Exponential integrators for the non-linear Schrödinger equation

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Abstract

We present numerical experiments from applying exponential integrators to the nonlinear Schrödinger equation. With periodic boundary conditions, the semi-discretised system becomes diagonal after a Fourier transform, and exponential integrators may therefore be implemented cheaply for our problem.

Our experiments indicate that the observed global error is not affected by the smoothness of initial data when the schemes due to Lawson (1967) are applied, as opposed to the Cox and Matthews and Lie group schemes. We present some analysis on a simplified problem to explain this.

(25 minute talk)

Overview

1. The Schrödinger equation
   - The non-linear Schrödinger equation
   - Semi-discretisation
2. Exponential integrators
   - Method format
   - Schemes
   - Numerical tests
3. Analysis
   - Local error
   - Global error
   - The end

The non-linear Schrödinger equation

Our aim is to solve the nonlinear Schrödinger equation,

$$\mathrm{i}\frac{\partial \psi}{\partial t} = -\frac{\partial^2 \psi}{\partial x^2} + (V(x) + C_{\mathrm{nl}}|\psi|^2)\psi, \quad x \in [-\pi, \pi]$$

where $V(x)$ is some potential and C_{nl} is the nonlinearity constant. We impose an initial condition and a periodic boundary condition,

$$\psi(x,0) = \psi_0(x), \quad x \in [-\pi,\pi]$$
$$\psi(-\pi,t) = \psi(\pi,t), \quad t > 0.$$

- We want an *explicit* integrator.

Semi-discretisation

We do a Fourier transform of the system, setting

$$\psi_n(x,t) = \sum_{k=-\frac{N_{\mathcal{F}}}{2}}^{\frac{N_{\mathcal{F}}}{2}-1} c_k(t)\mathrm{e}^{\mathrm{i}kx},$$

where $N_{\mathcal{F}}$ is a power of two, yielding

$$\begin{aligned} \frac{\mathrm{d}c}{\mathrm{d}t} &= Lc + N(c), \qquad \text{where} \\ N(c) &= -\mathrm{i}\cdot\mathcal{F}\Big(\big(V(x) + C_{\mathrm{nl}}|\mathcal{F}^{-1}(c)|^2\big)\mathcal{F}^{-1}(c)\Big) \\ L &= \mathrm{diag}(-\mathrm{i}k^2) \end{aligned}$$

Exponential integrators

We write all (explicit) integrators for solving $\dot{u} = Lu + N(u)$ in the format:

$$N_r = N\left(a_r^0(hL)u_0 + h\sum_{j=1}^{r-1} a_r^j(hL)N_j\right), \quad r = 1, \dots, s$$

$$u_1 = b^0(hL)u_0 + h\sum_{r=1}^{s} b^r(hL)N_r$$

and the coefficient functions $a_r^j(z)$ and $b^r(z)$ are written in the tableau

$$\begin{array}{c|cccc} c_1 & & & & \\ c_2 & a_2^1(z) & & & \\ \vdots & \vdots & \ddots & & \\ c_s & a_s^1(z) & \dots & a_s^{s-1}(z) & \\ \hline & b^1(z) & \dots & b^{s-1}(z) & b^s(z) \end{array}$$

For exponential integrators, $a_r^0(z) = \mathrm{e}^{c_r z}$, $b^0(z) = \mathrm{e}^z$.

Fourth order Lawson scheme

$$
\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2}e^{z/2} & & & \\
\frac{1}{2} & & \frac{1}{2} & & \\
1 & & & e^{z/2} & \\
\hline
 & \frac{1}{6}e^{z} & \frac{1}{3}e^{z/2} & \frac{1}{3}e^{z/2} & \frac{1}{6}
\end{array}
$$

In general, Lawson schemes may be written as

$$
a_r^j(z) = \alpha_r^{j,0} e^{(c_r - c_j)z} \quad \text{and} \quad b^r(z) = \beta^{r,0} e^{(1-c_r)z}.
$$

where $\alpha_r^{j,0}$, $\beta^{r,0}$ and c_r are the coefficients from the underlying Runge–Kutta scheme.

Commutator-free, order 4

$$
\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2}\phi_0(z/2) & & & \\
\frac{1}{2} & & \frac{1}{2}\phi_0(z/2) & & \\
1 & \frac{z}{4}\phi_0(z/2)^2 & & \phi_0(z/2) & \\
\hline
 & \frac{1}{2}\phi_0(z) - \frac{1}{3}\phi_0(z/2) & \frac{1}{3}\phi_0(z) & \frac{1}{3}\phi_0(z) & -\frac{1}{6}\phi_0(z) + \frac{1}{3}\phi_0(z/2)
\end{array}
$$

where

$$\phi_0(z) = \frac{e^z - 1}{z}$$

- Lie group method, with the affine Lie group action.

ETD4RK

$$
\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2}\phi_0(z/2) & & & \\
\frac{1}{2} & & \frac{1}{2}\phi_0(z/2) & & \\
1 & \frac{z}{4}\phi_0(z/2)^2 & & \phi_0(z/2) & \\
\hline
 & \phi_0 - 3\phi_1 + 2\phi_2 & 2\phi_1 - 2\phi_2 & 2\phi_1 - 2\phi_2 & -\phi_1 + 2\phi_2
\end{array}
$$

where

$$\phi_k(z) = \int_0^1 \mathrm{e}^{(1-\theta)z}\theta^k \, \mathrm{d}\theta$$

- Due to Cox & Matthews 2002.

Runge–Kutta–Munthe-Kaas, order 4

$$
\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2}\phi_0(z/2) & & & \\
\frac{1}{2} & \frac{z}{8}\phi_0(z/2) & \frac{1}{2}\left(1-\frac{z}{4}\right)\phi_0(z/2) & & \\
1 & & & \phi_0(z) & \\
\hline
 & \frac{\phi_0(z)}{6}\left(1+\frac{z}{2}\right) & \frac{\phi_0(z)}{3} & \frac{\phi_0(z)}{3} & \frac{\phi_0(z)}{6}\left(1-\frac{z}{2}\right)
\end{array}
$$

where

$$\phi_0(z) = \frac{e^z - 1}{z}$$

- Lie group method, with the affine Lie group action.
- CFREE4, ETD4RK and RKMK4 are exact on the affine scalar problem $y' = Ly + N$ for L, N constants. They may therefore be denoted *affine* exponential integrators.

Combined Commutator-free and Lawson, order 4

$$
\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2}\phi_0(z/2) & & & \\
\frac{1}{2} & & \frac{1}{2}\phi_0(z/2) & & \\
1 & \frac{z}{4}\phi_0(z/2)^2 & & \phi_0(z/2) & \\
\hline
 & \frac{1}{6}e^{z} & \frac{1}{3}e^{z/2} & \frac{1}{3}e^{z/2} & \frac{1}{6}
\end{array}
$$

- The scheme has $a_r^j(z)$-coefficients from the Commutator-free scheme, and $b^r(z)$-coefficients from the Lawson-scheme.
- This is not an affine integrator.

Crank–Nicolson

- Simplified Jacobian
- 4 Newton-iterations $\Rightarrow$ 4 stages

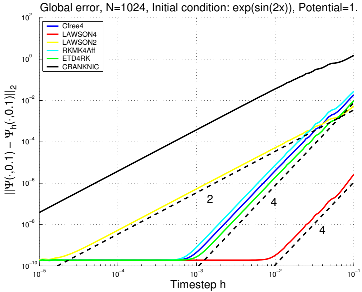
$$
\begin{array}{c|cccc}
0 & & & & \\
1 & \frac{2}{2-z} & & & \\
1 & \frac{1}{2-z} & \frac{1}{2-z} & & \\
1 & \frac{1}{2-z} & & \frac{1}{2-z} & \\
\hline
1 & \frac{1}{2-z} & & & \frac{1}{2-z}
\end{array}
$$

and with $a_r^0(z) = b^0(z) = \frac{1+z/2}{1-z/2}$.

In this form, Crank–Nicolson is also a W-method.

Numerical tests

IC	Potential	Lawson4	AcfreeBlawson	ETD4RK/CFREE4/RKMK4
IC = smooth	$V = \lambda$	4	4	4
	$V =$ smooth	4	4	4
	$V =$ hat	1.25 oscillating	1.25 oscillating	1.65
IC = hat	$V = \lambda$	4	1.75	0.75
	$V =$ smooth	> 2, staircase	2	0.75
	$V =$ hat	1.25 oscillating	1.25 oscillating	0.75



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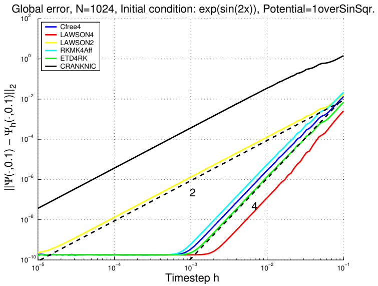

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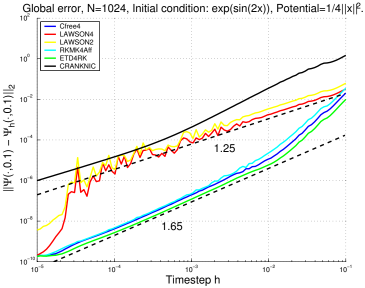

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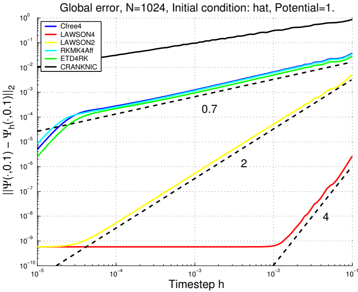

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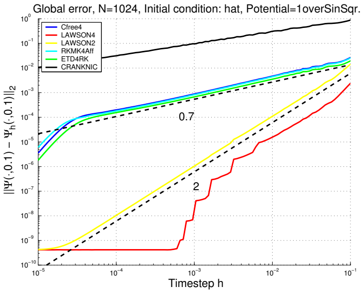

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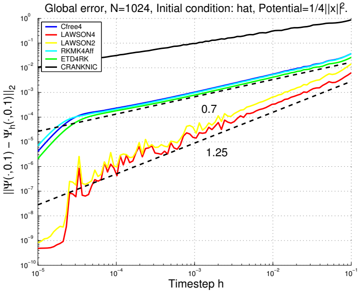


Local error

If $V(x)$ is constant and $C_{\text{nl}} = 0$ in the NLS-equation, one obtains a decoupled system of scalar ODEs. We write the equation for each Fourier mode as a scalar linear equation

$$\dot{y} = Ly + Ny \qquad y(0) = y_0 \tag{1}$$

with exact solution $y(h) = \mathrm{e}^{h(L+N)} y_0$, ($L = -\mathrm{i}k^2$).
The stability function $R(h, L, N)$ for each scheme gives us the local error

Lawson4	$\frac{h^5}{5!} N^5$
ETD4RK	$\frac{h^5}{2880}(3N{\color{red}L^4} - 7N^2L^3 - 4N^3L^2 + 30N^4L + 24N^5)$
RKMK4	$\frac{h^5}{2880}(11N{\color{red}L^4} + 20N^2L^3 + 15N^3L^2 + 30N^4L + 24N^5)$
CFREE4	$\frac{h^5}{480}(N{\color{red}L^4} + 5N^4L + 4N^5)$
AcfreeBlawson	$\frac{h^5}{2880}(15N^2{\color{red}L^3} + 10N^3L^2 - 30N^4L - 24N^5)$

Local error for Lawson-schemes

Proposition

The local error for an explicit p-th order Lawson scheme on the scalar initial value problem $\dot{y} = Ly + Ny, y(0) = 1, L, N \in \mathbf{C}$ *is*

$$\frac{h^{p+1}}{(p+1)!} N^{p+1} + \mathcal{O}(h^{p+2})$$

Proof.

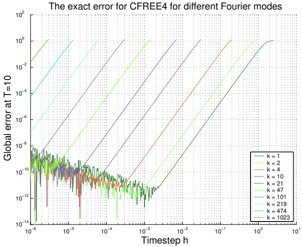
The "change of variables"-trick makes the stability function $\mathrm{e}^{hL} R(hN)$ where $R(hN)$ is the stability function for the underlying RK-scheme. Thus, the local error becomes

$$e = \mathrm{e}^{h(L+N)} - \mathrm{e}^{hL} R(hN) = \mathrm{e}^{hL} \mathcal{O}((hN)^{p+1}) \qquad \square$$

In the matrix case, this is true if $[L, N] = 0$.

The global error for the decoupled case

The effect of having L^4 in the local error for each Fourier mode:



- We have order-four behaviour for $h < h_{\text{crit}}$.
- h_{crit} dominated by the NL^4 term in the local error ($L = -\mathrm{i}k^2$ here).
- For $h > h_{\text{crit}}$, the error is bounded by 2 as long as $hN < 2\sqrt{2}$ (classical stability of RK4C).
- For the Lawson scheme, this plot is equivalent for all k.

Order reduction

For the CFREE/ETD-methods we bound the global error *for each Fourier mode* for the simplified case $y' = -\mathrm{i}k^2 y + Ny$, $y(0) = y_0^k$ by

$$|\mathrm{ge}_k| \leq \begin{cases} 2\left(\frac{hk^2}{S_B}\right)^4 |y_k^0|, & hk^2 \leq S_B \\ 2|y_k^0|, & hk^2 > S_B \end{cases}$$

Order reduction depends on the regularity of the initial function. The decay of the Fourier coefficients in the initial condition is governed by

$$y_k^0 \leq \frac{K_r}{k^r}$$

for some regularity r. For the hat function, $r = 1$.

Order reduction

Summing over all Fourier modes, we obtain

$$\begin{aligned}\frac{1}{4}||\mathrm{ge}||_2^2 &= \frac{1}{4}\sum_{k=-N_{\mathcal{F}}/2}^{N_{\mathcal{F}}/2-1} |\mathrm{ge}_k|^2 \\ &\leq \sum_{|k|\leq\sqrt{S_B/h}} \left(\frac{hk^2}{S_B}\right)^8 |y_k^0|^2 + \sum_{|k|>\sqrt{S_B/h}} |y_k^0|^2 \\ &\leq K_r^2\left(\frac{h}{S_B}\right)^8 \sum_{|k|\leq\sqrt{S_B/h}} k^{16-2r} + K_r^2 \sum_{|k|>\sqrt{S_B/h}} k^{-2r}\end{aligned}$$

Using Euler–MacLaurin with remainder term to find bounds for the sums, we eventually find the reduced global order for $r \leq 8$:

$$||\mathrm{ge}||_2 \leq Ch^{\frac{2r-1}{4}}$$

This is confirmed experimentally:

Predicted and observed order CFREE4:

Conclusions

- The Lawson scheme is competitive for the NLS-equation.
- Affine integrators (CFREE/ETD/RKMK) exhibits order reduction when the initial condition has low regularity.

- *Thank you for your attention!*
- Project webpage

http://www.math.ntnu.no/num/expint/