Avoiding order reduction when integrating nonlinear Schrödinger equation with Strang method

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Outline

1. Preliminaries
2. Technique to tackle non-homogeneous Dirichlet b.c.
3. Conserving symmetry
4. Possible future research

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Nonlinear Schrödinger equation with homogeneous Dirichlet boundary conditions

$$
\begin{aligned}
&u_t(x,t) = i(\Delta u(x,t) + f(|u(x,t)|^2)u(x,t)) \quad \text{real and smooth } f\\
&u(x,0) = u_0(x), \qquad x \in [a,b],\\
&{\color{red} u(a,t) = u(b,t) = 0}, \qquad t \in [0,T].
\end{aligned}
$$

Example: Finite-difference 2nd-order scheme for space discretization

$$
A_{h,0} = \frac{1}{h^2}\begin{bmatrix} -2 & 1 & 0 & & \\ 1 & -2 & 1 & \ddots & \\ 0 & 1 & -2 & \ddots & 0 \\ & \ddots & \ddots & \ddots & 1 \\ & & 0 & 1 & -2 \end{bmatrix}, \quad P_h w = \begin{bmatrix} w(a+h) \\ \vdots \\ w(b-h) \end{bmatrix}, \quad h = \frac{b-a}{N}
$$

$$
\begin{aligned}
\dot{U}_h &= i(A_{h,0}U_h + f(|U_h|.^2).U_h),\\
U_h(0) &= P_h u_0,
\end{aligned}
\qquad U_h(t) \approx \begin{bmatrix} u(a+h,t) \\ \vdots \\ u(b-h,t) \end{bmatrix}.
$$

Nonlinear Schrödinger equation with periodic boundary conditions

$$
\begin{aligned}
&u_t(x,t) = i(\Delta u(x,t) + f(|u(x,t)|^2)u(x,t)), \quad x \in [a,b],\\
&u(x,0) = u_0(x)\\
&u(a,t) = u(b,t)\\
&u_x(a,t) = u_x(b,t).
\end{aligned}
$$

Example: Pseudospectral space discretization:

$A_{h,0} = F_N^{-1}\mathrm{diag}(-(\frac{2\pi}{b-a})^2 j^2)_{j=-N}^{N-1} F_N$, F_N: discrete Fourier transform, $h = \frac{b-a}{N}$

$$
\begin{array}{rcl}
\dot{U}_h & = & i(A_{h,0}U_h + f(|U_h|.^2).U_h),\\
U_h(0) & = & P_h u_0,
\end{array}
\qquad U_h(t) \approx \begin{bmatrix} u(a+h,t) \\ \vdots \\ u(b-h,t) \end{bmatrix}.
$$

Strang method

Decomposition $\begin{cases} u_t = i\Delta u \\ u_t = if(|u|^2)u \rightarrow |u| \text{ is invariant by time} \end{cases}$

Weideman & Herbst (SIAM, 1986)

$$\frac{d}{dt}|u|^2 = u\bar{u}_t + u_t\bar{u} = -if(|u|^2)u\bar{u} + if(|u|^2)u\bar{u} = 0.$$

Each part can be solved as linear

After space discretization

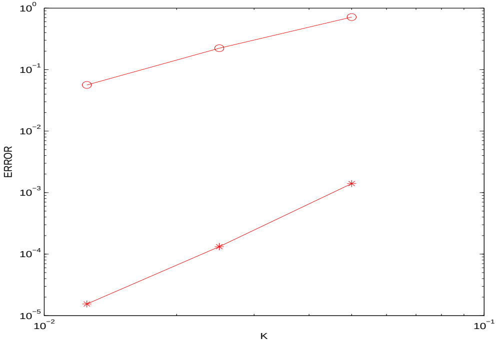
$$U_h^{n+1} = e^{\frac{k}{2}iD_{2,n}} e^{kiA_{h,0}} e^{\frac{k}{2}iD_{1,n}} U_h^n$$

$$D_{1,n} = \text{diag}(f(|U_h^n|.^2)),$$

$$D_{2,n} = \text{diag}(f(|W_h^n|.^2)), \quad W_h^n = e^{kiA_{h,0}} e^{\frac{k}{2}iD_{1,n}} U_h^n$$

Numerical result with 2nd order finite-differences

$$f(x) = 8x, [a,b] = [-50,50], u(x,t) = e^{it}\text{sech}(x)\frac{1+\frac{3}{4}\text{sech}(x)^2(e^{8it}-1)}{1-\frac{3}{4}\text{sech}(x)^4\sin(4t)^2}$$



$*$: Local error

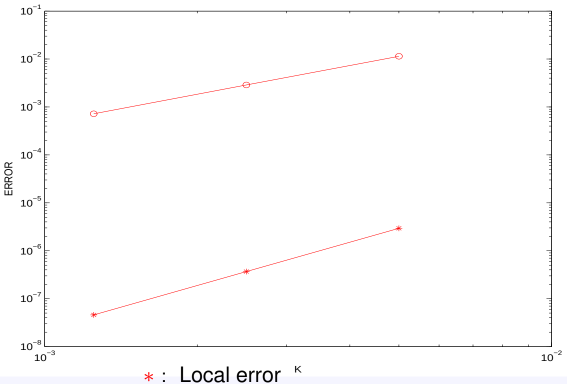
o : Global error till time $T = 1$

k	5×10^{-2}	2.5×10^{-2}	1.25×10^{-2}
Local order		3.41	3.10
Global order		1.68	1.99

$h = 3.125 \times 10^{-2}$

Numer. result with pseudospectral space discret.

$$f(x) = 8x, [a,b] = [-50,50], u(x,t) = e^{it}\mathrm{sech}(x)\frac{1+\frac{3}{4}\mathrm{sech}(x)^2(e^{8it}-1)}{1-\frac{3}{4}\mathrm{sech}(x)^4\sin(4t)^2}$$



$*$: Local error

o : Global error till time $T = 1$

k	5×10^{-3}	2.5×10^{-3}	1.25×10^{-3}
Local order		3.00	3.00
Global order		1.98	2.00

$N = 2000$

Non-homog. Dirichlet bound. cond. $\partial u(t) = g(t)$

If we first integrate in space and then in time:

$$\dot{U}_h(t) = iA_{h,0}U_h(t) + iC_h g(t) + if(|U_h|.^2).U_h$$

Example $\rightarrow$ 2nd-order symmetric FD

$$A_{h,0} = \frac{1}{h^2}\begin{bmatrix} -2 & 1 & 0 & & \\ 1 & -2 & 1 & \ddots & \\ 0 & 1 & -2 & \ddots & 0 \\ & \ddots & \ddots & \ddots & 1 \\ & & 0 & 1 & -2 \end{bmatrix}, \quad C_h g(t) = \frac{1}{h^2}\begin{bmatrix} g_a(t) \\ 0 \\ \vdots \\ 0 \\ g_b(t) \end{bmatrix}$$

As Strang method applied to $\dot{U} = A_1 U + A_2 U + F(t)$ leads to

$$U_h^{n+1} = e^{\frac{k}{2}A_1} e^{\frac{k}{2}A_2}(e^{\frac{k}{2}A_2} e^{\frac{k}{2}A_1} U_h^n + kF(t_n + \frac{k}{2})),$$

In our case, $U_h^{n+1} = e^{\frac{k}{2}iD_{2,n}} e^{\frac{k}{2}iA_{h,0}}(e^{\frac{k}{2}iA_{h,0}} e^{\frac{k}{2}iD_{1,n}} U_h^n + ikC_h g(t_n + \frac{k}{2})),$

$D_{1,n} = \text{diag}(f(|U_h^n|.^2)),$

$D_{2,n} = \text{diag}(f(|W_h^n|.^2)), \quad W_h^n = e^{\frac{k}{2}iA_{h,0}}(e^{\frac{k}{2}iA_{h,0}} e^{\frac{k}{2}iD_{1,n}} U_h^n + ikC_h g(t_n + \frac{k}{2}))$

Non-homog. Dirichlet bound. cond. $\partial u(t) = g(t)$

As we will see later, the results for

$$f(x) = 8x, u(x,t) = e^{it}\operatorname{sech}(x)\frac{1 + \frac{3}{4}\operatorname{sech}(x)^2(e^{8it} - 1)}{1 - \frac{3}{4}\operatorname{sech}(x)^4 \sin(4t)^2}, [a,b] = [0,1]$$

are very poor!!

Source of error:

$C_h g$ can take very big values and does not correspond to the values of any continuous function on $[a, b]$

Non-homog. Dirichlet bound. cond. $\partial u(t) = g(t)$

Another possibility: Considering

$$\Delta z(x,t) = 0, \quad x \in [a,b], \quad z(a,t) = g_a(t), \quad z(b,t) = g_b(t),$$

RK methods in linear problems (Calvo & Palencia (1997))
Splitting meths in diff-react prs (Einkemmer & Ostermann (2015))

Then, for $w = u - z$,

$$\begin{aligned} w_t &= i\Delta w - z_t + if(|w+z|^2)(w+z), \\ w(x,0) &= u_0(x) - z(x,0), \quad x \in [a,b], \quad w(a,t) = w(b,t) = 0. \end{aligned}$$

Decomposition $\begin{cases} w_t = i\Delta w + if(|z|^2)z - z_t, \\ w_t = if(|w+z|^2)(w+z) - if(|z|^2)z, \end{cases}$

Drawbacks:

1. In more dimensions, z and z_t must be numerically calculated
2. The linear eqn is not so directly solvable because of a source term
3. $|w+z|^2$ is not an invariant of the second equation any more

Our suggestion

From u^n,

(1) Integrate in time, with appropiate boundary values, the decomposition of

$$u_t = i\Delta u + if(|u|^2)u,$$

- Let $v/$
$$\left.\begin{array}{l} \dot{v}(s) = if(|u^n|^2)v(s), \\ v(0) = u^n \end{array}\right\} v(\tfrac{k}{2}) \approx u(t_n) + \tfrac{k}{2} if(|u(t_n)|^2)u(t_n)$$
- Let $w/$
$$\left\{\begin{array}{rcl} \dot{w}(s) &=& i\Delta w(s), \\ w(0) &=& v(\tfrac{k}{2}), \\ \partial w(s) &=& \partial[v(\tfrac{k}{2}) + si\Delta v(\tfrac{k}{2})] \\ &\approx& \partial[u(t_n) + \tfrac{k}{2} if(|u(t_n)|^2)u(t_n) + si\Delta u(t_n)]. \end{array}\right.$$
- Let $z/$ $\left\{\begin{array}{l} \dot{z}(s) = if(|w(k)|^2)z(s), \\ z(0) = w(k) \end{array}\right.$
- $u^{n+1} = z(\tfrac{k}{2})$

Boundary of w can be calculated in terms of data

$$i\partial\Delta u(t_n) = \partial[u_t(t_n) - if(|u(t_n)|^2)u(t_n)] = g_t(t_n) - if(|g(t_n)|^2)g(t_n).$$

However, higher order terms of asymptotic expansions cannot be calculated since

$$\begin{aligned}
v(\frac{k}{2}) &\approx u(t_n) + \frac{k}{2}if(|u(t_n)|^2)u(t_n) - \frac{k^2}{4}f(|u(t_n)|^2)^2u(t_n),\\
\partial w(s) &= \partial[v(\frac{k}{2}) + si\Delta v(\frac{k}{2}) - \frac{s^2}{2}\Delta^2 v(\frac{k}{2})]\\
&\approx \partial[u(t_n) + \frac{k}{2}if(|u(t_n)|^2)u(t_n) - \frac{k^2}{4}f(|u(t_n)|^2)^2u(t_n)\\
&\quad +si\Delta u(t_n) - \frac{sk}{2}\Delta(f(|u(t_n)|^2)u(t_n)) - \frac{s^2}{2}\Delta^2 u(t_n)].
\end{aligned}$$

All terms can be calculated except for $\partial\Delta(f(|u(t_n)|^2)u(t_n))$ and $\partial(\Delta^2 u(t_n))$ at the same time.

$$\begin{aligned}
\partial\Delta u_t(t_n) &= \partial[i\Delta^2 u(t_n) + i\Delta(f(|u(t_n)|^2)u(t_n))]\\
&= -ig_{tt}(t_n) - \frac{d}{dt}f(|g(t)|^2)g(t)|_{t=t_n}.
\end{aligned}$$

Our suggestion

(2) Integrate in space each above problem. Considering $U_h^0 = P_h u(0)$, from each U_h^n,

- $\hat{V}_h = V_h(\frac{k}{2}) = e^{\frac{k}{2} i \mathrm{diag}(f(|U_h^n|.^2))} U_h^n$,
- $\begin{cases} \dot{W}_h(s) &= iA_{h,0} W_h(s) + iC_h \partial[u(t_n) + \frac{k}{2} f(|u(t_n)|^2) u(t_n)) + si\Delta u(t_n)] \\ W_h(0) &= \hat{V}_h \end{cases}$

$$\begin{aligned} \hat{W}_h &= W_h(k) = e^{ikA_{h,0}} \hat{V}_h + i \int_0^k e^{i(k-s)A_{h,0}} C_h \partial[u(t_n) + \frac{k}{2} f(|u(t_n)|^2) u(t_n)) + si\Delta u(t_n)] ds \\ &= e^{ikA_{h,0}} \hat{V}_h + ik\varphi_1(ikA_{h,0}) C_h \partial[u(t_n) + \frac{k}{2} f(|u(t_n)|^2) u(t_n)] - k^2 \varphi_2(ikA_{h,0}) C_h \partial \Delta u(t_n), \end{aligned}$$

where $\varphi_j(itA_{h,0}) = \frac{1}{t^j} \int_0^t e^{i(t-\tau)A_{h,0}} \frac{\tau^{j-1}}{(j-1)!} d\tau, \quad j \geq 1.$

$\varphi_1(z) = \frac{e^z - 1}{z}, \quad \varphi_2(z) = \frac{\varphi_1(z) - 1}{z} = \frac{e^z - 1 - z}{z^2}.$

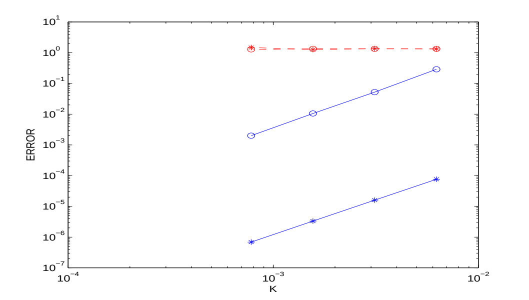
- $U_h^{n+1} = \hat{Z}_h = Z_h(\frac{k}{2}) = e^{i\frac{k}{2} \mathrm{diag}(f(|\hat{W}_h^n|.^2))} \hat{W}_h^n.$

Remarks on $\varphi_1(ikA_{h,0})$ and $\varphi_2(ikA_{h,0})$

- The information on the boundary enters at each step through multiplication by these matrices
- For fixed stepsize k, they can be calculated once and for all at the very beginning.
- For 2nd-order symmetric FD, $C_h g$ is a vector which just has 2 non-vanishing components $\Rightarrow$ Just the first and last column of $\varphi_j(ikA_{h,0})$ are in fact necessary.
- For fixed stepsize k and 2nd-order FD, once those two columns are calculated at the very beginning, just a suitable linear combination of those two columns must be added to the method at each step with this procedure.

Numer. result avoiding and without avoiding O. R.

$$f(x) = 8x, [a, b] = [0, 1], u(x, t) = e^{it}\mathrm{sech}(x)\frac{1+\frac{3}{4}\mathrm{sech}(x)^2(e^{8it}-1)}{1-\frac{3}{4}\mathrm{sech}(x)^4\sin(4t)^2}$$



$\color{red}{*}$: Local error without avoiding order reduction

$\color{red}{o}$: Global error till time $T = 1$ without avoiding order reduction

$\color{blue}{*}$: Local error avoiding order reduction

$\color{blue}{o}$: Global error till time $T = 1$ avoiding order reduction

k	6.25×10^{-3}	3.125×10^{-3}	1.5625×10^{-3}	7.8125×10^{-4}
Local order		2.26	2.26	2.27
Global order		2.47	2.31	2.40

$h = 2.5 \times 10^{-3}$

Local error

Local error of the time discretization: Whenever $u \in C([0,T], H^4([a,b]))$, $f(|u|^2)u \in C([0,T], H^2([a,b]))$, $f(|u|^2)^2 u \in C([0,T], L^2([a,b]))$,

$$\rho_{n+1} = \|u(t_{n+1}) - \overline{u}^{n+1}\|_{L^2(a,b)} = O(k^2).$$

Local error after full discretization: Whenever f is locally Lipschitz continuous, $e^{i\frac{k}{2}f(|u|^2)}u$, $\Delta(f(|u|^2)u)$, $\Delta^2 u$ exist and belong to $C([0,T], H^4([a,b]))$, for 2nd-order symmetric FD,

$$\rho_{n+1,h} = \|P_h u(t_{n+1}) - \overline{U}_h^{n+1}\|_{L_h^2(a,b)} = O(k^2 + kh^2).$$

In our experiments, kh^2 is negligible compared to k^2.

Idea of the proof

- Let $\overline{v}/$ $\left.\begin{array}{l}\dot{\overline{v}}(s) = if(|u(t_n)|^2)\overline{v}(s), \\ \overline{v}(0) = u(t_n)\end{array}\right\} \overline{v}(\frac{k}{2}) = e^{\frac{k}{2} if(|u(t_n)|^2)} u(t_n)$
- Let $\overline{w}/$ $\left\{\begin{array}{rcl}\dot{\overline{w}}(s) & = & i\Delta\overline{w}(s), \\ \overline{w}(0) & = & \overline{v}(\frac{k}{2}) = e^{\frac{k}{2} if(|u(t_n)|^2)} u(t_n), \\ \partial\overline{w}(s) & = & \partial w(s) = \partial w_B(s)\end{array}\right.$

  $w_B(s) = u(t_n) + \frac{k}{2} if(|u(t_n)|^2) u(t_n) + si\Delta u(t_n)$
- Let $\overline{z}/$ $\left\{\begin{array}{l}\dot{\overline{z}}(s) = if(|\overline{w}(k)|^2)\overline{z}(s), \\ \overline{z}(0) = \overline{w}(k)\end{array}\right.$
- $\overline{u}^{n+1} = \overline{z}(\frac{k}{2})$

Idea of the proof

$$
\begin{aligned}
\dot{\overline{w}}(s) - \dot{w}_B(s) &= i\Delta\overline{w}(s) - i\Delta u(t_n) = i\Delta(\overline{w}(s) - w_F(s)) + i\Delta(w_F(s) - u(t_n)) \\
&= i\Delta(\overline{w}(s) - w_B(s)) - \frac{k}{2}\Delta(f(|u(t_n)|^2)u(t_n) - s\Delta^2 u(t_n) \\
\overline{w}(0) - w_F(0) &= O(k^2) \\
\partial[\overline{w}(s) - w_B(s)] &= 0.
\end{aligned}
$$

Through variation-of-constants formula

$$
\overline{w}(s) - w_B(s) = e^{ik\Delta_0}O(k^2) - \frac{k^2}{2}\varphi_1(ik\Delta_0)\Delta(f(|u(t_n)|^2)u(t_n)) - k^2\varphi_2(ik\Delta_0)\Delta^2 u(t_n),
$$

where

Δ_0: Laplacian operator applied over functions which vanish on the boundary
$e^{ik\Delta_0}, \varphi_1(ik\Delta_0), \varphi_2(ik\Delta_0)$: well-known to be bounded operators

$$
\begin{aligned}
\Rightarrow \overline{w}(k) &= u(t_n) + \frac{k}{2} if(|u(t_n)|^2)u(t_n) + ki\Delta u(t_n) + O(k^2) \\
\Rightarrow \overline{u}^{n+1} &= \overline{z}(\frac{k}{2}) = e^{i\frac{k}{2}f(|\overline{w}(k)|^2)}\overline{w}(k) \\
&= u(t_n) + kif(|u(t_n)|^2)u(t_n) + ki\Delta u(t_n) + O(k^2) = u(t_{n+1}) + O(k^2).
\end{aligned}
$$

Global error after full discretization

Classical argument for global error $\rightarrow$ Order 1

Under more assumptions of regularity, $\rightarrow$ Order 2

using

1. $$\|ki\Delta_0 \sum_{r=1}^{n-1} e^{irk\Delta_0} u\|_{L^2(\Omega)} \leq T\|u\|_{H^2(\Omega)}.$$

   G. Dujardin (APNUM, 2009)
2. a summation-by-parts argument ($\Delta_0^{-1}\rho_n = O(k^3)$)

Is symmetry lost with this technique?

When looking at time discretization, the suggested values for the boundary of w are based on asymptotic expansions of $v(\frac{k}{2})$ on t_n. If we want to preserve symmetry, when integrating backwards from t_{n+1}, that boundary should be the same.

We can try to approximate $\partial[v(\frac{k}{2}) + si\Delta v(\frac{k}{2})]$ through values of the solution on $t_{n+\frac{1}{2}} = t_n + \frac{k}{2}$:

$$\begin{aligned} v(\frac{k}{2}) &\approx u(t_n) + \frac{k}{2} if(|u(t_n)|^2)u(t_n) + O(k^2) \\ &= u(t_{n+\frac{1}{2}}) - \frac{k}{2} i\Delta u(t_{n+\frac{1}{2}}) + O(k^2) \\ \Delta v(\frac{k}{2}) &\approx \Delta u(t_n) = \Delta u(t_{n+\frac{1}{2}}) + O(k) \end{aligned}$$

Therefore, we suggest $\partial w(s) = \partial[u(t_{n+\frac{1}{2}}) + (s - \frac{k}{2}) i\Delta u(t_{n+\frac{1}{2}})]$

Both terms can also be calculated in terms of data!!

Proof of symmetry

Starting from $u^{n+1}= e^{i\frac{k}{2}f(|w(k)|^2)}w(k) \to |u^{n+1}| = |w(k)|$, and advancing $-k$, we arrive at u^n

- $\left\{ \begin{array}{l} \dot{\tilde{v}}(s) = if(|u^{n+1}|^2)\tilde{v}(s), \\ \tilde{v}(0) = u^{n+1} \end{array} \right.$ $\tilde{v}(-\frac{k}{2}) = e^{-i\frac{k}{2}f(|u^{n+1}|^2)}e^{i\frac{k}{2}f(|w(k)|^2)}w(k) = w(k)$

- $\left\{ \begin{array}{rcl} \dot{\tilde{w}}(s) & = & i\Delta\tilde{w}(s), \\ \tilde{w}(0) & = & w(k), \\ \partial\tilde{w}(s) & = & \partial[u(t_{n+\frac{1}{2}}) + (s+\frac{k}{2})i\Delta u(t_{n+\frac{1}{2}})]. \end{array} \right.$

$\tilde{w}(s) = w(s+k)$

$$\left\{ \begin{array}{l} \text{They satisfy the same equation} \\ \text{Same value at } s=0 \to \tilde{w}(0) = w(k), \\ \text{Same boundary } \to \partial w(s+k) = \partial[u(t_{n+\frac{1}{2}}) + (s+\frac{k}{2})i\Delta u(t_{n+\frac{1}{2}})] \\ \qquad\qquad\qquad\qquad\qquad\qquad = \partial\tilde{w}(s). \end{array} \right.$$

$\Rightarrow \tilde{w}(-k) = w(0)$

Proof of symmetry

- $\left\{ \begin{array}{l} \dot{\tilde{z}}(s) = if(|\tilde{w}(-k)|^2)\tilde{z}(s), \\ \tilde{z}(0) = \tilde{w}(-k) = w(0) \end{array} \right. \quad \tilde{z}(-\frac{k}{2}) = e^{-i\frac{k}{2}f(|w(0)|^2)}w(0)$

  As $w(0) = v(\frac{k}{2})$, $v(\frac{k}{2}) = e^{i\frac{k}{2}f(|u^n|^2)}u^n \rightarrow |v(\frac{k}{2})| = |u^n|$,

  $\tilde{z}(-\frac{k}{2}) = e^{-i\frac{k}{2}f(|v(\frac{k}{2})|^2)}v(\frac{k}{2}) = e^{-i\frac{k}{2}f(|u^n|^2)}e^{i\frac{k}{2}f(|u^n|^2)}u^n = u^n$

Symmetry is proved!

Is symmetry also conserved exactly after space discretization?

Starting from $U_h^{n+1} = e^{i\frac{k}{2}\mathrm{diag}(|f(\hat{W}_h)|.^2)}\hat{W}_h$ and advancing with stepsize $-k$, do we arrive at U_h^n?

$$
\begin{aligned}
\hat{\tilde{V}}_h &= \tilde{V}_h(-\frac{k}{2}) = e^{-\frac{k}{2}i\mathrm{diag}(f(|\hat{W}_h^n|.^2))}e^{\frac{k}{2}i\mathrm{diag}(f(|\hat{W}_h^n|.^2))}\hat{W}_h^n = \hat{W}_h^n,\\
\hat{\tilde{W}}_h &= \tilde{W}_h(-k) = e^{-ikA_{h,0}}\hat{W}_h - ik\varphi_1(-ikA_{h,0})C_h\partial[u(t_{n+\frac{1}{2}}) + i\frac{k}{2}Au(t_{n+\frac{1}{2}})]\\
&\qquad -k^2\varphi_2(-ikA_{h,0})C_h\partial\Delta u(t_{n+\frac{1}{2}})\\
&= e^{-ikA_{h,0}}\Big[e^{ikA_{h,0}}\hat{V}_h + ik\varphi_1(ikA_{h,0})C_h\partial[u(t_{n+\frac{1}{2}}) - i\frac{k}{2}Au(t_{n+\frac{1}{2}})]\\
&\qquad -k^2\varphi_2(ikA_{h,0})C_h\partial\Delta u(t_{n+\frac{1}{2}})\Big]\\
&\qquad -ik\varphi_1(-ikA_{h,0})C_h\partial[u(t_{n+\frac{1}{2}}) + i\frac{k}{2}Au(t_{n+\frac{1}{2}})] - k^2\varphi_2(-ikA_{h,0})C_h\partial\Delta u(t_{n+\frac{1}{2}})\\
&= \hat{V}_h + ik[e^{-ikA_{h,0}}\varphi_1(ikA_{h,0}) - \varphi_1(-ikA_{h,0})]C_h\partial u(t_{n+\frac{1}{2}})\\
&\quad +k^2[\frac{1}{2}(e^{-ikA_{h,0}}\varphi_1(ikA_{h,0}) + \varphi_1(-ikA_{h,0})) - e^{-ikA_{h,0}}\varphi_2(ikA_{h,0}) - \varphi_2(-ikA_{h,0})]C_h\partial Au(t_{n+\frac{1}{2}})
\end{aligned}
$$

Is symmetry also conserved exactly after space discretization?

Coeffs of k and k^2 vanish

$$\varphi_1(z)=\frac{e^z-1}{z};\ e^{-z}\varphi_1(z)=\frac{1-e^{-z}}{z}=\varphi_1(-z);\ \varphi_2(z)=\frac{\varphi_1(z)-1}{z};\ e^{-z}\varphi_2(z)=\frac{\varphi_1(-z)-e^{-z}}{z};$$

$$\begin{aligned}
k &: e^{-z}\varphi_1(z)-\varphi_1(-z)=0;\\
k^2 &: \frac{1}{2}(e^{-z}\varphi_1(z)+\varphi_1(-z))-e^{-z}\varphi_2(z)-\varphi_2(-z)\\
&= \varphi_1(-z)-\frac{\varphi_1(-z)-e^{-z}}{z}+\frac{\varphi_1(-z)-1}{z}=0;
\end{aligned}$$

$$\begin{aligned}
\hat{\tilde{W}}_h &= \hat{V}_h\\
\hat{\tilde{Z}}_h &= e^{-i\frac{k}{2}\mathrm{diag}(f(|\hat{\tilde{W}}_h|.^2))}\hat{\tilde{W}}_h=e^{-i\frac{k}{2}\mathrm{diag}(f(|\hat{V}_h|.^2))}\hat{V}_h=U_h^n
\end{aligned}$$

$$\hat{V}_h=e^{i\frac{k}{2}\mathrm{diag}(f(|U_h^n|.^2))}U_h^n\Rightarrow|\hat{V}_h|=|U_h^n|$$

Quantative possible benefits of symmetry

- From a qualitative point of view, with symmetry, reversibility of equation is conserved
- But, how symmetry can benefit in a quantitative way the integration of the problem?

  * For ODEs, PDEs with periodic or homogeneous boundary conditions, symmetry $\Rightarrow$ better quantitative behaviour in the long term

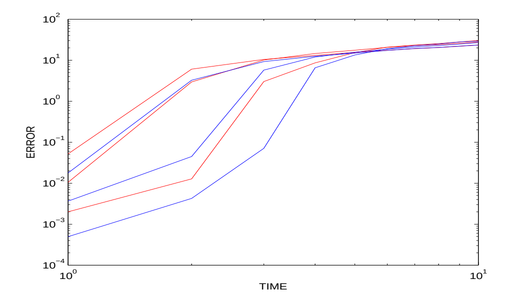
  Good approximation of conserved quantities is observed

  Calvo & Hairer (1995) $\rightarrow$ one-step methods integrating Hamiltonian ODEs
  Cano & Sanz-Serna (1997) $\rightarrow$ one-step methods integrating periodic orbits of ODEs
  Cano & Sanz-Serna (1998) $\rightarrow$ multistep methods integrating periodic orbits of ODEs
  Cano & Durán (2003) $\rightarrow$ adaptive multistep methods integrating periodic orbits of ODEs
  Hairer & Lubich (2004) $\rightarrow$ multistep methods integrating Hamiltonian ODEs
  Cano (2013) $\rightarrow$ multistep cosine methods integrating nonlinear wave eqns with period. b.c.

  * For PDEs with non-homogeneous boundary conditions, the continuous problem does not conserve those quantities any more.

Error growth in the problem at hand

$$f(x) = 8x, [a,b] = [0,1], u(x,t) = e^{it}\mathrm{sech}(x)\frac{1+\frac{3}{4}\mathrm{sech}(x)^2(e^{8it}-1)}{1-\frac{3}{4}\mathrm{sech}(x)^4\sin(4t)^2}$$



– : Global error with non-symmetric technique to avoid O. R.
– : Global error with symmetric technique to avoid O. R.

$$k = 3.125 \times 10^{-3}, 1.5625 \times 10^{-3}, 7.8125 \times 10^{-4}, \qquad h = 2.5 \times 10^{-3}$$