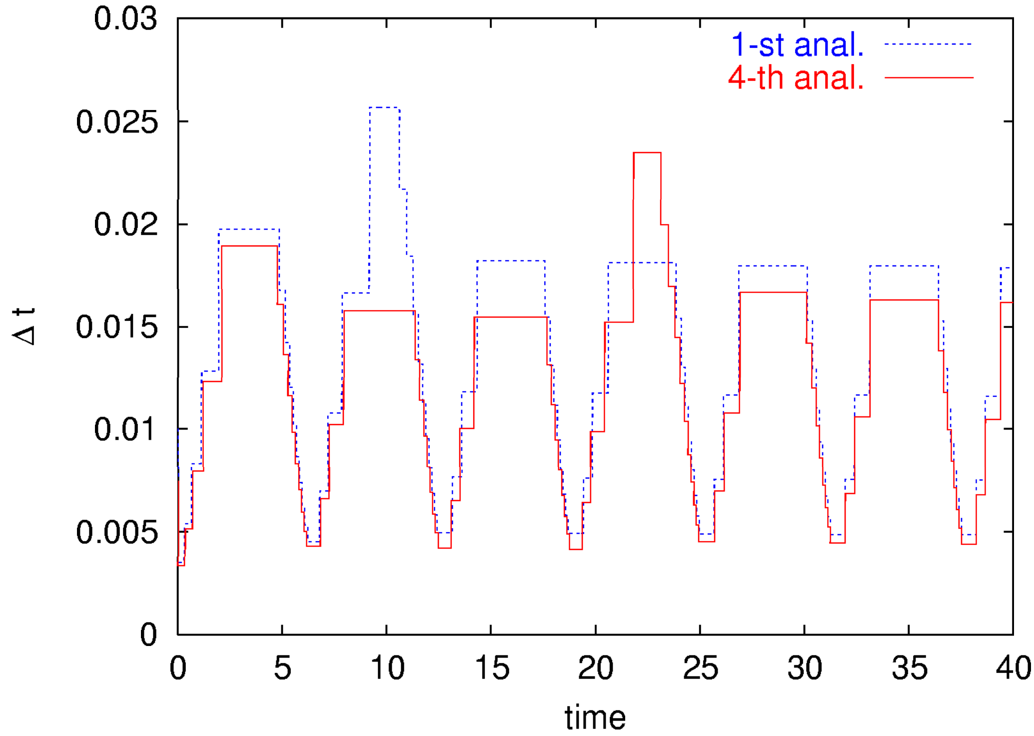
- adap. scheme reduces error for complete time range, in 3-rd anal. $emax < gtol$
- better results for time before 'bifurcation' (at $t \approx 125$),
- after $t \approx 125$ reasonable results, but not 'perfect' error reduction

Time step adaptation

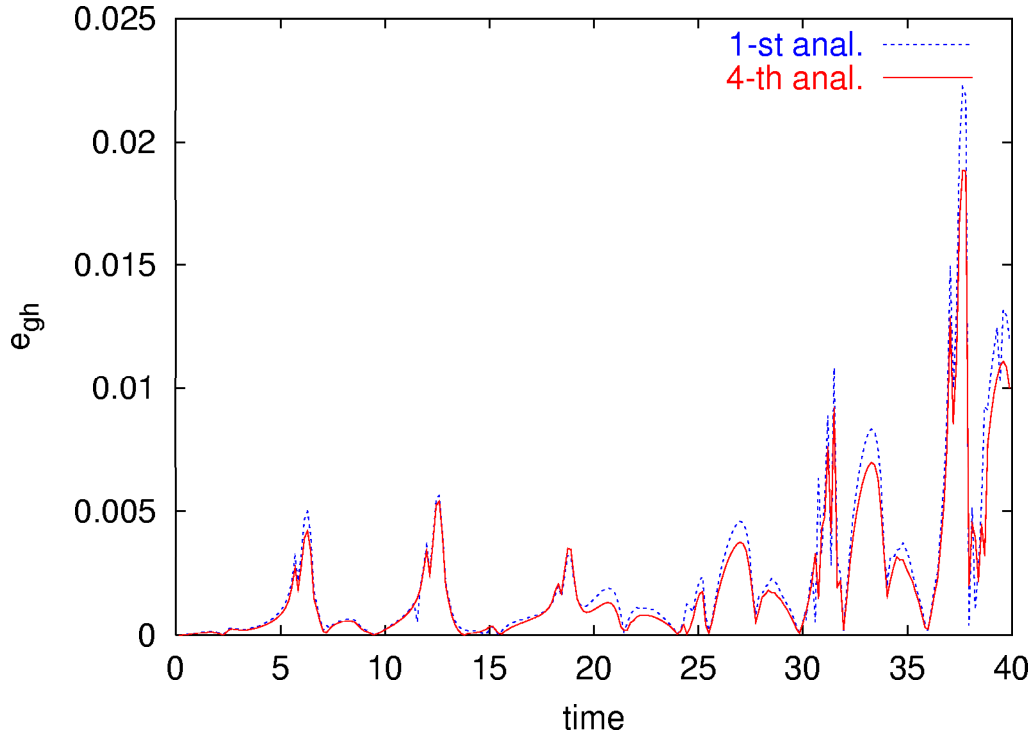
Two body interaction: starting tolerances:

$$lower\ ltol = 5.0 \cdot 10^{-8},\ upper\ ltol = 3.0 \cdot 10^{-7},\ gtol = 0.02$$

Results: • $\Delta t(t)$ - time step size



• Estimated global error $e_{gh}(CG2 - newm)$



→ in 2-nd analysis $emax < gtol$

J. Neumann, K. Schweizerhof
Mechanik, Universität Karlsruhe

Conclusions

- effectivity and efficiency of local and global error indicator / estimator for structural dynamic problems shown
- simple local and FD-based global indicator for linear problems reasonably applicable
- FE-based global estimator
  - high efficiency for linear and mildly nonlinear problems
  - less efficient for highly nonlinear problems
- Time step adaptation scheme based on combination of global FE estimator and local FD indicator works reasonably well for linear and nonlinear problems