22, 23 y 24 de Octubre de 2008. El Escorial (Madrid)

Cuarta reunión de la red temática Dance

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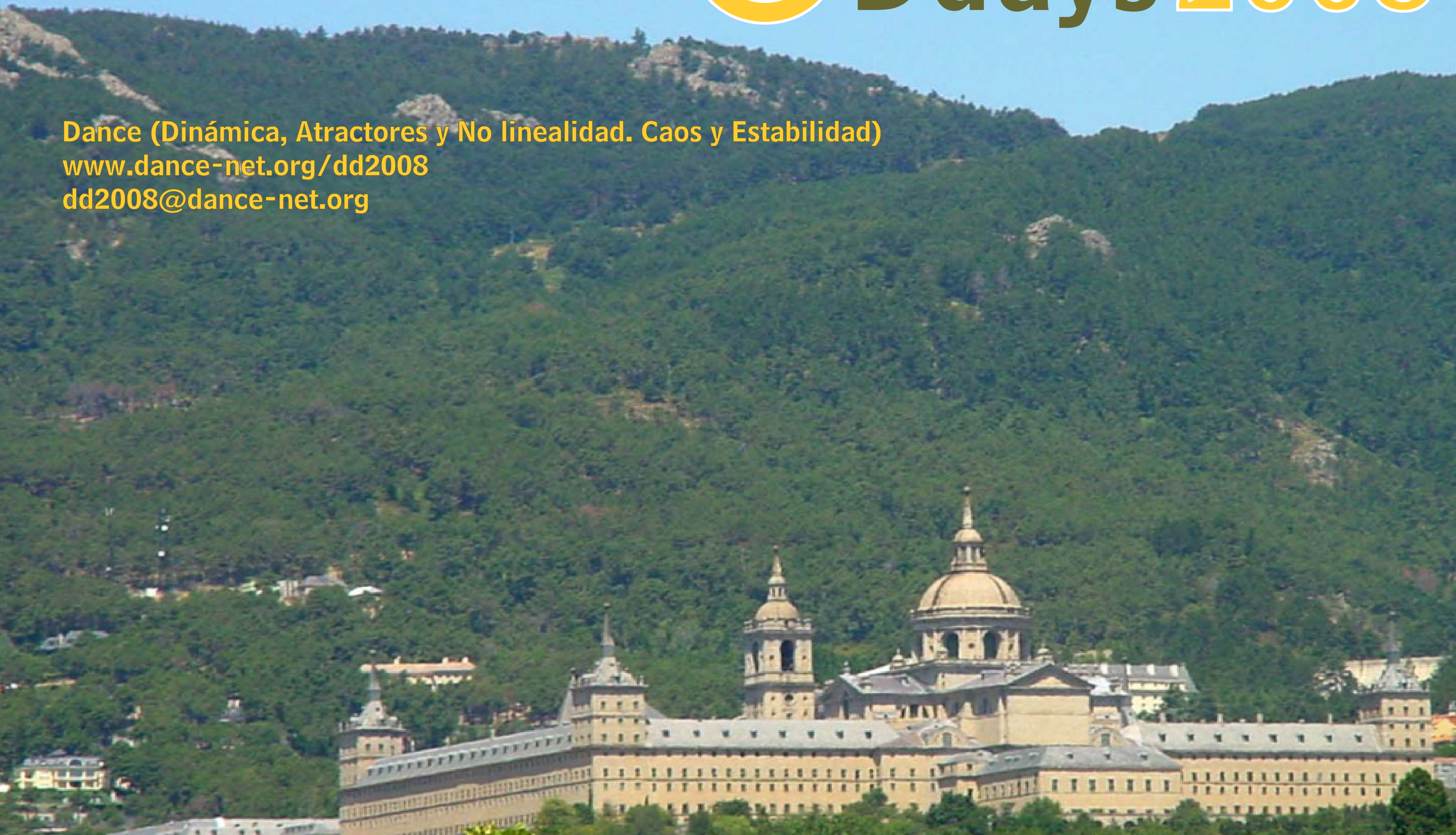

Multistep cosine methods for second-order partial differential equations

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AIM: Efficient numerical integration of PDEs of second-order in time with qualitative properties to imitate

$$
\begin{aligned}
u_{tt}(x,t) &= Au(x,t) + g(t, u(x,t)),\ x \in [a,b],\ 0 < t < T \\
u(x,0) &= u_0(x) \\
u_t(x,0) &= v_0(x)
\end{aligned}
$$

periodic boundary conditions

$Au = u_{xx} \rightarrow$ nonlinear wave equation

$Au = -u_{xxxx} \rightarrow$ Euler-Bernoulli equation

Important assumption: Enough regularity of the solution

Literature

- Integration of highly oscillatory problems

  energy of the solution being bounded

  stiff part easy to integrate

Gautschi-type methods

Hochbruch&Lubich, Numer. Math (1999)
Hairer & Lubich, SIAM J. Numer. (2000)
Grimm & Hochbruch, J. Phys. A Math. Gen. (2006)

Mollified impulse methods

García-Archilla, Sanz-Serna, Skeel, SIAM J. Sci. Comp. (1998)
Sanz-Serna, SIAM J. Numer. (2008)

second-order accurate

Literature

- Integration of parabolic PDEs with exponential integrators

  stiff and linear part integrated exactly

$\longrightarrow$ explicit and stable methods of arbitrary high order

Norsett, Lecture Notes (1969)
Cox & Matthews, JCP (2002)
Hochbruch & Ostermann, APNUM (2005)
Hochbruch & Ostermann, SIAM J. Num. Anal. (2005)
Calvo & Palencia, Numer. Math. (2006)

no qualitative properties to imitate

We will use symmetric explicit multistep cosine methods

explicit multistep	$\Longrightarrow$	1 funct.eval./step
cosine	$\Longrightarrow$	stiff part integrated exactly
symmetric	$\Longrightarrow$	qualitative properties are conserved

Literature on symmetric multistep methods for ODEs of second-order in time $\ddot{y} = f(y)$

$$\rho(E)y_n = h^2\sigma(E)f(y_n), \quad \rho(x) = x^k\rho(\tfrac{1}{x}), \quad \sigma(x) = x^k\sigma(\tfrac{1}{x}).$$

If 1 is the only double root of ρ $\longrightarrow$ good qualitative behaviour

In another case $\longrightarrow$ exponential error growth with time in general

Cano & Sanz-Serna, IMA J. Numer. Anal. (1998)
Hairer & Lubich, Numer. Math. (2004)
Cano, Numer. Math. (2006) $\longrightarrow$ generalization to PDEs

After pseudospectral discretization in space,

$$\ddot{Y}(t) = -\Omega^2 Y(t) + G(t, Y(t)), \quad \Omega \rightarrow \text{diagonal and real}$$

Construction of methods

$$Y(t_n+h) = \cos(h\Omega)Y(t_n) + h\,\text{sinc}(h\Omega)\dot{Y}(t_n) + \int_0^h \Omega^{-1}\sin((h-s)\Omega)G(t_n+s, Y(t_n+s))ds$$

$h \rightarrow -h$ and adding

$$Y(t_n+h) - 2\cos(h\Omega)Y(t_n) + Y(t_n-h)$$
$$= \int_0^h \Omega^{-1}\sin((h-s)\Omega)[G(t_n+s, Y(t_n+s)) + G(t_n-s, Y(t_n-s))]ds.$$

When $G(t_n+s, Y(t_n+s)) \approx G(t_n, Y_n)$ $\longrightarrow$ Gautschi method

$$Y_{n+2} - 2\cos(h\Omega)Y_{n+1} + Y_n = h^2\gamma_1(h\Omega)G_{n+1}, \quad \gamma_1(\epsilon) = 2\epsilon^{-2}(1-\cos(\epsilon)),$$

If $G(t_n+s, Y(t_n+s)) \approx \sum_{l=0}^{k-1} G(t_{n-l}, Y_{n-l}) L_{-l,h}(s) \rightarrow$ higher order method

$L_{-l,h}$: Lagrange polynomial $\{0, -h, \ldots, -\overset{\curlyvee}{l}h, \ldots, -(k-1)h\}$

$k = 3$ MC3

$$Y_{n+3} - 2\cos(h\Omega) Y_{n+2} + Y_{n+1} = h^2[\gamma_2(h\Omega) G_{n+2} + \gamma_1(h\Omega) G_{n+1} + \gamma_0(h\Omega) G_n]$$

$$\begin{aligned}
\gamma_0(\epsilon) &= \epsilon^{-2}[1 - 2\epsilon^{-2} + 2\epsilon^{-2}\cos(\epsilon)]. \\
\gamma_1(\epsilon) &= \epsilon^{-2}[-2 + 4\epsilon^{-2} - 4\epsilon^{-2}\cos(\epsilon)], \\
\gamma_2(\epsilon) &= \epsilon^{-2}[3 - 2\cos(\epsilon) - 2\epsilon^{-2} + 2\epsilon^{-2}\cos(\epsilon)].
\end{aligned}$$

$\Omega \rightarrow 0$: 3rd-order explicit Störmer multistep method, not symmetric

SMC4

$$Y(t_n+2h) - \delta(h\Omega)Y(t_n+h) - 2(\cos(2h\Omega) - \delta(h\Omega)\cos(h\Omega))Y(t_n) - \delta(h\Omega)Y(t_n-h) + Y(t_n-2h)$$
$$= \int_0^{2h} \Omega^{-1}\sin((2h-s)\Omega)[G(t_n+s, Y(t_n+s)) + G(t_n-s, Y(t_n-s))]ds$$
$$-\delta(h\Omega)\int_0^{h} \Omega^{-1}\sin((h-s)\Omega)[G(t_n+s, Y(t_n+s)) + G(t_n-s, Y(t_n-s))]ds.$$

Interpolation in $\{-h, 0, h\}$ $\longrightarrow$ symmetry

$\delta(\epsilon) = \cos(\epsilon)$ $\begin{cases} \rho_0(x) = x^4 - x^3 - x + 1 = (x-1)^2(x^2+x+1) \\ \text{stability} \rightarrow \text{roots of } \rho_\epsilon(x) \text{ of unit modulus} \end{cases}$

$$x_1(\epsilon) = \frac{-\cos(\epsilon) + i\sqrt{4-\cos^2(\epsilon)}}{2}, \quad x_2(\epsilon) = \frac{-\cos(\epsilon) - i\sqrt{4-\cos^2(\epsilon)}}{2},$$
$$x_3(\epsilon) = \cos(\epsilon) + i\sin(\epsilon), \quad x_4(\epsilon) = \cos(\epsilon) - i\sin(\epsilon).$$

$$Y_{n+4} - \cos(h\Omega)Y_{n+3} + (-2\cos(2h\Omega) + 2\cos(h\Omega)^2)Y_{n+2} - \cos(h\Omega)Y_{n+1} + Y_n$$
$$= h^2[\gamma_1(h\Omega)G_{n+3} + \gamma_2(h\Omega)G_{n+2} + \gamma_1(h\Omega)G_{n+1}],$$

$$\gamma_1(\epsilon) = \epsilon^{-2}(4-\cos(\epsilon)) + 2\epsilon^{-4}[\cos(2\epsilon) - 1 + \cos(\epsilon)(1-\cos(\epsilon))]$$
$$\gamma_2(\epsilon) = 2\epsilon^{-2}(-3-\cos(2\epsilon)+\cos^2(\epsilon)) + 4\epsilon^{-4}(1-\cos(2\epsilon)-\cos(\epsilon)(1-\cos(\epsilon)))$$

Gautschi $\rightarrow q = 2$
MC3 $\rightarrow q = 3$
SMC4 $\rightarrow q = 4$

Local truncation error (d_n)

By using error of interpolation

- If $\frac{d^q}{dt^q} G(t, Y(t))$ exists and $|\left(\frac{d^q}{dt^q} G(t, Y(t))\right)_\lambda| \le K_{\lambda,q}$

$|d_{n,\lambda}| \le C_q K_{\lambda,q} h^{q+2}$, $C_2 = 1, \quad C_3 = (1 + 2\sqrt{3}/5)/2, \quad C_4 = (4 + \frac{\sqrt{3}}{54})$

- Under any of the following assumptions of regularity

(i) $\frac{d^q}{dt^q} g(t, u(t, x))$ can be extended to a holomorphic function on a complex band $|\text{Im}(z)| \le \hat{B}$ for $0 \le t \le T$, and there $|\frac{d^q}{dt^q} g(t, u(t, z))| \le \hat{C}$,

(ii) $\frac{d^q}{dt^q} g(t, u(t, x))$ admits $m \ge 0$ continuous and periodic derivatives with respect to x and $\frac{d^{m+1}}{dx^{m+1}} \frac{d^q}{dt^q} g(t, u(t, x))$ exists and is piecewise C^1 in $[a, b]$.

$$\|d_n\| = O(h^{q+2})$$

Global error

$$\bar{Y}_n = [Y_{n+k-1}, \ldots, Y_n]^T, \quad \bar{G}(\bar{Y}_n) = [G(Y_{n+k-1}), \ldots, G(Y_n)]^T$$

$$\bar{Y}_{n+1} = R(h\Omega)\bar{Y}_n + h^2 B(h\Omega)\bar{G}(\bar{Y}_n), \quad B(\epsilon) = \begin{pmatrix} \gamma_{k-1}(\epsilon) & \ldots & \gamma_1(\epsilon) & 0 \\ 0 & 0 & \ldots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & \ldots & \ldots & 0 \end{pmatrix},$$

Gautschi $\rightarrow R(\epsilon) = \begin{pmatrix} 2\cos(\epsilon) & -1 \\ 1 & 0 \end{pmatrix}$, MC3 $\rightarrow R(\epsilon) = \begin{pmatrix} 2\cos(\epsilon) & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$

SMC4 $\rightarrow R(\epsilon) = \begin{pmatrix} \cos(\epsilon) & 2\cos(2\epsilon) - 2\cos(\epsilon)^2 & \cos(\epsilon) & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$

$$\|B(h\Omega)\| \leq \sup_{\lambda \in \sigma(\Omega)} \|B(h\lambda)\|$$

Stability $\|R^j(\epsilon)\| \le \bar{C} j, \quad \epsilon \in \mathbb{R}$

Eigenvalues of $R(\epsilon)$ $\left\{ \begin{array}{r} \text{of modulus} \le 1 \\ \text{those of unit modulus} \\ \text{at most double} \end{array} \right\} \rightarrow$ Schur decomposition

Gautschi $\epsilon = 2m\pi, \pi + 2m\pi, \rightarrow x_{1,2} = e^{\pm i\epsilon} = +1, -1$

SMC4

	$\epsilon = 2m\pi$	$\epsilon = \frac{\pi}{2} + 2m\pi$	$\epsilon = 3\frac{\pi}{2} + 2m\pi$	$\epsilon = \pi + 2m\pi$
x_1	$\frac{-1+i\sqrt{3}}{2}$	i	i	$\frac{1+i\sqrt{3}}{2}$
x_2	$\frac{-1-i\sqrt{3}}{2}$	$-i$	$-i$	$\frac{1-i\sqrt{3}}{2}$
x_3	1	i	$-i$	-1
x_4	1	$-i$	i	-1

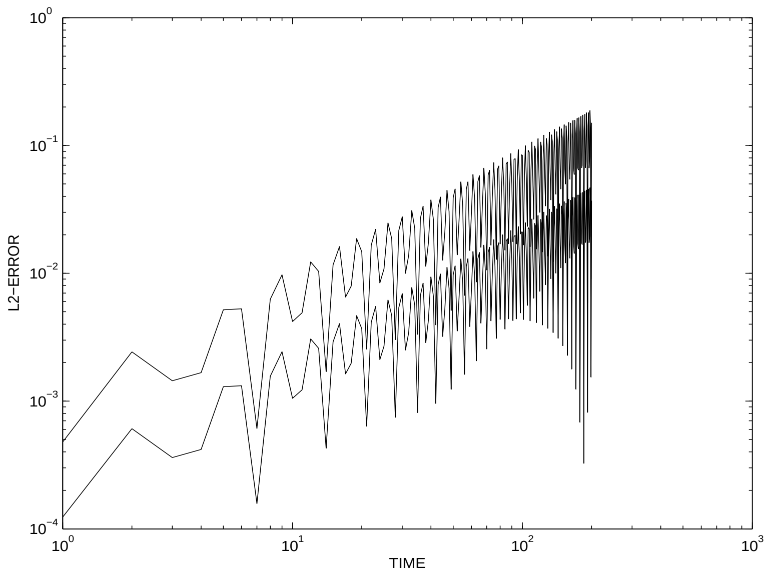
• Under the mentioned assumptions of regularity, whenever $Y(t_\nu) - Y_\nu = O(h^{q+1}), \nu = 0, 1, \ldots, k-1$, $Y(t_n) - Y_n = O(h^q)$, $0 \le nh \le T$.

Growth of error with time for the nonlinear wave equation

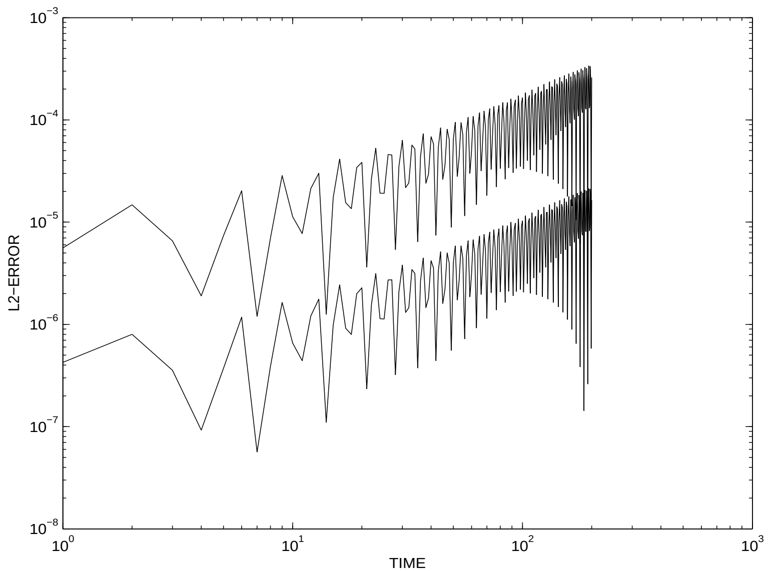
Pseudospectral discretization in space ($M = 250$)

$$\Omega = \text{diag}(\lambda_k)_{k=-M}^{M} = \text{diag}(\tfrac{2\pi k}{b-a})_{k=-M}^{M} = \text{diag}(\tfrac{2\pi k}{100})_{k=-M}^{M}$$

Gautschi



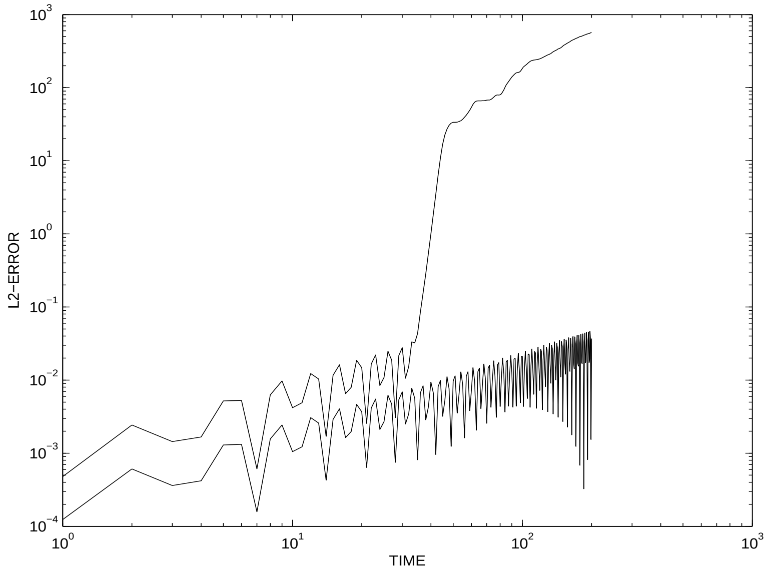
SMC4

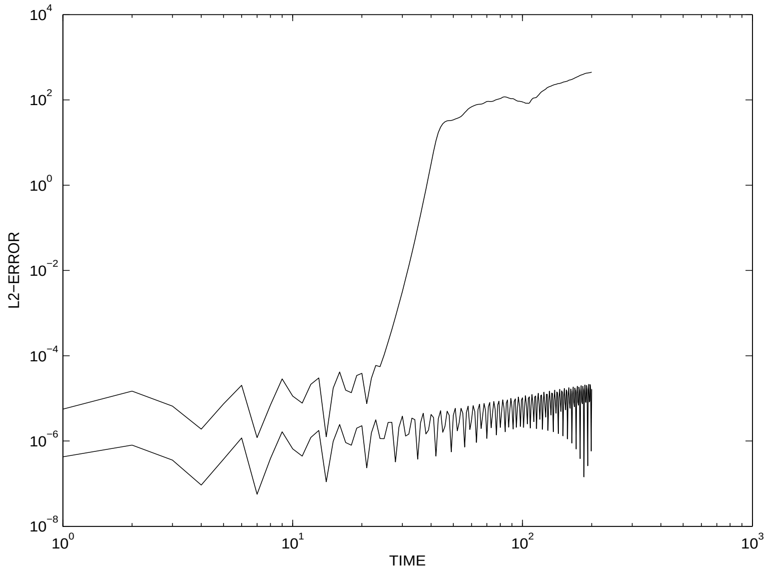


$h = 1/10, 1/20,$ $\quad |\lambda_k h| \leq 5\pi h \leq \pi/2$

Resonances

$h = 1/10, 1/20,$ $\qquad\qquad$ $M = 500$





$h = 1/10, \lambda_M h = \pi \rightarrow$ leads to double root of $\rho_\epsilon(x)$

$h = 1/20, |\lambda_k h| \leq \pi/2$

Explanation for resonances

Simplified problem $\ddot{y}(t) = -\lambda^2 y(t) - y(t)$

Numerical solution for stepsize h, $Y_n = \sum_{j=1}^{k} \delta_j [x_j(\lambda h, h)]^n$

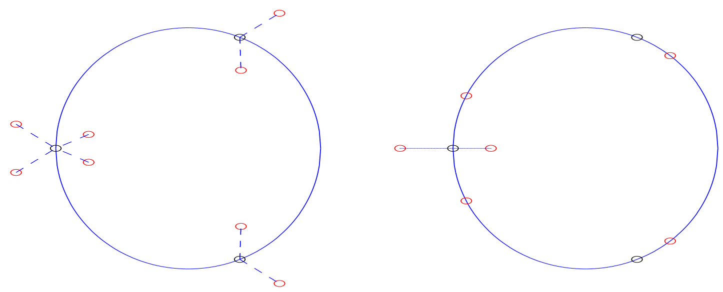
$$x_j(\epsilon, h) \rightarrow \text{roots of } r_{\epsilon,h}(x) \equiv \rho_\epsilon(x) + h^2 \sigma_\epsilon(x)$$

$\rho_\epsilon(x) = \alpha_k(\epsilon)x^k + \cdots + \alpha_0(\epsilon), \quad \sigma_\epsilon(x) = \gamma_{k-1}(\epsilon)x^{k-1} + \cdots + \gamma_1(\epsilon),$

Symmetric methods $\left\{ \begin{array}{ll} \alpha_j(\epsilon) = \alpha_{k-j}(\epsilon), & \gamma_j(\epsilon) = \gamma_{k-j}(\epsilon), \\ \rho_\epsilon(x) = x^k \rho_\epsilon(1/x), & \sigma_\epsilon(x) = x^k \sigma_\epsilon(1/x), \end{array} \right.$

$x_j(\epsilon, h)$ root of $r_{\epsilon,h}(x) \Longrightarrow \left\{ \begin{array}{l} \overline{x_j(\epsilon, h)} \\ 1/x_j(\epsilon, h) \end{array} \right\}$ also roots of $r_{\epsilon,h}(x)$

Stable methods$\longrightarrow$ roots of unit modulus of $r_{\epsilon,0}(x)$ at most double



Gautschi small h

- If ϵ far from $m\pi$ $(m \in \mathbb{Z})$, $|x_j(\epsilon, h)| = 1, \quad j = 1, 2.$

- If ϵ near $m\pi$ $(m \in \mathbb{Z})$,

$|x_j(\epsilon, h)| = 1, \quad j = 1, 2.$

or

$$\left.\begin{array}{l} x_1(\epsilon, h) \text{ real and } |x_1(\epsilon, h)| > 1, \\ x_2(\epsilon, h) = 1/x_1((\epsilon, h) \end{array}\right\} \Longrightarrow \text{resonance}$$

By using Taylor series expansion of $r_{\epsilon,h}(x)$ around $\epsilon = \epsilon_l$, $h = 0$, $x = x_l$ with x_l double root of $r_{\epsilon_l,0}$, $\epsilon = \epsilon_l + \eta$, $x = x_l + r$

$$\epsilon_l = m\pi \left\{ \begin{array}{l} \text{even } m \Longrightarrow r \text{ purely imaginary in first approximation} \\ \text{odd } m \Longrightarrow r \text{ real} \Longrightarrow \text{resonance} \end{array} \right.$$

SMC4 small h

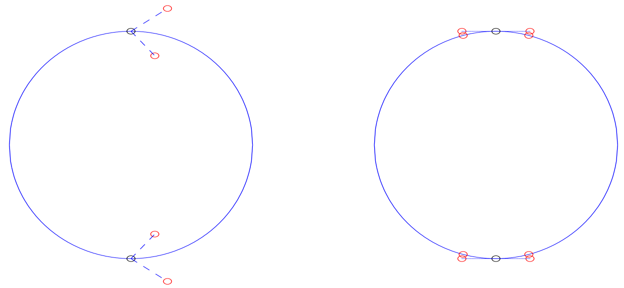
- If ϵ far from $m\pi, \pi/2 + m\pi$ $(m \in \mathbb{Z})$, $|x_j(\epsilon, h)| = 1$.
- If ϵ near $m\pi$, $|x_j(\epsilon, h)| = 1$, or

$$\left.\begin{array}{l} x_1(\epsilon,h) \text{ real and } |x_1(\epsilon,h)| > 1, \\ x_2(\epsilon,h) = 1/x_1((\epsilon,h) \end{array}\right\} \Longrightarrow \text{resonance}$$

By Taylor expansion around $\epsilon = \epsilon_l$, $h = 0$, $x = x_l$, $\epsilon = \epsilon_l + \eta$, $x = x_l + r$,

$$\left\{\begin{array}{l} \text{even } m \Longrightarrow r \text{ purely imaginary } \Longrightarrow \text{no resonance} \\ \text{odd } m \Longrightarrow r \text{ real} \Longrightarrow \text{resonance} \end{array}\right.$$

- If ϵ near $\pi/2 + m\pi$, by Taylor expansion,



$$r = (-1)^m \frac{2\eta \pm \sqrt{4\eta^2 + 16(ch^2 + 2\eta^2)}}{8}, \quad c > 0$$

$$\text{real} \left\{\begin{array}{l} \text{positive} \\ \text{negative} \end{array}\right. \Longrightarrow |x_j(\epsilon,h)| = 1 \Longrightarrow \text{no resonance}$$

Filters to avoid resonances

- Annihilating components $\rightarrow$ resonant frequencies

$$\ddot{Y}(t) = -\Omega^2 Y(t) + G(t, Y(t)), \qquad \Omega = \mathrm{diag}(\lambda_r),$$

If $|\lambda_r h - \epsilon_l| < \eta_0(\epsilon_l)$ then $Y_r = 0$

ϵ_l one of the values which leads to resonance
$\eta_0(\epsilon_l)$ deduced from Taylor expansion before

Under our assumptions of regularity, convergence conserved

- Standard filters: filter function ϕ

$$\sum_{l=0}^{k} \alpha_l(h\Omega) Y_{n+l} = h^2 \sum_{l=0}^{k} \gamma_l(h\Omega) G(\phi(h\Omega) Y_{n+l}), \; n \geq 0$$

When applied to linear problem $\ddot{y}(t) = -\lambda^2 y(t) - y(t)$, control of roots of $\tilde{r}_{\epsilon,h}(x) = \rho_\epsilon(x) + h^2 \tilde{\sigma}_\epsilon(x)$, $\tilde{\sigma}_\epsilon(x) = \phi(\epsilon)\sigma_\epsilon(x)$.

Gautschi method

- To avoid resonance in simplified problem,

$\phi(0) \geq 0$,
$\phi(\pi + 2m\pi) \leq 0, \quad m \in \mathbb{Z}$, (Taylor expansion)
If $\phi(\pi + 2m\pi) = 0$ then $\phi'(\pi + 2m\pi) = 0$.

- To conserve consistency of order 2 for the more general problem, with the assumptions of regularity, g Lipschitz in L^2-norm on its second variable and $\|Au\|_2$ bounded,

$\frac{\phi(\epsilon)-1}{\epsilon^2}$ bounded for real ϵ (local truncation error revisited)

Possible filter functions: $(\frac{\sin(\epsilon)}{\epsilon})^2, \quad (\frac{\sin(\epsilon)}{\epsilon})^2(1 + \frac{1-\cos(\epsilon)}{2})$

Hochbruch & Lubich (1999)

SMC4 method

- To avoid resonance in simplified problem,

$$\begin{aligned}
&\phi(0) > 0,\\
&\phi(\tfrac{\pi}{2} + 2m\pi) > 0,\\
&\phi(\pi + 2m\pi) \leq 0, \quad m \in \mathbb{Z},\\
&\text{If } \phi(\pi + 2m\pi) = 0 \text{ then } \phi'(\pi + 2m\pi) = 0.
\end{aligned}$$

- To conserve consistency of order 4 for the more general problem, with the assumptions of regularity, g Lipschitz in L^2-norm on its second variable and $\|A^2 u\|_2$ bounded,

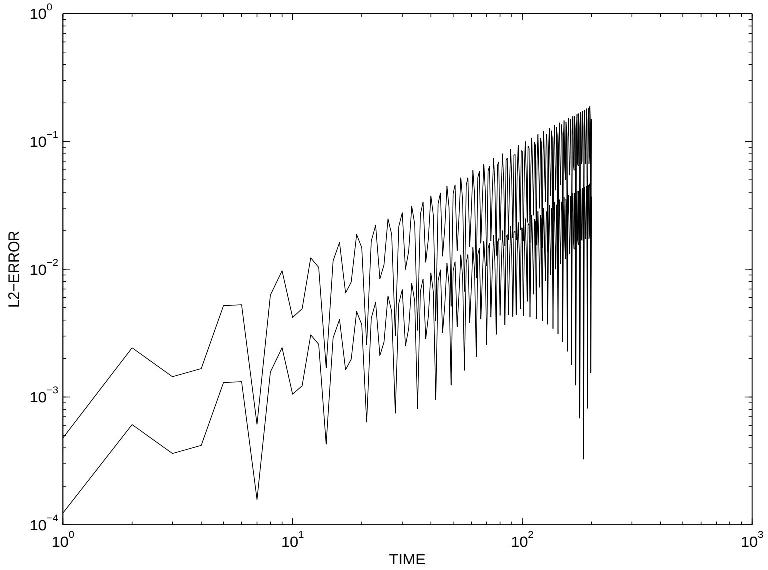
$\frac{\phi(\epsilon)-1}{\epsilon^4}$ bounded for real ϵ

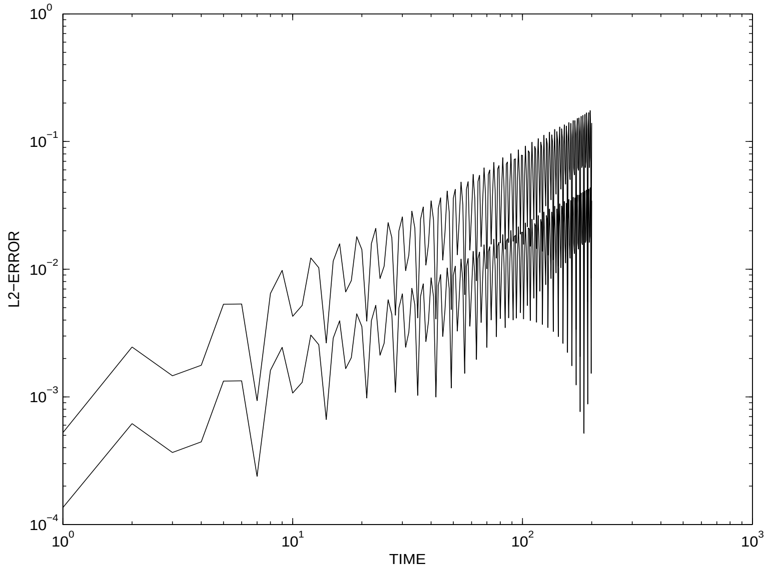
Possible filter function: $(\frac{\sin(\epsilon)}{\epsilon})^2[1 + \frac{2}{3}(1 - \cos(\epsilon))]$

Numerical comparison

Growth of error with time for the nonlinear wave equation

Gautschi ($h = 1/10, 1/20$), pseudospectral ($M = 500$)





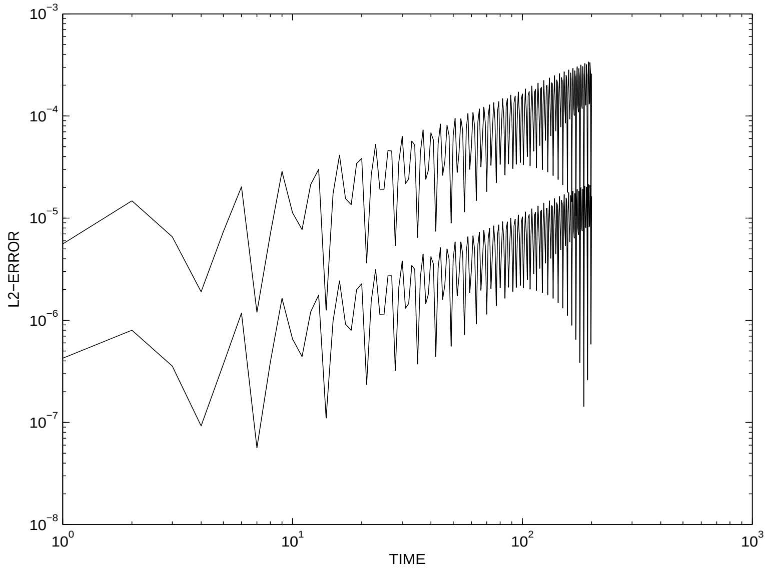
Annihilating frequencies

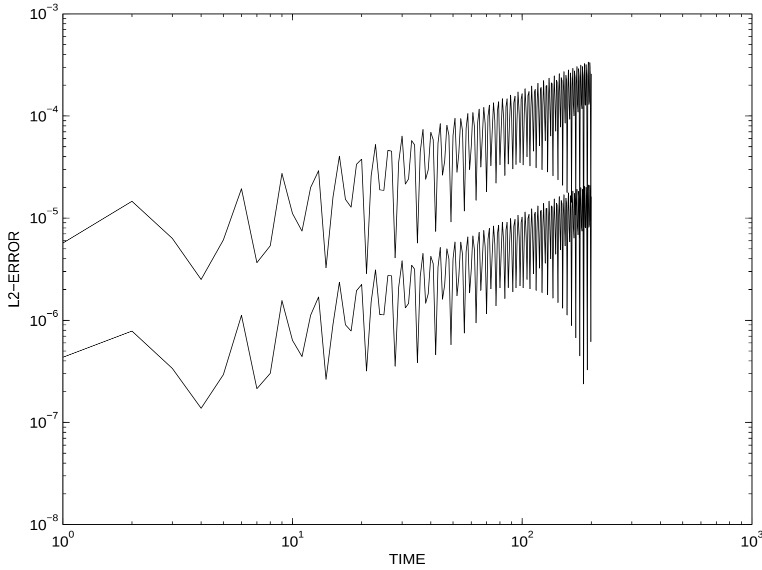
filter function
$\phi(\epsilon) = (\frac{\sin(\epsilon)}{\epsilon})^2(1 + \frac{1-\cos(\epsilon)}{2})$

Numerical comparison

Growth of error with time for the nonlinear wave equation

SMC4 ($h = 1/10, 1/20$), pseudospectral ($M = 500$)





Annihilating frequencies

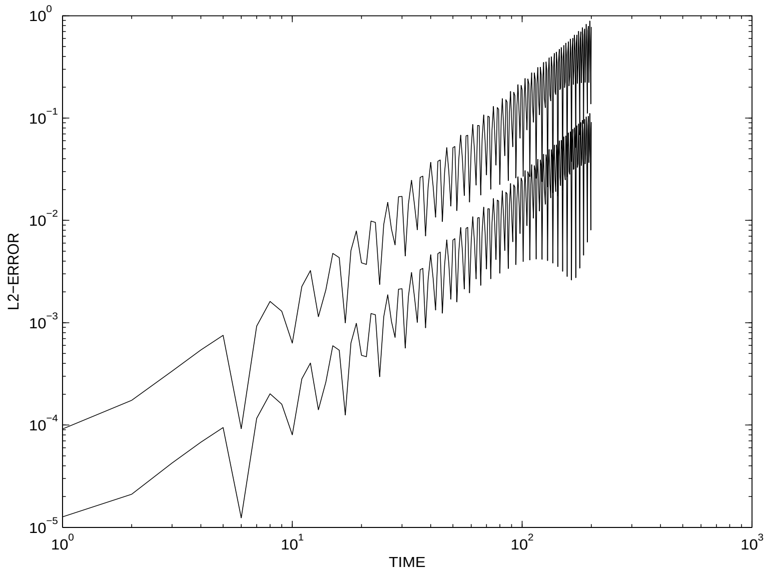
filter function
$\phi(\epsilon) = (\frac{\sin(\epsilon)}{\epsilon})^2[1 + \frac{2}{3}(1 - \cos(\epsilon))]$

Qualitative properties of symmetric methods

Better behaviour with respect to growth of error with time

MC3 (not symmetric) ($h = 1/10, 1/20$),

pseudospectral ($M = 250$)



Quadratic error growth while linear before

Numerical integration of Euler-Bernoulli equation

$$
\begin{aligned}
u_{tt} &= -u_{xxxx} - 0{,}4u^3, \quad x \in [0, 2\pi], \quad 0 \leq t \leq T, \\
u(x,0) &= \frac{5}{2}e^{\frac{\cos(x)}{5}} - \frac{5}{2}, \\
v(x,0) &= e^{\frac{\sin(x)}{5}} - \frac{5}{2},
\end{aligned}
$$

periodic boundary conditions

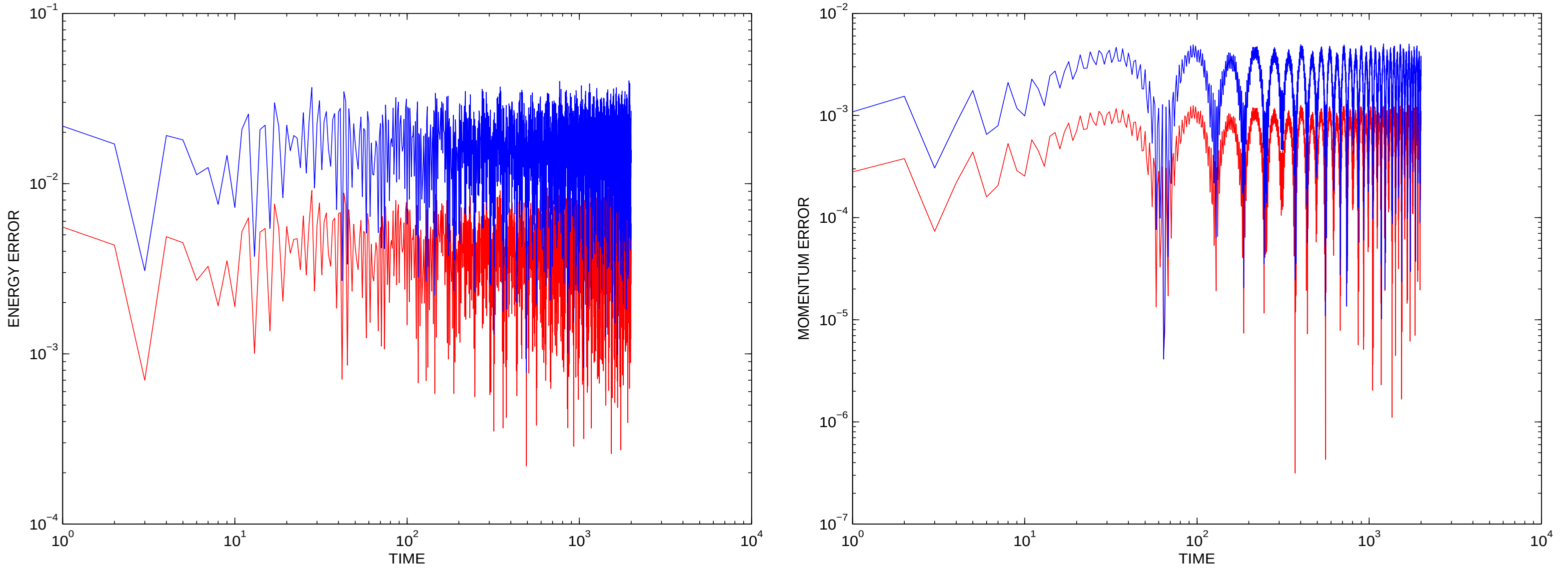
Conserved quantities

$$
\begin{aligned}
H &= \int_a^b [\frac{1}{2}u_t^2 + \frac{1}{2}u_{xx}^2 + 0{,}1u^4)]dx, \\
M &= -\int_a^b u_t u_x dx.
\end{aligned}
$$

Growth of energy and momentum error with time

Gautschi (filtered) ($h = 1/20, 1/40$),

pseudospectral ($M = 10$)



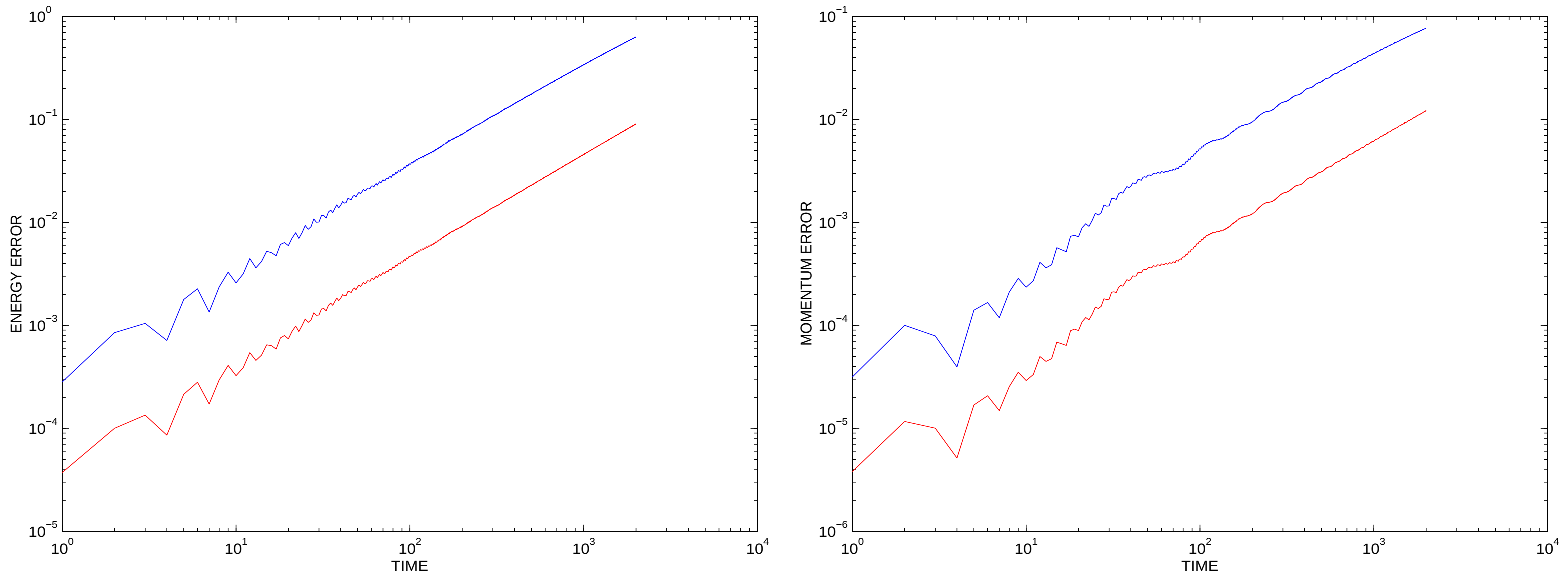
‘bounded ’

$$h = 1/20, \to \lambda_M h = 20, \quad h = 1/40, \to \lambda_M h = 10$$

Growth of energy and momentum error with time

MC3 (filtered) ($h = 1/20, 1/40$),

pseudospectral ($M = 10$)

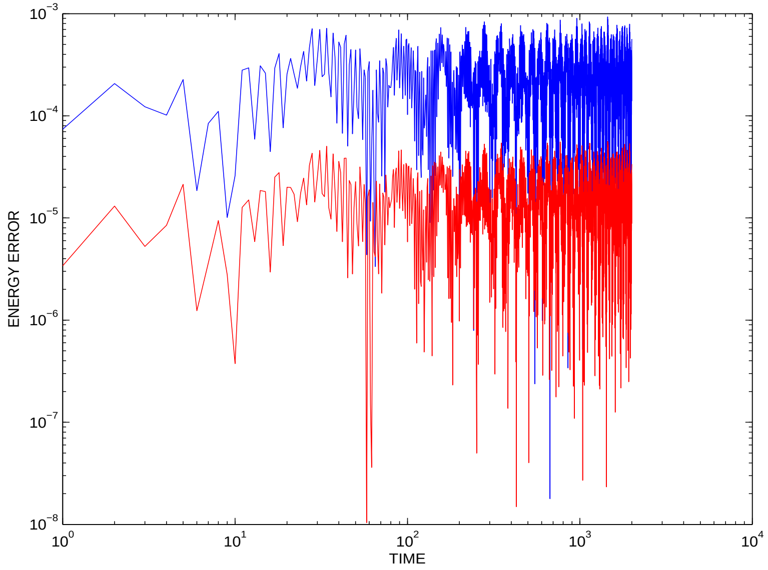


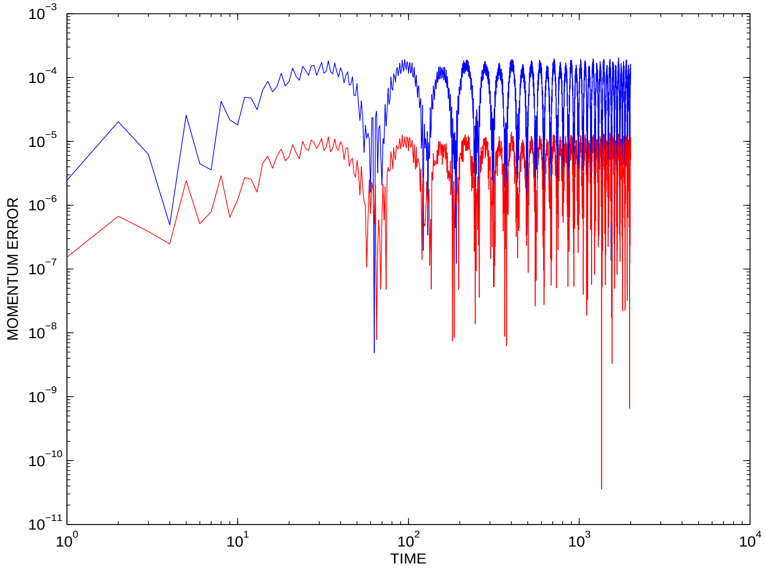
linear error growth

Growth of energy and momentum error with time

SMC4 (filtered) ($h = 1/20, 1/40$),

pseudospectral ($M = 10$)





‘bounded ’