Fourth order exponential integrators for the nonlinear Schrödinger equation

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Abstract

We explore the numerical properties of the the fourth order Lawson exponential integrator and the fourth order ETD4RK on the nonlinear Schrödinger equation. The Lawson (integrating factor) scheme does not satisfy the stiff order conditions derived by Hochbruck and Ostermann, but works better in some cases for this equation nevertheless.
By varying the regularity of the potential and the initial condition, order reduction is observed and explained for both integrators but in different scenarios.

(25 minute talk)

Overview

1. The Schrödinger equation.
2. Lawson4 vs. ETD4RK in the smooth case.
3. Dependency on the regularity of the potential.
4. Dependency on the regularity of initial conditions.
5. EXPINT: A MATLAB package for exponential integrators.

The nonlinear Schrödinger equation

Our aim is to solve the nonlinear Schrödinger equation,

$$
\begin{aligned}
\mathrm{i}\psi_t &= -\psi_{xx} + (V(x) + \lambda|\psi|^2)\psi, \quad x \in [-\pi, \pi] \\
\psi(x, 0) &= \psi_0(x), \quad x \in [-\pi, \pi] \\
\psi(-\pi, t) &= \psi(\pi, t), \quad t > 0.
\end{aligned}
$$

where $V(x)$ is some potential, λ is the nonlinearity constant and ψ_0 is some initial condition.

After a spectral discretization, we have the system of equations

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

The format of an exponential Runge–Kutta scheme

One step of an exponential integrator of Runge–Kutta type applied to a problem

$$\dot{y} = Ly + N(y,t)$$

is written

$$Y_i = h \sum_{j=1}^{s} a_{ij}(hL)\, N(Y_j, t_{n-1} + c_j h) + \mathrm{e}^{c_i hL} y_{n-1}, \quad i = 1, \ldots, s,$$

$$y_n = h \sum_{i=1}^{s} b_i(hL) N(Y_j, t_{n-1} + c_j h) + \mathrm{e}^{hL} y_{n-1}.$$

and coefficient functions are written up in a Butcher-like tableau.

Fourth order Lawson scheme based on cRK4

The Lawson4 scheme in this format reads:

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

where $z = hL$.

In general, Lawson schemes may be written as

$$a_{ij}(z) = \tilde{a}_{ij}e^{(c_i - c_j)z} \quad \text{and} \quad b_i(z) = \tilde{b}_i e^{(1-c_i)z}.$$

where $\tilde{a}_{ij}$, $\tilde{b}_i$ and c_i are the coefficients from the underlying Runge–Kutta scheme.

ETD4RK

$$
\begin{array}{c|cccc}
0 & & & & \\
\frac{1}{2} & \frac{1}{2}\varphi_1(z/2) & & & \\
\frac{1}{2} & & \frac{1}{2}\varphi_1(z/2) & & \\
1 & \varphi_1(z/2)(e^{z/2}-1) & & \varphi_1(z/2) & \\
\hline
 & \varphi_1 - 3\varphi_2 + 4\varphi_3 & 2\varphi_2 - 4\varphi_3 & 2\varphi_2 - 4\varphi_3 & -\varphi_2 + 4\varphi_3
\end{array}
$$

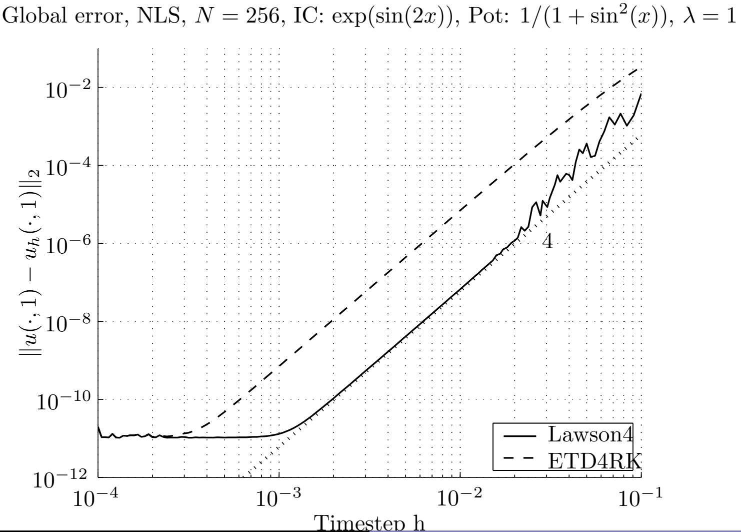
where

$$\varphi_k(z) = \frac{1}{(k-1)!}\int_0^1 e^{(1-\theta)z}\theta^k \, d\theta$$

- Due to Cox & Matthews 2002.
- Computing $\varphi_k(z)$ is not a trivial task.
  (6,6)-Padé-approximations together with scaling and corrected squaring is used here.

Lawson is order 4

An introductory numerical test with smooth IC and smooth potential:



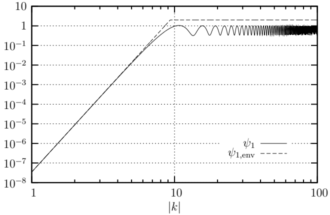
The stiff order conditions

Hochbruck and Ostermann (2004) introduced stiff order conditions for analyzing exponential integrators on semilinear parabolic problems.

- The first one reads

$$h\varphi_1(z)N(u(t_0)) - h\sum_{i=1}^{s} b_i(z)N(u(t_0)) = h\psi_1(z)N(u(t_0))$$

  so they require $\psi_1(z) = 0$.
- But for Lawson, $\psi_1(z)$ looks like



- For ETD-schemes, $\psi_1(z) = 0$, because they use $\varphi_1(z)$.

Dependency on potential $V(x)$

From the first stiff order condition, we get a contribution less than order 4 to the error depending on the regularity of N. N does not have a higher regularity than the potential $V(x)$.

Proposition

If the regularity r of N is ≤ 8, assuming smooth initial conditions, we have an error contribution from the first stiff order condition

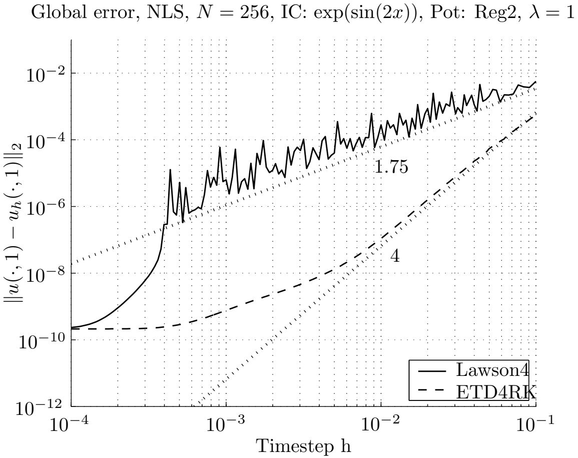
$$||h\psi_1 N||_2 = \mathcal{O}(h^{1+\frac{r}{2}-\frac{1}{4}})$$

The proof is done by using the $\psi_{1,\text{env}}$-function to bound ψ_1, and then summing over each Fourier coeffient, where Fourier coefficients of N decays by r.

- With regard to dependency on potential-regularity, we have that local order *equals* global order (seen numerically).

Numerical experiment with varying potential

Setting $V(x)$ to be a random function with Fourier decay k^{-2} , we get the following result



and the expression $Ch^{1+\frac{r}{2}-\frac{1}{4}}$ gives exactly order 1.75.

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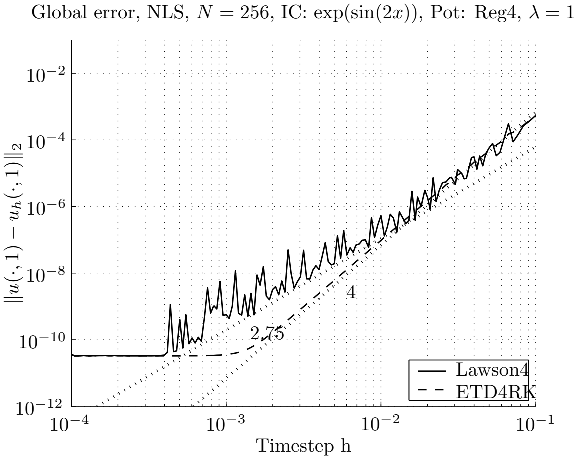
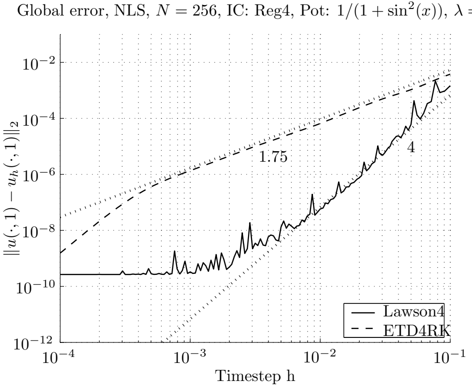


and the expression $Ch^{1+\frac{r}{2}-\frac{1}{4}}$ gives exactly order 2.75.

Dependency on the initial condition

- ETD-schemes suffer from order reduction when the initial condition has low regularity, the error contribution being $Ch^{\frac{r}{2}-\frac{1}{4}}$.
- Lawson is less sensitive to the regularity of the initial condition. At regularity 4 we almost regain classical order:



Linear problem, $\lambda = 0$

We observe numerically that most of the dependency on the IC-regularity is still present for Lawson when we set $\lambda = 0$. Then the problem is linear.

- Applying the Lawson4 stepper to the simpler equation

$$\dot{u} = Lu + Vu$$

yields the following expression

$$\begin{aligned} u_{n+1} = \Big[& EE + \frac{h}{6}(EEV + 4EVE + VEE) \\ & + \frac{h^2}{6}(EVEV + EVVE + VEVE) \\ & + \frac{h^3}{12}(EVVEV + VEVVE) + \frac{h^4}{24} VEVVEV \Big] u_n \end{aligned}$$

where $E = \mathrm{e}^{hL/2}$.

The exact solution of the linear problem

Following Jahnke and Lubich (2000), we write the exact solution of $\dot{u} = (L + V)u$ as given by the variation of constants formula;

$$e^{h(L+V)}u_0 = e^{hL}u_0 + \int_0^h e^{sL} V e^{(h-s)(L+V)} u_0 \, ds$$

and we may recursively apply this formula to the red part above. This yields

$$\begin{aligned} e^{h(L+V)}u_0 &= e^{hL}u_0 \\ &\quad + \int_0^h e^{s_1 L} V e^{(h-s_1)L} u_0 \, ds_1 \\ &\quad + \int_0^h e^{s_1 L} V \int_0^{h-s_1} e^{s_2 L} V e^{(h-s_1-s_2)(L+V)} u_0 \, ds_2 ds_1 \end{aligned}$$

and this should be done three more times.

The Lawson approximation

Lawson solves each of these multi-dimensional integral to a sufficient degree of accuracy, for example:

$$\int_0^h e^{s_1 L} V e^{(h-s_1)L} u_0 \, ds_1 = \frac{h}{6}(VE^2 + 4EVE + E^2 V)u_0 + \frac{h^5}{2880} f^{(4)}(\xi) u_0$$

which is the Simpson rule, exact for cubic polynomials.

- The error term is

$$f^{(4)}(\xi) = e^{\xi L}[L,[L,[L,[L,V]]]]e^{(h-\xi)L} = e^{\xi L}\mathrm{ad}_L^4(V)e^{(h-\xi)L}.$$

- Regarding $\bar{u} = e^{(h-s)L} u$ as a continous function and $L = \frac{d^2}{dx^2}$ and V as operators on functions, we find the error term to be

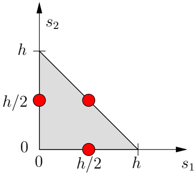
$$e^{sL}\left(V^{(8)}\bar{u} + 4V^{(7)}\bar{u}^{(1)} + 6V^{(6)}\bar{u}^{(2)} + 4V^{(5)}\bar{u}^{(3)} + V^{(4)}\bar{u}^{(4)}\right)$$

(in general, we have $\mathrm{ad}_L^m(V)u = \sum_{i=0}^m 2^i \binom{m}{i} V^{(2m-i)} u^{(i)}$)

The Lawson approximation

The double integral

$$\int_0^h e^{s_1 L} V \int_0^{h-s_1} e^{s_2 L} V e^{(h-s_1-s_2)L} u_0 \, ds_2 ds_1$$



is approximated in the points in the figure by the quadrature rule

$$\frac{h^2}{6}(EVEV + EVVE + VEVE)$$

with degree of precision 2. The error term is

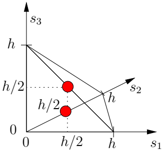
$$\int_0^h \int_0^{h-s_1} g(s_1, s_2) \, ds_1 ds_2 = \frac{h^2}{6}(EVEV + EVVE + VEVE) + CM_3 h^5$$

where the third derivatives of g is bounded by M_3.

The Lawson approximation

The triple integral

$$\int_0^h \mathrm{e}^{s_1 L} V \int_0^{h-s_1} \mathrm{e}^{s_2 L} V \int_0^{h-s_1-s_2} \mathrm{e}^{s_3 L} V \mathrm{e}^{(h-s_1-s_2-s_3)L} u_0 \,\mathrm{d}s_3 \mathrm{d}s_2 \mathrm{d}s_1$$



is approximated in the two points

$$(s_1, s_2, s_3) = \left\{ \left(\tfrac{h}{2}, 0, \tfrac{h}{2}\right), \left(0, \tfrac{h}{2}, 0\right) \right\}$$

by $\frac{h^3}{12}(EVVEV + VEVVE)$ with degree of precision 1 (exact on linear functions).

The last quadruple integral is evaluated at one point, $\frac{h^4}{24} VEVVEV$ and is exact for constant functions.

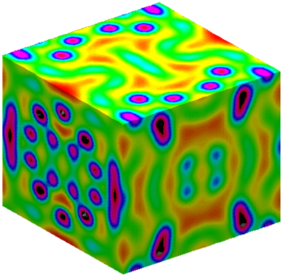
Lawson dependency on initial condition

- The error formula for the Simpson quadrature requires u_0 to be 4 times differentiable for order 4 of Lawson (and also the potential to be 8 times differentiable).
- The error terms from the double, triple and quadruple integral requires less regularity.
- Lawson on a constant potential shows no dependency on the initial condition, then $[L, V] = 0$.
- When mixing low regularity potential and low regularity initial condition, the differences in performance between Lawson and ETD are small.

Numerical implementation in MATLAB

All computations are performed in a now released MATLAB-package, EXPINT, featuring:

- Easy implementation and comparison of exponential integrators (more than 30 included).
- Numerous examples of discretizations of common PDEs.
- φ-functions computed by (6,6)-Padé-approximations together with scaling and corrected squaring.



The EXPINT-package and an accompanying technical report may be downloaded from

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

The end

- Cox and Matthews: *Exponential time differencing for stiff systems*, J. Comp. Physics, 2002.
- Hochbruck and Ostermann: *Explicit exponential Runge–Kutta methods for semilinear parabolic problems*, 2004.
- Jahnke and Lubich: *Error bounds for exponential operator splittings*, BIT 2000.
- Lawson: *Generalized Runge–Kutta Processes for Stable Systems with Large Lipschitz Constants*, SIAM J. Num. Anal., 1967.