Pf: (symplectic $\Rightarrow$ Hamiltonian)

$$0 = \frac{d}{dt}\left(\left(\frac{\partial \varphi_t}{\partial u_0}\right)^T J \left(\frac{\partial \varphi_t}{\partial u_0}\right)\right)$$

$$= \left(\frac{\partial \varphi_t}{\partial u_0}\right)^T \underbrace{\left(\nabla f(\varphi_t(u_0))^T J + J \nabla f(\varphi_t(u_0))\right)}_{=0} \left(\frac{\partial \varphi_t}{\partial u_0}\right)$$

$t=0$.

$$\nabla f(u_0)^T J + J \nabla f(u_0) = 0, \quad \forall u_0 \in \mathbb{R}^{2d}.$$

$J^T = -J \Rightarrow J \nabla f(u) = (J \nabla f(u))^T, \quad \forall u.$

By integrability lemma, $\exists$ $H(u)$

$$J f(u) = \nabla H(u) \Rightarrow f(u) = J^{-1} \nabla H(u) \quad \square.$$

Thm (existence of modified Hamiltonian)

$u_{n+1} = \Phi_h(u_n)$ applied to $\dot{u} = J^{-1} \nabla H(u)$

w. smooth $H: \mathbb{R}^{2d} \to \mathbb{R}$. then modified eq is Hamiltonian. i.e.

for each term f_j in backward error analysis.

there exists $H_j : \mathbb{R}^{2d} \to \mathbb{R}$. s.t

$$f_j(u) = J^{-1} \nabla H_j(u), \quad \forall u.$$

Pf: Induction.

$j=1$, true. $f_1 \equiv f = J^{-1} \nabla H$

Assume truncated modified eq.

$$\dot{\tilde{u}} = f(\tilde{u}) + h f_2(\tilde{u}) + \cdots + h^{r-1} f_r(\tilde{u}).$$

$\rightarrow$ flow map $\tilde{\varphi}_{r,t}(u_0)$ is symplectic

scheme

$$\Psi_h(u_0) = \tilde{\varphi}_{r,h}(u_0) + h^{r+1} f_{r+1}(u_0) + O(h^{r+2})$$

induction

$$\nabla \Psi_h(u_0) = \nabla \tilde{\varphi}_{r,h}(u_0) + h^{r+1} \nabla f_{r+1}(u_0) + O(h^{r+2})$$

$$J = \left(\nabla \Psi_h(u_0)\right)^T J \left(\nabla \Psi_h(u_0)\right)$$

$$= \nabla \tilde{\varphi}_{r,h}^T(u_0)\, J\, \nabla \tilde{\varphi}_{r,h}(u_0) \qquad \nabla \varphi_{r,h}(u_0) \approx I + O(h)$$

$$+ h^{r+1}\Big(\nabla \tilde{\varphi}_{r,h}^T(u_0)\, J\, \nabla f_{r+1}(u_0)$$

$$+ \nabla f_{r+1}(u_0)^T J\, \nabla \varphi_{r,h}\Big) + O(h^{r+2})$$

$$= J + h^{r+1} \underbrace{\left(J \nabla f_{r+1}(u_0) + \left(\nabla f_{r+1}(u_0)\right)^T J\right)}_{= 0} + O(h^{r+2})$$

$\Rightarrow$ $J \nabla f_{r+1}$ is symmetric $\Rightarrow$ $f_{r+1} = J^{-1} \nabla H_{r+1}$ $\square$.

Thm. (long time preservation of energy).

$H: \mathbb{R}^{2d} \to \mathbb{R}$ smooth.

order p

$u_{n+1} = \Phi_h(u_n)$ symp. w. constant step size h.

$\{u_n\} \subset K$. K is a compact set. then

$h \to 0$, for any m.

modified Hamiltonian

$$\tilde{H}^{(m)} = H(u) + h^p H_{p+1}(u) + \cdots + h^{m-1} H_m(u)$$

we have

$$\tilde{H}^{(M)}(u_N) = \tilde{H}^{(M)}(u_0) + O(th^M)$$

$$H(u_N) = H(u_0) + O(h^p)$$

over time interval $[0, t = Nh]$, $t \leq Ch^{p-M}$.

Remark:

1. constant M is arbitrary if $H \in C^\infty$.

sharper bound can be given if H is real analytic. conservation of energy holds on $[0,t]$, $t \le C e^{+\frac{\gamma}{h}}$, $\gamma > 0$.

2. Fact on compact set.

$\tilde{H}^{(M)}$ locally Lip. cont. $\Rightarrow$ globally Lip. cont.

i.e. $\exists\ L > 0$. s.t.

$$|\tilde{H}^{(M)}(u) - \tilde{H}^{(M)}(v)| \le L \|u-v\|, \quad \forall u, v \in K.$$

$$|H^{p+1}(u) + h H^{p+2}(u) + \cdots + h^{M-1-p} H^{M}(u)| \le C, \quad \forall u \in K.$$

Pf: $\left|\tilde{H}^{(m)}(u_N) - \tilde{H}^{(m)}(u_0)\right|$

$\tilde{H}^{(m)}(u_n) = \tilde{H}^{(m)}(\tilde{\varphi}_{m,h}(u_n))$

Ham. dyn. flow induced by $\tilde{H}^{(m)}$

$$= \left|\sum_{n=0}^{N-1} \tilde{H}^{(m)}(u_{n+1}) - \tilde{H}^{(m)}(u_n)\right|$$

$$= \left|\sum_{n=0}^{N-1} \tilde{H}^{(m)}(u_{n+1}) - \tilde{H}^{(m)}(\tilde{\varphi}_{m,h}(u_n))\right|$$

$$\leq L \sum_{n=0}^{N-1} \left\| u_{n+1} - \tilde{\varphi}_{m,h}(u_n) \right\|$$

$$\leq L\, C \sum_{n=0}^{N-1} h^{m+1} \leq \tilde{C} N h^{m+1} =: O(t h^m)$$

consistency error

Using $|H(u) - \tilde{H}^{(m)}(u)|$ uniformly bounded.

$$\Rightarrow |H(u_N) - H(u_0)| \le O(h^p) + |\tilde{H}^{(m)}(u_N) - \tilde{H}^{(m)}(u_0)|$$

$$\le O(h^p)$$

if $t h^m \le C h^p$. $\square$.

$$\dot{u}(t) = L\,u(t) + N(u(t), t)$$

linear — nonlinear

stiff — non-stiff

implicit — explicit.

Ex. $u_t = \alpha\, u_{xx} + N(u(t), t)$

diffusion. — reaction / source term

Implicit - Explicit method (IMEX)

Ex. Backward - Forward Euler.

$$u_{n+1} = u_n + hL\,u_{n+1} + hN(u_n, t_n)$$

RAS $\quad N(u(t),t) = \lambda u(t), \quad L = c \in \mathbb{R}.$

$$\dot{u} = (c+\lambda)u = cu + \lambda u. \qquad \mathrm{Re}(\lambda + c) < 0.$$

$$u_{n+1} = u_n + ch\,u_{n+1} + \lambda h\,u_n$$

Introduce $\omega = ch$, $z = \lambda h$.

$$(1-\omega)\, u_{n+1} = (1+z)\, u_n .$$

$$R(z;\omega) = \frac{1+z}{1-\omega} .$$

decaying sol $\Rightarrow$ $|1+z| \le |1-\omega|$.

If $|\omega| >> 1$. $|1-\omega| \approx |\omega|$. $\Rightarrow$ $|1+z| \lesssim |\omega|$

Exponential time differencing (ETD)

Use Duhamel's principle.

$$u(t) = e^{Lt} u(0) + \int_0^t e^{L(t-s)} N(u(s), s)\, ds.$$

"ultimate" way of using info of L.

Need to evaluate e^{Lt} matrix exponential.

First focus on scalar case $L = c \in \mathbb{R}$.

ETD-1: Forward Euler for integral.

$$u_{n+1} = e^{ch} u_n + \int_{t_n}^{t_{n+1}} e^{c(t_{n+1}-s)} N(u_n, t_n)\, ds$$

$$= e^{ch} u_n + \frac{e^{ch}-1}{c} N(u_n, t_n)$$

LTE. $\left| u(t_{n+1}) - e^{ch} u(t_n) - \frac{e^{ch}-1}{c} N(u(t_n), t_n) \right|$

$$= \left| \int_{t_n}^{t_{n+1}} e^{c(t_{n+1}-s)} \big(N(u(s), s) - N(u_n, t_n) \big)\, ds \right|$$

$$\le L_N \int_{t_n}^{t_{n+1}} e^{c(t_{n+1}-s)} |u(s) - u(t_n)| \, ds$$

$$\le L_N \max_{0 \le t \le T} |u'(t)| \int_{t_n}^{t_{n+1}} e^{c(t_{n+1}-s)} \cdot |s - t_n| \, ds$$

$\sim O(h^2)$ 1st order method.

vector case ETD-1:

$$u_{n+1} = e^{Lh} u_n + L^{-1}(e^{Lh} - 1) N(u_n, t_n).$$

similarly ETD-n. $\rightarrow$ AB-like.

ETD-RKn $\rightarrow$ RK-like.

How to compute matrix exponentials?

① Taylor expansion.

$A \in \mathbb{C}^{n\times n}$.

$$e^{At} := \sum_{n=0}^{\infty} \frac{t^n}{n!} A^n$$

$$\|e^{At}\|_2 \le \sum_{n=0}^{\infty} \frac{t^n}{n!} \|A\|_2^n = e^{t\|A\|_2} < \infty.$$

well defined for any t, A.

Numerically.

truncate

$$e^{At} \approx \sum_{n=0}^{N} \frac{t^n}{n!} A^n$$

often not efficient enough.

② diagonalization.

Assume A diagonalizable $\begin{cases} \text{theoretically.} \\ \text{practically. } n \text{ not too large.} \end{cases}$

$A = VDV^{-1}$. D diagonal.

$$e^{At} := \sum_{n=0}^{\infty} \frac{t^n}{n!} (VDV^{-1})^n$$

$$= V\left(\sum_{n=0}^{\infty} \frac{t^n}{n!} D^n\right) V^{-1}$$

$$= V e^{tD} V^{-1}$$

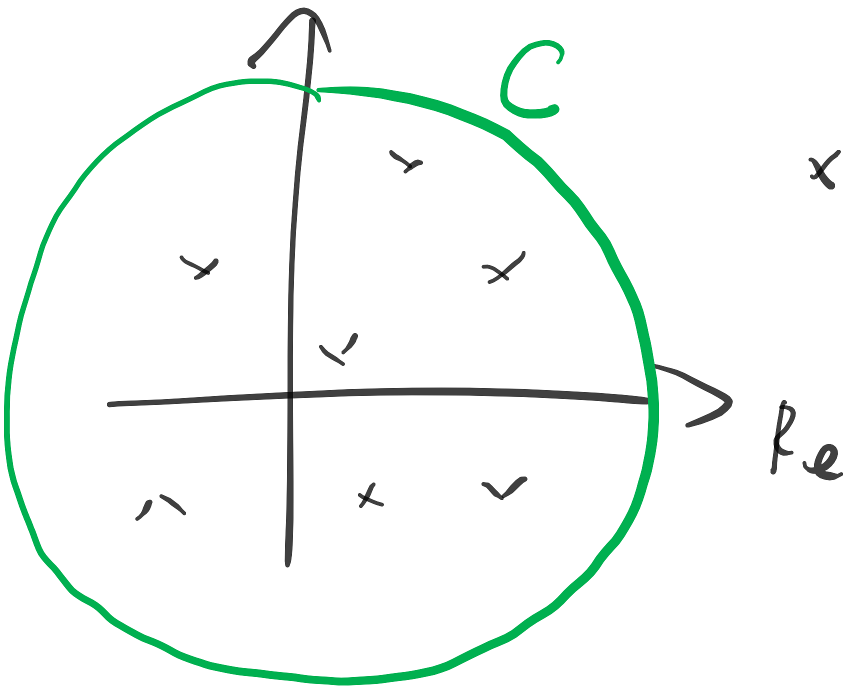
no approximation.

not always efficient enough.

③ Contour integral.

well defined for any matrix A.

For simplicity, A diagonalizable.



× eigenvalues of A

Cauchy contour integral formula.

$$e^{z} = \frac{1}{2\pi i} \oint_C \frac{e^{s}}{s-z}\, ds .$$

<u>Def</u> $e^A := \frac{1}{2\pi i} \oint_c e^s (sI - A)^{-1} ds$

show consistency w. prev. def when A diagonalizable.

$A = V D V^{-1}$

diagonal.

$$\text{RHS} = \frac{1}{2\pi i} \oint_c e^s (sVV^{-1} - VDV^{-1})^{-1} ds$$

$$= \frac{1}{2\pi i} \oint_c e^s V (sI - D)^{-1} V^{-1} ds$$

$$= V \left(\frac{1}{2\pi i} \oint_c e^s (sI - D)^{-1} ds \right) V^{-1}$$

$$= V e^D V^{-1} = e^A$$

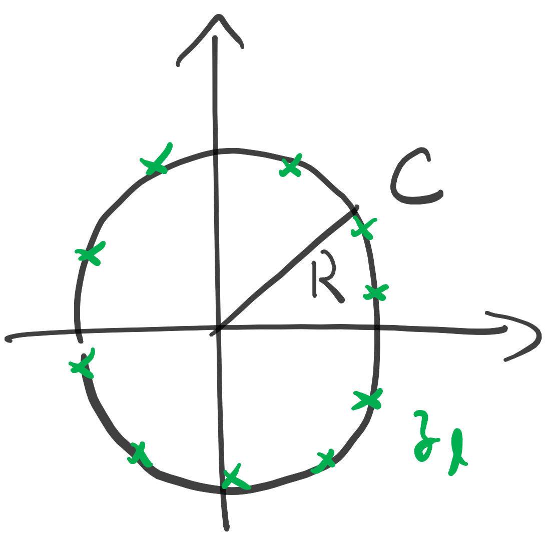
Numerical use?

quadrature on the contour (in $\mathbb{C}$)

parameterize contour using a single real parameter, say $t \in [0,1]$

$\to$ standard contour.

Ex.



$C = \{ z \mid |z| = R \}$.

$= \{ z(\theta) = Re^{i\theta} \mid 0 \le \theta < 2\pi \}$.

$$\frac{1}{2\pi i}\oint_c f(z)\,dz$$

$$= \frac{1}{2\pi i}\int_0^{2\pi} f(Re^{i\theta})\, R i e^{i\theta}\, d\theta$$

$$\approx \frac{1}{2\pi i}\sum_{\ell} \omega_\ell \left(f(Re^{i\theta_\ell})\, R i e^{i\theta_\ell} \right)$$

Apply to e^A.

$$e^A \approx \sum_{\ell=1}^{?} \tilde{\omega}_\ell \,(z_\ell I - A)^{-1}$$

Compute $e^A v \longrightarrow$ requires solving linear eq.

$$(z_\ell I - A)\, u = v$$

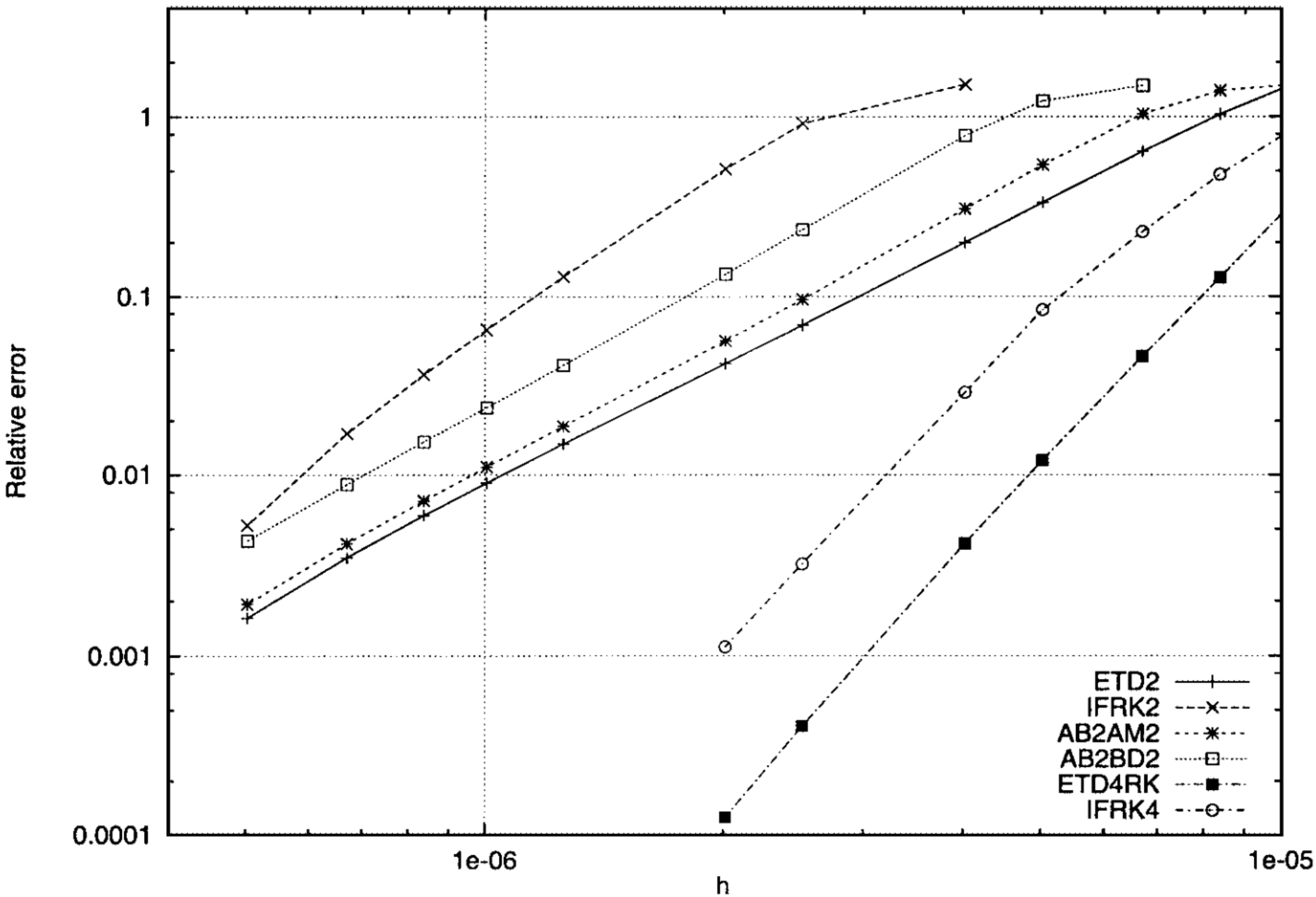


FIG. 9. Error after one soliton period for the KdV equation (59) for six methods.

$$a_n = e^{Lh/2} u_n + L^{-1} \left(e^{Lh/2} - I \right) \mathcal{N}(u_n, t_n)$$

$$b_n = e^{Lh/2} u_n + L^{-1} \left(e^{Lh/2} - I \right) \mathcal{N}(a_n, t_n + h/2)$$

$$c_n = e^{Lh/2} a_n + L^{-1} \left(e^{Lh/2} - I \right) \left(2\mathcal{N}(b_n, t_n + h/2) - \mathcal{N}(u_n, t_n) \right)$$

$$u_{n+1} = e^{Lh} u_n + h^{-2} L^{-3} \left\{ \left[-4 - Lh + e^{Lh} \left(4 - 3Lh + (Lh)^2 \right) \right] \mathcal{N}(u_n, t_n) + \right.$$

$$\left. \cdot\, 2 \left[2 + Lh + e^{Lh} (-2 + Lh) \right] \left(\mathcal{N}(a_n, t_n + h/2) + \mathcal{N}(b_n, t_n + h/2) \right) + \left[-4 - 3Lh - (Lh)^2 + e^{Lh} (4 - Lh) \right] \mathcal{N}(c_n, t_n + h) \right\}$$

[1] S.M. Cox, P.C. Matthews, Exponential Time Differencing for Stiff Systems, J. Comput. Phys. 176 (2002) 430–455.

[2] A.-K. Kassam, L.N. Trefethen, Fourth-Order Time-Stepping for Stiff PDEs, SIAM J. Sci. Comput. 26 (2005) 1214–1233.