Fourth Order Exponential Time Integrators for the Nonlinear Schrödinger Equation

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Introduction

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,

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

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

$$\frac{\mathrm{d}c}{\mathrm{d}t} = Lc + N(c), \qquad \text{where}$$

$$N(c) = -\mathrm{i}\cdot\mathcal{F}\big((V(x)+C_{\mathrm{nl}})|\mathcal{F}^{-1}(c)|^2)\mathcal{F}^{-1}(c)\big)$$

$$L = \mathrm{diag}(-\mathrm{i}k^2)$$

Splitting scheme

The semi-discretised system $\dot{c} = Lc + N(c)$ calls for methods utilizing the splitting into a linear part L and a nonlinear part $N(c)$.

The scheme must cope with the unbounded linear part L (the Laplacian). We focus on the following schemes:

- **IF** Integrating factor methods (Maday, Patera, Rønquist)
- **ETD** Exponential Time Differencing (Cox, Matthews, now also Krogstad)
- **LGI** Lie group integrators with affine actions (Munthe-Kaas and others).

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- All these approaches integrate the linear part *exactly* to cope with the unbounded L. The alternative is to use some implicit integrator, which we want to avoid.

Integrating factor

By a change of variables, an integrating factor *ameliorates* the "stiff" part L.

The exact integrating factor e^{tL} applied on the semi-discretised system $\dot{c}(t) = Lc(t) + N(c(t))$ results in

$$\mathrm{e}^{tL}\dot{c}(t) = \mathrm{e}^{tL}Lc(t) + \mathrm{e}^{tL}N(c(t))$$

which is integrated to

$$c(h) = \mathrm{e}^{-hL}c(0) + \mathrm{e}^{-hL}\int_0^h \mathrm{e}^{tL}N(c(t))\,\mathrm{d}t.$$

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- Our methods OIFS, ETD and LGI can all be thought of as *arising from different ways of evaluating the integral above*.

Unified Method format

Framework (Runge–Kutta-like) for all the methods herein:

$$k_i = hN\left(a_{i0}(hL)c_0 + \sum_{j=1}^{i-1} a_{ij}(hL)k_j\right),$$

for $\quad i = 1, \ldots, s$

$$c_1 = b_0(hL)c_0 + \sum_{i=1}^{s} b_i(hL)k_i$$

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- “Variable coefficients” Runge–Kutta method.
- When $L = 0$, the order conditions reduce to standard theory. Our $a_{ij}(0)$ and $b_i(0)$ should correspond to Kutta’s classical fourth order method. Note also $a_{i0}(0) = 1$ and $b_i(0) = 1$.

Unified method format

We will write all our fourth order methods in the four stages, where $z := hL$,

$$
\begin{aligned}
k_1 &= hN\big(a_{10}(z)c_0\big)\\
k_2 &= hN\big(a_{20}(z)c_0 + a_{21}(z)k_1\big)\\
k_3 &= hN\big(a_{30}(z)c_0 + a_{31}(z)k_1 + a_{32}(z)k_2\big)\\
k_4 &= hN\big(a_{40}(z)c_0 + a_{41}(z)k_1 + a_{42}(z)k_2 + a_{43}(z)k_3\big)\\
\hline
c_1 &= b_0(z)c_0 + b_1(z)k_1 + b_2(z)k_2 + b_3(z)k_3 + b_4(z)k_4
\end{aligned}
$$

which is again written in the tableau

$$
\begin{array}{ccccc}
a_{10}(z) & & & & \\
a_{20}(z) & a_{21}(z) & & & \\
a_{30}(z) & a_{31}(z) & a_{32}(z) & & \\
a_{40}(z) & a_{41}(z) & a_{42}(z) & a_{43}(z) & \\
\hline
b_0(z) & b_1(z) & b_2(z) & b_3(z) & b_4(z)
\end{array}
$$

Operator–Integration–Factor methods (OIFS)

A methodology for generating time-splitting schemes. We use the integrating factor $Q(t) = \mathrm{e}^{-tL}$ as we have an autonomous linear part. This corresponds to using an exact solver for the inner time-step in OIFS-methods.

RK4/Exact:

$$k_1 = hN\big(c_0\big)$$

$$k_2 = hN\big(\mathrm{e}^{\frac{hL}{2}} c_0 + \tfrac{1}{2}\mathrm{e}^{\frac{hL}{2}} k_1)\big)$$

$$k_3 = hN\big(\mathrm{e}^{\frac{hL}{2}} c_0 + \tfrac{1}{2} k_2\big)$$

$$k_4 = hN\big(\mathrm{e}^{hL} c_0 + \mathrm{e}^{\frac{hL}{2}} k_3)\big)$$

$$y_1 = \mathrm{e}^{hL} c_0 + \tfrac{1}{6}\big(\mathrm{e}^{hL} k_1 + 2\mathrm{e}^{\frac{hL}{2}}(k_2 + k_3) + k_4\big)$$

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RK4/Exact, Unified method format

Let $hL =: z$,

$$
\begin{array}{ccccc}
1 & & & & \\
\mathrm{e}^{\frac{z}{2}} & \frac{1}{2}\mathrm{e}^{\frac{z}{2}} & & & \\
\mathrm{e}^{\frac{z}{2}} & & \frac{1}{2} & & \\
\mathrm{e}^{z} & & & \mathrm{e}^{\frac{z}{2}} & \\
\hline
\mathrm{e}^{z} & \frac{1}{6}\mathrm{e}^{z} & \frac{1}{3}\mathrm{e}^{\frac{z}{2}} & \frac{1}{3}\mathrm{e}^{\frac{z}{2}} & \frac{1}{6}
\end{array}
$$

Explicit Time Differentiation (ETD)

Cox and Matthews proposed to solve the integral $\int_0^h \mathrm{e}^{tA} b(c(t))\,\mathrm{d}t$ by approximating $b(c(t))$ by an interpolating polynomial.

First order method, ETD1:

$$b(c(t)) \approx b(c_0) \quad \Rightarrow \quad \int_0^h \mathrm{e}^{tA} b(c_0)\,\mathrm{d}t = \frac{\mathrm{e}^{hA}-1}{A} b(c_0)$$

Second order method, ETDRK2:

$$b(c(t)) \approx b(c_0) + t\frac{b(c_1)-b(c_0)}{h} \quad \Rightarrow$$

$$\int_0^h \mathrm{e}^{tA}\left(b(c_0) + t\frac{b(c_1)-b(c_0)}{h}\right)\mathrm{d}t = \frac{\mathrm{e}^{hA}-1-hA}{hA^2}\left(b(c_1)-b(c_0)\right)$$

where c_1 is an approximation of $c(h)$ done via ETD1.

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Fourth order, ETDRK4:

Let $z = hL$,

$$\begin{aligned}
\tilde{k}_1 &= \mathrm{e}^{\frac{z}{2}} c_0 + h\tfrac{1}{2}\alpha(z/2)N(c_0) \\
\tilde{k}_2 &= \mathrm{e}^{\frac{z}{2}} c_0 + h\tfrac{1}{2}\alpha(z/2)N(\tilde{k}_1) \\
\tilde{k}_3 &= \mathrm{e}^{\frac{z}{2}} k_1 + h\tfrac{1}{2}\alpha(z/2)(2N(\tilde{k}_2) - N(c_0)) \\
c_1 &= \mathrm{e}^{z} c_0 + h\beta_1(z)N(c_0) + h\beta_2(z)\left(N(\tilde{k}_1) + N(\tilde{k}_2)\right) + h\beta_3(z)N(\tilde{k}_3)
\end{aligned}$$

and

$$\begin{aligned}
\alpha(z) &= z^{-1}(\mathrm{e}^z - 1) \\
\beta_1(z) &= z^{-3}\left(-4 - z + \mathrm{e}^z(4 - 3z + z^2)\right) \\
\beta_2(z) &= z^{-3}(2 + z + \mathrm{e}^z(-2 + z)) \cdot 2 \\
\beta_3(z) &= z^{-3}\left(-4 - 3z - z^2 + \mathrm{e}^z(4 - z)\right)
\end{aligned}$$

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Fourth, order, ETDRK4, Unifi ed method format:

$$
\begin{aligned}
k_1 &= hN(c_0) \\
k_2 &= hN(\mathrm{e}^{\frac{z}{2}} c_0 + \tfrac{1}{2}\alpha(z/2)k_1) \\
k_3 &= hN(\mathrm{e}^{\frac{z}{2}} c_0 + \tfrac{1}{2}\alpha(z/2)k_2) \\
k_4 &= hN(\mathrm{e}^{z} c_0 + \tfrac{z}{4}\alpha(z/2)^2 k_1 + \alpha(z/2)k_3)
\end{aligned}
$$

$$
\begin{array}{c|cccc}
1 & & & & \\
\mathrm{e}^{\frac{z}{2}} & \frac{1}{2}\alpha(z/2) & & & \\
\mathrm{e}^{\frac{z}{2}} & & \frac{1}{2}\alpha(z/2) & & \\
\mathrm{e}^{z} & \frac{z}{4}\alpha(z/2)^2 & & \alpha(z/2) & \\
\hline
\mathrm{e}^{z} & \beta_1(z) & \beta_2(z) & \beta_2(z) & \beta_3(z)
\end{array}
$$

Lie group integrator — Affine action (LGI)

We have the *affine Lie group*, with elements (A, b) acting on $\mathbb{C}^N$ via the group action $(A, b) \cdot c = Ac + b$, $A \in \mathrm{GL}_N(\mathbb{C})$. The group becomes $\mathrm{GL}_N(\mathbb{C}) \rtimes \mathbb{C}^N$.

The associated *affine Lie algebra* has the exponential map

$$\mathrm{Exp}\,(t(A, b)) = \left(\mathrm{e}^{tA}, \frac{\mathrm{e}^{tA} - 1}{A} b \right)$$

This is put into the framework of Runge–Kutta–Munthe-Kaas methods and we get a RKMK4 method from Kutta's classical 4th order method, and the commutator in $\mathfrak{g}$

$$[(A_2, b_2), (A_1, b_1)] = ([A_2, A_1], A_1 b_2 - A_2 b_1)\,.$$

Commutator-free schemes (LGI)

Commutator-free methods are also based on the *affine Lie group* and is an LGI-method, but unlike RKMK, they avoid the necessity of forming commutators in $\mathfrak{g}$ by extra evaluations of the exponentials. We use the standard 4th order method, denoted CFREE4 with 5 exponentials.

$$
\begin{aligned}
k_1 &= hN(c_0) \\
U_2 &= e^{\frac{hL}{2}} c_0 + \tfrac{1}{2}\alpha(\tfrac{hL}{2}) k_1 \\
k_2 &= hN(U_2) \\
k_3 &= hN(e^{\frac{hL}{2}} c_0 + \tfrac{1}{2}\alpha(\tfrac{hL}{2}) k_2) \\
k_4 &= hN(e^{\frac{hL}{2}} U_2 + \alpha(\tfrac{hL}{2})(k_3 - \tfrac{1}{2}k_1)) \\
U_s &= e^{\frac{hL}{2}} c_0 + \tfrac{1}{12}\alpha(\tfrac{hL}{2})(3k_1 + 2k_2 + 2k_3 - k_4) \\
c_1 &= e^{\frac{hL}{2}} U_s + \tfrac{1}{12}\alpha(\tfrac{hL}{2})(-k_1 + 2k_2 + 2k_3 + 3k_4)
\end{aligned}
$$

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\begin{array}{c|cccc}
1 & & & & \\
e^{\frac{z}{2}} & \frac{1}{2}\alpha(z/2) & & & \\
e^{\frac{z}{2}} & & \frac{1}{2}\alpha(z/2) & & \\
e^{z} & \frac{z}{4}\alpha(z/2)^2 & & \alpha(z/2) & \\
\hline
e^{z} & \frac{\alpha(z/2)}{12}\left(3e^{\frac{z}{2}}-1\right) & \frac{\alpha(z/2)}{6}\left(e^{\frac{z}{2}}+1\right) & \frac{\alpha(z/2)}{6}\left(e^{\frac{z}{2}}+1\right) & \frac{\alpha(z/2)}{12}\left(3-e^{\frac{z}{2}}\right)
\end{array}
$$

- The $a_{ij}(z)$ functions are the same for CFREE4 and ETD4RK.

Runge–Kutta–Munthe-Kaas fourth order (LG

From Munthe-Kaas & Owren (1999) we derive

$$k_1 = hN(c_0)$$

$$k_2 = hN(\mathrm{e}^{\frac{z}{2}} c_0 + \tfrac{1}{2}\alpha(z/2)k_1)$$

$$C_1 = L(k_2 - k_1)$$

$$k_3 = hN(\mathrm{e}^{\frac{z}{2}} c_0 + \alpha(z/2)(\tfrac{1}{2}k_2 - \tfrac{1}{8}C_1)\mathrm{k}_2 - \tfrac{1}{8}\mathrm{C}_1))$$

$$k_4 = hN(\mathrm{e}^{z} c_0 + \alpha(z)k_3)$$

$$C_2 = L(k_1 - 2k_2 + k_4)$$

$$c_1 = \mathrm{e}^{z} c_0 + \tfrac{1}{6}\alpha(z)(k_1 + 2k_2 + 2k_3 + k_4 - C_1 - \tfrac{1}{2}C_2)$$

where C_1 and C_2 represents the two commutators needed.

Runge–Kutta–Munthe-Kaas fourth order (LG

In the unified method format,

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

Crank–Nicolson

- Physicists seem to use Crank–Nicolson almost exclusively, as it is regarded the “best” solver for these problems.
- It is implemented for reference, with Newton-iterations making it comparable to our methods in terms of computational cost.

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- Trapezoidal rule in time, spectral in space:

$$c_1 = c_0 + \frac{h}{2}\left(Lc_0 + Lc_1 + N(c_0) + N(c_1)\right)$$

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- It is implemented for reference, with Newton-iterations making it comparable to our methods in terms of computational cost.
- Trapezoidal rule in time, spectral in space:

$$c_1 = c_0 + \frac{h}{2}\left(Lc_0 + Lc_1 + N(c_0) + N(c_1)\right)$$

- Newton: Solve $F(c_1) = 0$ where

$$F(c_1) = c_1 - c^k - \frac{h}{2}\left(Lc^k + Lc_1 + N(c^k) + N(c_1)\right)$$

and $F'(c_1) = 1 - \frac{hL}{2} - \frac{hN'(c_1)}{2}$ which gives the iteration:

$$c^{k+1} = (1 - hL/2)^{-1}\left(\frac{h}{2}N(c^k) + (1 + hL/2)c_0 + \frac{h}{2}N(c_0)\right)$$

Crank–Nicolson, unified method format

Crank–Nicolson, with simplified Jacobian and 4 iterations, may be put into the framework common for our methods as follows:

$$
\begin{array}{ccccc}
1 & & & & \\
\frac{1+z/2}{1-z/2} & \frac{2}{2-z} & & & \\
\frac{1+z/2}{1-z/2} & \frac{1}{2-z} & \frac{1}{2-z} & & \\
\frac{1+z/2}{1-z/2} & \frac{1}{2-z} & & \frac{1}{2-z} & \\
\hline
\frac{1+z/2}{1-z/2} & \frac{1}{2-z} & & & \frac{1}{2-z}
\end{array}
$$

where we recognise $\frac{1+z/2}{1-z/2}$ as the $(1,1)$ Padé approximant to e^z. This is also a W-method.

Spatial resolution

- The number of Fourier modes, $N_{\mathcal{F}}$, is chosen big, $N_{\mathcal{F}} = 1024$ in all our experiments.
- When $hN_{\mathcal{F}}^2 \lesssim 1$ all methods attain classical order for all initial conditions and potentials tested.
- For $N_{\mathcal{F}} = 1024$ we typically look at the interval $h \in [10^{-6}, 10^{-1}]$, where classical order is *not* expected.

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- For $N_{\mathcal{F}} = 1024$ we typically look at the interval $h \in [10^{-6}, 10^{-1}]$, where classical order is *not* expected.
- $N_{\mathcal{F}} = 1024$ *pose such big "problems" for our integrator, that we can set the nonlinearity constant* $C_{\mathrm{nl}} = 0$.

Initial conditions

- Crucial for observed order (order reduction).
- Decay in Fourier coefficients is connected to differentiability. If a function $c_0(x)$ is p times continuously differentiable, then there exists a K_p such that
$$|c_k^0| < \frac{K_p}{k^p}$$
where $\psi_0(x) = \sum c_k^0(t)\mathrm{e}^{\mathrm{i}kx}$.
- Examples used in experiments
  - Hat function: $\psi_0(x) = \mathrm{abs}(x)$ on $[-\pi, \pi]$, $p = 1$.
  - Smooth function: $\psi_0(x) = \exp(2\sin(x))$ on $[-\pi, \pi]$, $p = \infty$.
  - Randomly generated functions with prescribed regularity $p \in \{1, 2, 3, 4, 5, 6\}$

Potentials

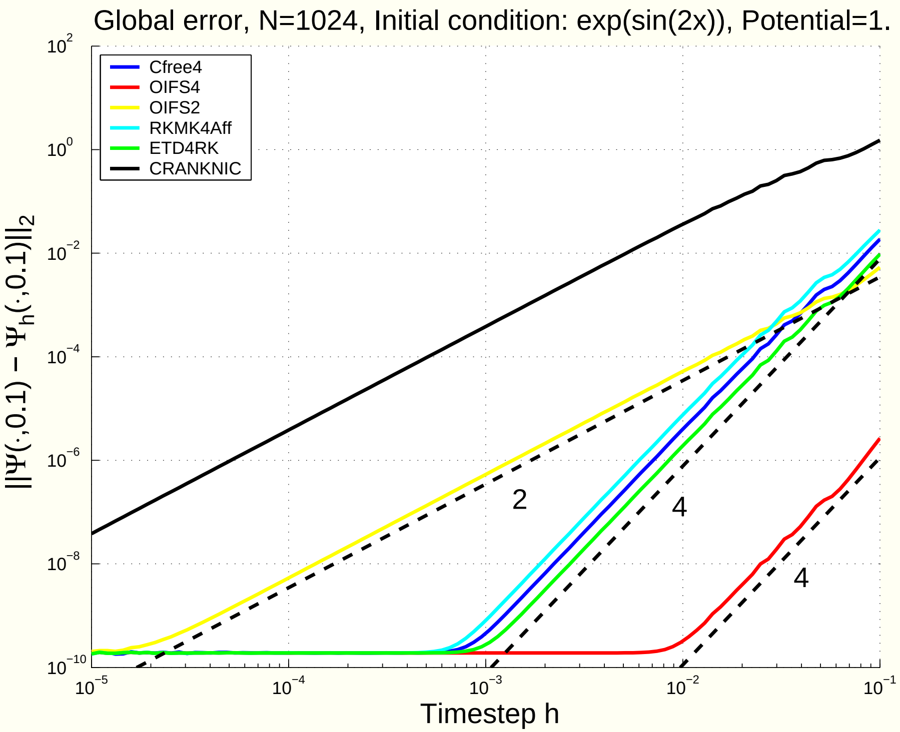
Various potensials $V(x)$ have been used.

- Smooth potential
- Hat potential
- Random potential with prescribed regularity
- Constant potential, $V(x) \equiv \lambda$. The system of equations decouples.

We will see that a potential with low regularity also leads to order reduction.

Numerical tests

IC	Potential	OIFS4 order	ETD4/RKMK4/CFREE4 order
IC = smooth	$V = \lambda$	4	4
	$V =$ smooth	4	4
	$V =$ hat	1.25 oscillating	1.65
IC = hat	$V = \lambda$	4	0.7
	$V =$ smooth	$2 <$ order, staircase	0.7
	$V =$ hat	1.25 oscillating	0.7



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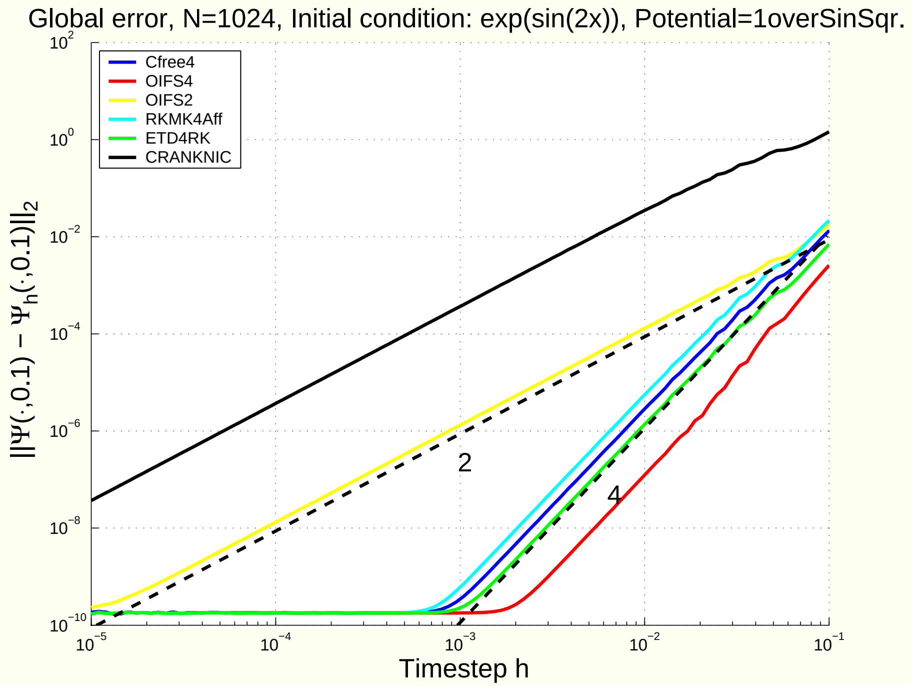

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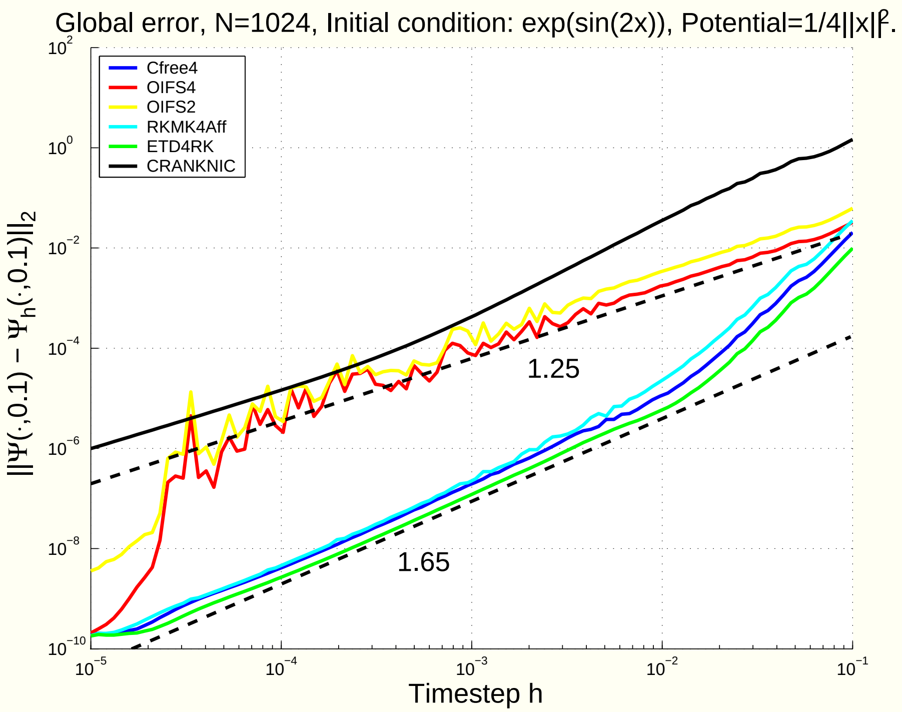

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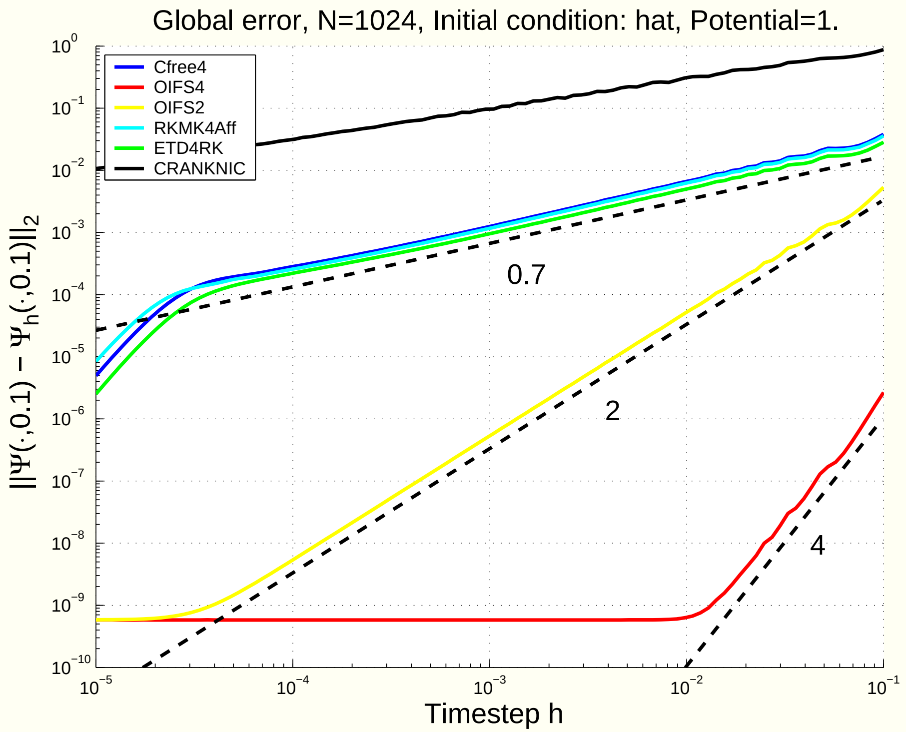

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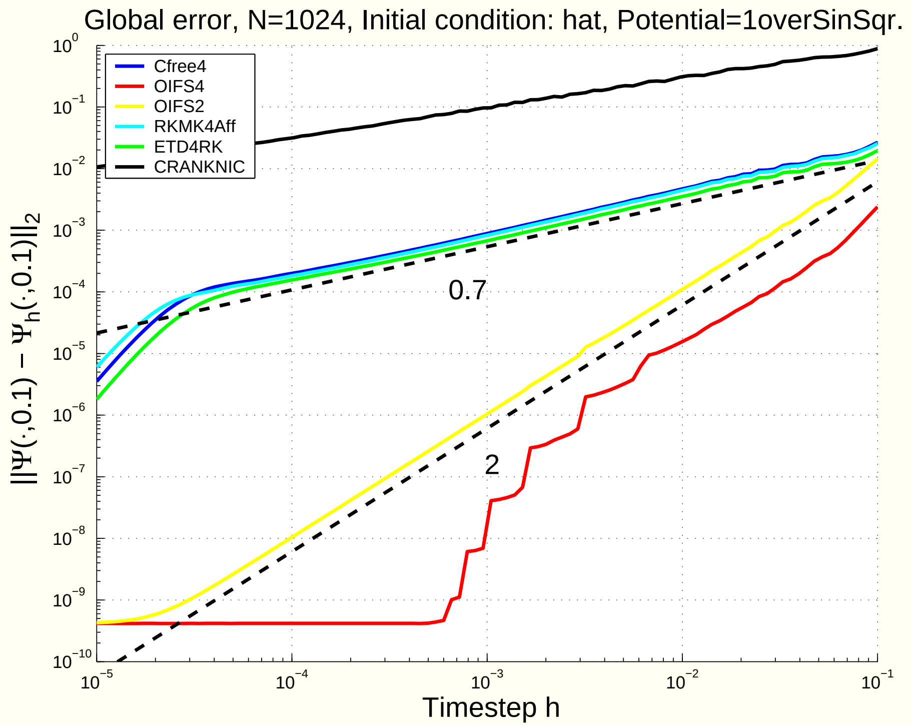

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IC = hat	$V = \lambda$	$\mathbf{4}$	$\mathbf{0.7}$
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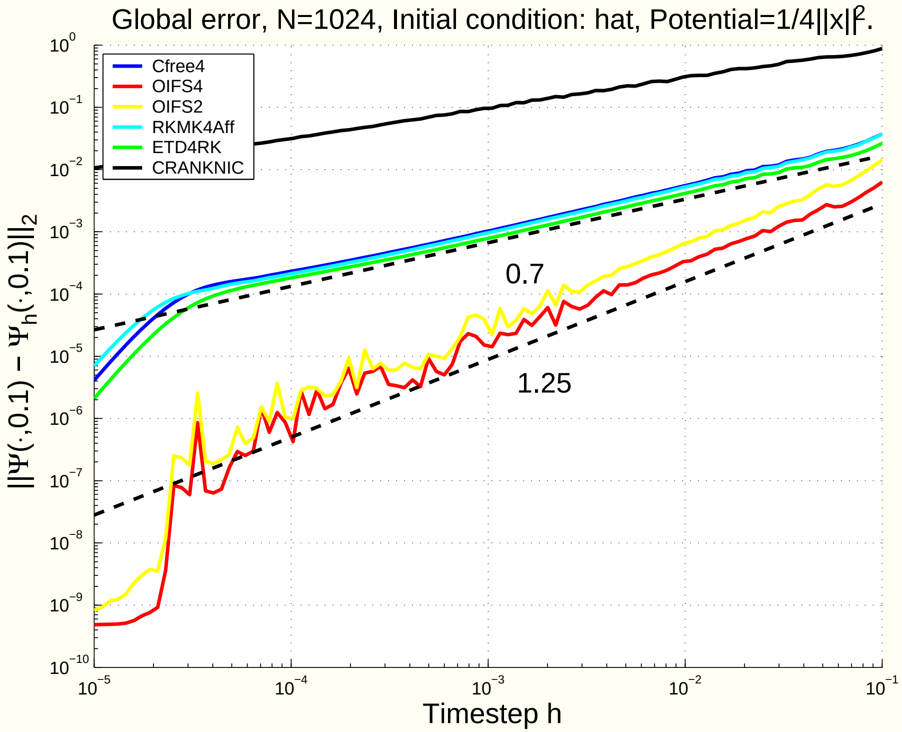

Conclusions from numerical tests

- $C_{\mathbf{nl}}$ does not affect numerical results when $N_{\mathcal{F}} = 1024$.
- ETDRK4/RKMK4/CFREE4 performs very similarly.
- OIFS4 more sensitive to potential, also senses the subtle difference smooth vs. constant potential.
- OIFS4 less sensitive to initial condition.
- ETDRK4/RKMK4/CFREE4 bad on hat initial condition, regardless of potential.

Analysis for CFREE4, constant potential

Observe the global error for each Fourier mode:

Decoupled case, $V(x) = \lambda$:

$$\dot{c}_k = -\mathrm{i}k^2 c_k - \mathrm{i}\lambda c_k$$

with exact solution

$$c_k(t) = \exp(-\mathrm{i}(k^2 + \lambda)t)c_k^0$$

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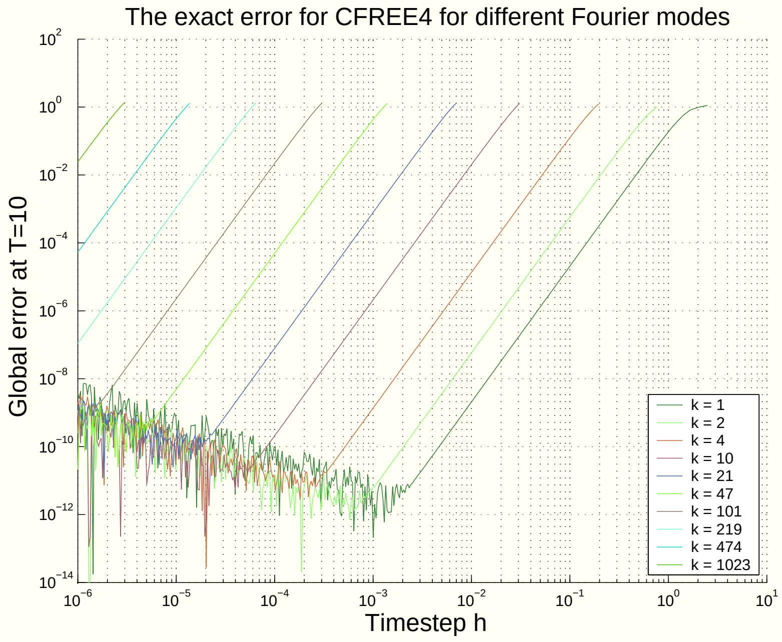

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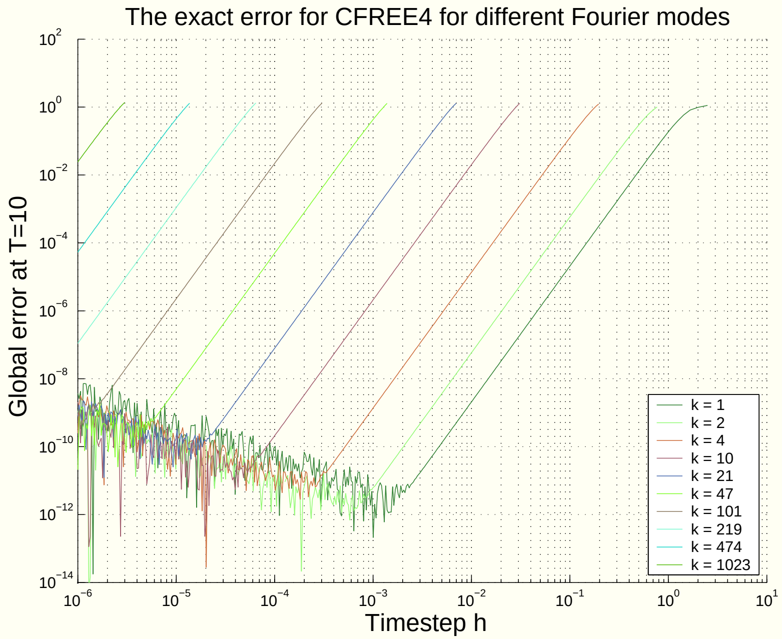
Global error for each component goes like

$$||\mathrm{ge}_k|| \approx \left(\frac{hk^2}{S_B}\right)^4$$

when $hk^2 < S_B$.



For $hk^2 > S_B$, the error is bounded by 2. S_B is given by $\frac{960}{T|\lambda|}^{1/4}$ which is 3.13 here.

Analysis for CFREE4, constant potential

The global error for each Fourier mode is now bounded by

$$|\mathbf{ge}_k| < \begin{cases} 2\left(\frac{hk^2}{S_B}\right)^4 |c_k^0| & hk^2 \le S_B \\ 2|c_k^0| & hk^2 > S_B \end{cases}$$

Remember $|c_k^0| < \frac{K_p}{k^p}$.

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Remember $|c_k^0| < \frac{K_p}{k^p}$. Compute

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

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Using the Euler–MacLaurin with remainder term to fi nd bounds for the sums, we eventually fi nd for $p \le 8$

$$||\mathrm{ge}||_2 \le K\left(\frac{h}{S_B}\right)^{\frac{2p-1}{4}}$$

Analysis for CFREE4, constant potential

We have

$$||\mathbf{ge}|| = \sum_k ||\mathbf{ge}_k|| \approx Ch^{\frac{2p-1}{4}} \qquad p \leq 8$$

Predicted and observed order, CFREE4:

IC:	Reg1	Reg2	Reg3	Reg4	Reg5	Reg6	Smootl
$V(x) = 1$	0.25	0.75	1.25	1.75	2.25	2.75	4*

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$V(x) = 1$	0.25	0.75	1.25	1.75	2.25	2.75	4*

Observed order, CFREE4, ETD4, RKMK:

$V = \frac{1}{4}\|\|x\|\|^2$	0.35	0.75	1.25	1.25	1.75	1.75	1.6
Smooth V	0.25	0.75	1.25	1.75	2.25	2.75	4

Analysis for OIFS4, constant potential

Accordingly for OIFS4:

Each mode behaves the same, with the result that OIFS4 has order 4 on all constant potentials. Verifi ed experimentally.

$$\|ge\|_2^2 = \sum_{k=-N_{\mathcal{F}}/2}^{N_{\mathcal{F}}/2-1} |ge_k|^2$$

$$= K_h h^4 |c_k^0|$$

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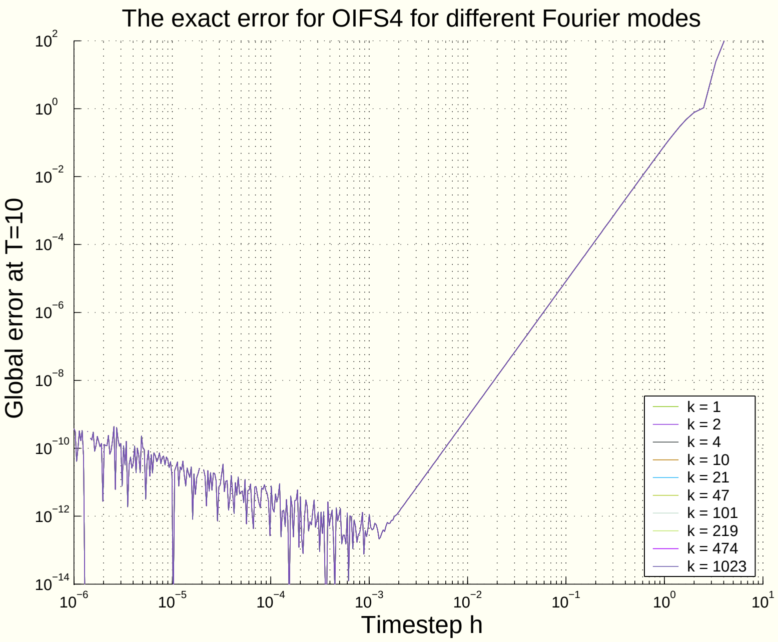
$$= K_h \|c^0\|_2^2 \, h^4.$$



The end

References

- See Borko & Will’s slides for a reference list..

The end

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Conclusions (or an attempt thereat)

- OIFS seems best for our Schrödinger application