Geometric Integrators for the Nonlinear Schrödinger Equation

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2. Is it useful for GI problems to consider the abstract problem with no discretisation in space?
3. What is the role of energy conservation vs various forms of symplecticity (cf talk of E. Hairer) in the Hamiltonian PDE situation?

The Nonlinear Schrödinger equation on the d-torus

$$\mathrm{i}\, u_t + \Delta u = \lambda |u|^{2\sigma} u, \qquad \mathbf{x} \in \mathbf{T}^d,\ \ t \geq 0, \qquad u(\mathbf{x}, 0) = u_0(\mathbf{x})$$

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For $u_0(\mathbf{x}) \in L^2(\mathbf{T}^d)$, one has $dN/dt = 0$ where

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Whenever the problem is well posed in $H^1(\mathbf{T}^d)$ one has $dE/dt = 0$ with

$$E(t) = \int_{\mathbf{T}^d} \frac{1}{2} |\nabla u|^2 + \frac{\lambda}{2\sigma + 2} |u|^{2\sigma+2} d\mathbf{x}$$

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$d = 1$

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- $\sigma = 1 \;\Rightarrow\; u \in C(\mathbf{R}, H^s(\mathbf{T})),\; u_0 \in H^s(\mathbf{T}))$

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- Globally well posed in $H^1(\mathbf{T}^3)$ for $1 \leq \sigma \leq 2$ and small initial data in $H^1(\mathbf{T}^3)$

Main case: $d = \sigma = 1$

Mostly we consider here the case of the completely integrable cubic 1D NLS.

$$\mathrm{i}\, u_t + u_{xx} = \lambda |u|^2 u, \qquad u(x,t) = u(x+L,t), \quad u(x,0) = u_0(x)$$

We recall the conservation laws

$$N(t) = \int_{\mathbf{T}} |u|^2\, dx$$

$$E(t) = \int_{\mathbf{T}} \left(\frac{1}{2} |u_x|^2 + \frac{\lambda}{4} |u|^4 \right) dx$$

Ideas for geometric integrators

1. Splitting methods
2. Conservative schemes, like the Besse scheme and the Fei scheme.
3. Multisymplectic formulation and multisymplectic schemes
4. Semidiscretisation in space given by the long known completely integrable Ablowitz-Ladik space discretisation. Many possible choices for how to discretize in time.
5. Schemes arising from Lie group- or exponential integrators

Linear - Nonlinear

$$H_1 = \frac{1}{2}\int_{\mathbf{T}} |u_x|^2 \, dx, \qquad H_2 = \frac{\lambda}{4}\int_{\mathbf{T}} |u|^4 \, dx$$

Leads to partial flows

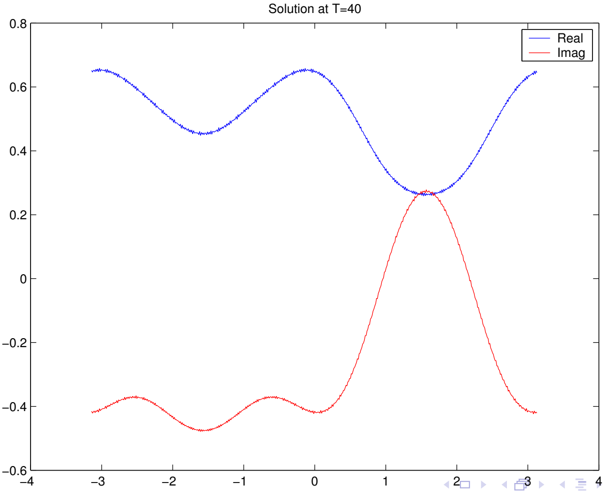
1. Schrödinger group $\exp(\mathrm{i}t\Delta)$ calculated efficiently by FFT.
2. The nonlinear flow is an ODE with parameter x, having solution

$$u(x,t) = \exp\left(-\mathrm{i}t\lambda \left|f(x)\right|^2 t\right) \, f(x), \quad u(x,0) = f(x).$$

Problem: This type of splitting often results in resonance for large Δt.

Resonance in Strang splitting

$$u_0(x) = \frac{1}{2+\sin x}, \quad \Delta t = 0.015, \quad T = 40.$$



Resonance – spectrum

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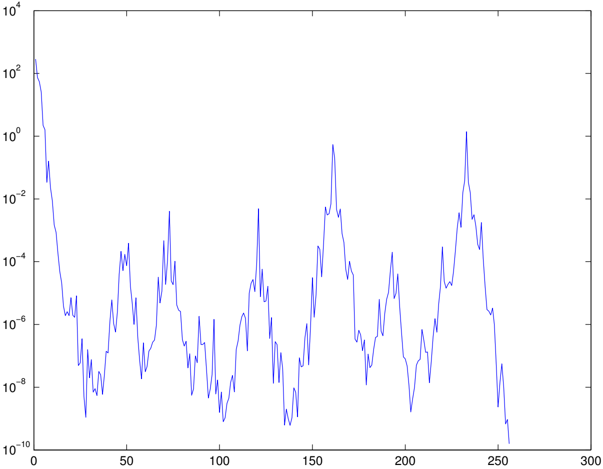

Formulation

Rewrite the d-dim NLSE as a system

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The method of Besse

$$\frac{\phi^{n+\frac{1}{2}} + \phi^{n-\frac{1}{2}}}{2} = |u^n|^2$$

$$\mathrm{i}\,\frac{u^{n+1} - u^n}{\Delta t} + \Delta\left(\frac{u^{n+1} + u^n}{2}\right) = \lambda\left(\frac{u^{n+1} + u^n}{2}\right)\phi^{n+\frac{1}{2}}$$

Properties of the Besse method

Besse (2004) works with pure initial value problem, $x \in \mathbf{R}^d$.
He proves

1. Regularity results. For sufficiently large s the solution of the extended scheme converges to $(u, |u|^2)$ in

$$L^\infty([0,T]; H^s \times H^s)$$

2. The scheme is conservative in the sense that

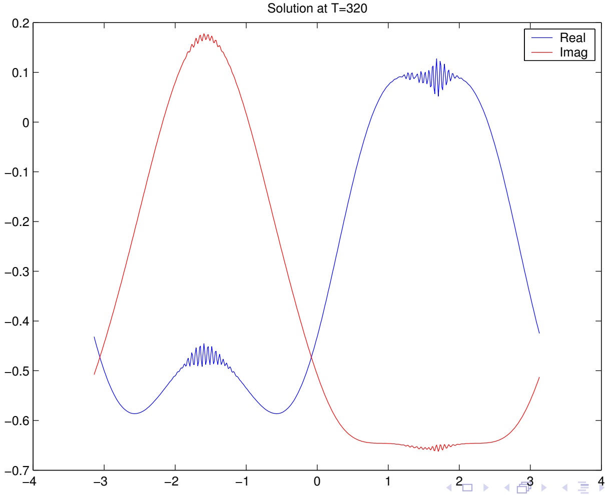
$$\int_{\mathbf{R}^d} |u^n|^2 \, dx = \int_{\mathbf{R}^d} |u^0|^2 \, dx$$

and if

$$E_n = \int_{\mathbf{R}^d} \left(|\nabla u^n|^2 + \frac{\lambda}{2} \phi^{n-\frac{1}{2}} \phi^{n+\frac{1}{2}} \right) dx$$

then $E_n = E_0$ for every n.

$$T = 320, \qquad \Delta t = 0.04.$$



Besse – conservation in practice

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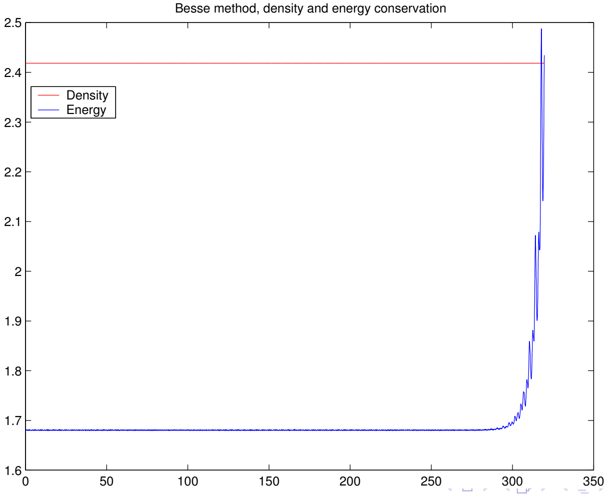

FD scheme of Fei et al.

$$\mathrm{i}\frac{u_\ell^{n+1} - u_\ell^{n-1}}{2\Delta t} + \frac{\delta_x^2(u_\ell^{n+1} + u_\ell^{n-1})}{2\Delta x^2} = \frac{\lambda}{2}|u_n|^2(u_\ell^{n+1} + u_\ell^{n-1})$$

The scheme is symmetric and conservative in the sense that

$$N_n = \sum_\ell \frac{\Delta x}{2}\left(|u_\ell^n|^2 + |u_\ell^{n+1}|^2\right)$$

$$E_n = \sum_\ell \frac{\Delta x}{4}\left(\left|\frac{u_{\ell+1}^{n+1} - u_\ell^{n+1}}{\Delta x}\right|^2 + \left|\frac{u_{\ell+1}^n - u_\ell^n}{\Delta x}\right|^2 + \lambda\,|u_\ell^{n+1}|^2 \cdot |u_\ell^n|^2\right)$$

are preserved for all time steps.

Behaviour of Fei scheme

Focusing case: $\lambda, 0$. The scheme behaves well and conserves also my "home made energy" mod truncation error

$$\bar{E}_n = \Delta x \sum_{\ell} \left(\frac{1}{2} \left| \frac{u_{\ell+1} - u_\ell}{\Delta x} \right|^2 + \frac{\lambda}{4} |u_\ell|^4 \right)$$

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Defocusing case: The parasitic solution is unstable, causing an oscillation in time. "My energy" deviates strongly from the Fei energy, a situation which is incompatible with continuity in time.

Multisymplectic formulation (Reich 2000)

$$u(x,t) = p(x,t) + \mathrm{i}\, q(x,t), \quad v = p_x, \quad w = q_x$$

Define

$$\mathbf{M} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \mathbf{K} = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, Z = \begin{pmatrix} p \\ q \\ v \\ w \end{pmatrix}$$

$$S(Z) = \frac{1}{2}(v^2 + w^2) - \frac{\lambda}{4}(p^2 + q^2)^2$$

Then the NLSE takes the form

$$\mathbf{M} Z_t + \mathbf{K} Z_x = \nabla_Z S(Z)$$

Multisymplecticity

M and **K** define forms

$$\omega(U, V) = \langle \mathbf{M} U, V \rangle, \qquad \kappa(U, V) = \langle \mathbf{K} U, V \rangle$$

Conservation law. One has

$$\partial_t \omega(U, V) + \partial_x \kappa(U, V) = 0$$

where U and V are solutions of the variational equation
$\mathbf{M} dZ_t + \mathbf{K} dZ_x = D_{ZZ} S(Z) dZ$.
This law can be imposed on the discretised level

$$\delta_t \omega(U_i^j, V_i^j) + \delta_x \kappa(U_i^j, V_i^j) = 0$$

U_i^j, V_i^j being solutions of the discrete variational equations, δ_t, δ_x being approximations to ∂_t and ∂_x.

Multisymplectic scheme

Centered box scheme of second order

$$\mathbf{M}\left(\frac{Z_{i+\frac{1}{2}}^{j+1} - Z_{i+\frac{1}{2}}^{j}}{\Delta t}\right) + \mathbf{K}\left(\frac{Z_{i+1}^{j+\frac{1}{2}} - Z_{i}^{j+\frac{1}{2}}}{\Delta x}\right) = \nabla_Z S(Z_{i+\frac{1}{2}}^{j+\frac{1}{2}})$$

$$Z_{i+1/2}^{m} = \frac{Z_i^m + Z_{i+1}^m}{2}, \qquad Z_\ell^{j+1/2} = \frac{Z_\ell^j + Z_\ell^{j+1}}{2}.$$

$$Z_{i+1/2}^{j+1/2} = \frac{Z_{i+1}^{j+1} + Z_i^{j+1} + Z_{i+1}^{j} + Z_i^{j}}{4}$$

The Ablowitz-Ladik discretization

With $u(x,t) = p(x,t) + \mathrm{i}\, q(x,t)$, discretize in space

$$p(x_k,t) \approx P_k(t), \qquad q(x_k,t) \approx Q_k(t), \quad , k = 1, \dots, N,$$

$$\frac{d}{dt}P_k = -\frac{Q_{k+1} - 2Q_k + Q_{k-1}}{\Delta x^2} + \frac{\lambda}{2}(P_k^2 + Q_k^2)(Q_{k-1} + Q_{k+1})$$

$$\frac{d}{dt}Q_k = \frac{P_{k+1} - 2P_k + P_{k-1}}{\Delta x^2} - \frac{\lambda}{2}(P_k^2 + Q_k^2)(P_{k-1} + P_{k+1})$$

Noncanonical Hamiltonian system

Ablowitz-Ladik, noncanonical Hamiltonian system

$$\begin{pmatrix} \dot{P} \\ \dot{Q} \end{pmatrix} = \begin{pmatrix} 0 & -D(P,Q) \\ D(P,Q) & 0 \end{pmatrix} \begin{pmatrix} \nabla_P H(P,Q) \\ \nabla_Q H(P,Q) \end{pmatrix}$$

$$H(P,Q) = \frac{1}{\Delta x^2} \sum_{k=1}^{N} (P_k P_{k-1} + Q_k Q_{k-1}) + \frac{2}{\lambda \Delta x^4} \sum_{k=1}^{N} \log\left(1 - \frac{\lambda}{2} \Delta x^2 (P_k^2 + Q_k^2)\right)$$

$$D(P,Q) = \mathrm{diag}(d_k(P,Q)), \qquad d_k(P,Q) = 1 - \frac{\lambda}{2} \Delta x^2 (P_k^2 + Q_k^2)$$

Ablowitz-Ladik time discretization

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   e.g. by means of generating function approach.
3. Bring the system to a canonical form by a symplectic transformation (several such are known), and apply a standard symplectic scheme to the transformed variables.

Numerical tests

We are interested in checking

- Integration over long times
- With a large number of spatial degrees of freedom, (but still fairly large time step)
- Use density and energy conservation as quality measures

Parameter choices

$N = 512$	Spatial degrees of freedom
$\lambda = 4$	Nonlinear constant
Δt	Constant time step in range $0.001 - 0.3$

Time interval T: Run up to $T = 1000$ or until energy deviation exceeds 20% from initial point.

Results

Long time behaviour for a range of step sizes

Method	Succeeds	Fails	Failure reason
Multisymp (∞)	< 0.2	Never	
Multisymp (4)	< 0.06	> 0.07	Drift
Strang splitting	$< 4 \cdot 10^{-4}$	$> 6 \cdot 10^{-3}$	Resonance
Besse method	< 0.008	> 0.01	Instability
ETD4RK	< 0.02	> 0.02	Drift

We count time consumption per step, using `Matlab sparse` functions for linear algebra. One unit is Strang splitting

Timings

Strang splitting	1.00
Expint (ETD4RK)	1.37
Besse scheme	15.12
Multisymp (0.010)	60.00
Multisymp (0.025)	79.25
Multisymp (0.050)	100.25
Multisymp (0.100)	138.43

Multisymplectic depends on time step. All runs are for ' $N = 500$ space points.

Conclusions

1. Geometric integrators for the NLSE perform very well over long times for moderate spatial degrees of freedom N
2. For large N, several GIs encounter problems, with resonance or poor convergence
3. The multisymplectic integrators behave well as N increases, but are expensive for large time steps. Nonlinear systems must be solved accurately.
4. Abstract schemes conservative in the limit may deteriorate after space discretisation
5. The "non-geometric" exponential integrators show expected drift, but can probably compete with GIs because of superior efficiency.