Geometric Integrators for the Nonlinear Schrödinger Equation
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Some questions in Geometric Integration of PDEs

1. How much are we willing to pay (or are we capable of paying) in extra computational cost for a Geometric Integrator? How to make a compromise?

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?
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The Nonlinear Schrödinger equation on the $d$-torus

\begin{align*}
  i u_t + \Delta u &= \lambda |u|^{2\sigma} u, \quad x \in T^d, \ t \geq 0, \quad u(x, 0) = u_0(x)
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\[ N(t) = \int_{T^d} |u(\mathbf{x}, t)|^2 \, d\mathbf{x} \]

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

\[ E(t) = \int_{T^d} \frac{1}{2} |\nabla u|^2 + \frac{\lambda}{2\sigma + 2} |u|^{2\sigma + 2} \, d\mathbf{x} \]
Summary of wellposedness of NLS on $T^d$

$\text{Locally well posed in } H^s(T) \text{ for } \sigma \leq 2/(1-2s)$

$\text{Globally well posed in } L^4(T \times \mathbb{R}_{loc}) \text{ whenever } \sigma \leq 1$ and $u_0 \in L^2(T)$.

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

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$\text{Globally well posed in } H^1(T^2) \text{ for } \sigma = 1 \text{ and } L^2\text{-}small \text{ initial data in } H^1(T^2)$.

$\text{Globally well posed in } H^1(T^3) \text{ for } 1 \leq \sigma \leq 2 \text{ and small initial data in } H^1(T^3)$.
Summary of wellposedness of NLS on $\mathbb{T}^d$

$d = 1$

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

\(d = 2\)
- Locally well posed in $H^\sigma(\mathbb{T}^2)$ $1 \leq \sigma \leq 1/(1 - s)$, $0 \leq s \leq 1$
- Globally well posed in $H^1(\mathbb{T}^2)$ for $\sigma = 1$ and $L^2$-small initial data in $H^1(\mathbb{T}^2)$. 
Summary of wellposedness of NLS on $\mathbb{T}^d$

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$d = 3$

- Globally well posed in $H^1(\mathbb{T}^3)$ for $1 \leq \sigma \leq 2$ and small initial data in $H^1(\mathbb{T}^3)$
Main case: \( d = \sigma = 1 \)

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

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

We recall the conservation laws

\[
N(t) = \int_T |u|^2 \, dx
\]

\[
E(t) = \int_T \left( \frac{1}{2} |u_x|^2 + \frac{\lambda}{4} |u|^4 \right) \, dx
\]
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
Abstract problem – Splitting methods

Linear - Nonlinear

\[
H_1 = \frac{1}{2} \int_T |u_x|^2 \, dx, \quad H_2 = \frac{\lambda}{4} \int_T |u|^4 \, dx
\]

Leads to partial flows

1. Schrödinger group \( \exp(it\Delta) \) calculated efficiently by FFT.
2. The nonlinear flow is an ODE with parameter \( x \), having solution

\[
u(x, t) = \exp\left( -it\lambda |f(x)|^2 t \right) f(x), \quad u(x, 0) = f(x).
\]

Problem: This type of splitting often results in resonance for large \( \Delta t \).
Resonance in Strang splitting

\[ u_0(x) = \frac{1}{2 + \sin x}, \quad \Delta t = 0.015, \quad T = 40. \]
Resonance – spectrum

\[ u_0(x) = \frac{1}{2 + \sin x}, \quad \Delta t = 0.015, \quad T = 40. \]
Formulation
Rewrite the \(d\)-dim NLSE as a system

\[
\phi(u) = |u|^2 \\
i u_t + \Delta u = \lambda \phi(u) u
\]
Abstract schemes – Besse’s method

Formulation
Rewrite the $d$-dim NLSE as a system

$$\phi(u) = |u|^2$$

$$iu_t + \Delta u = \lambda \phi(u) u$$

The method of Besse

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

$$i\frac{u^{n+1} - u^n}{\Delta t} + \Delta \left( \frac{u^{n+1} + u^n}{2} \right) = \lambda \left( \frac{u^{n+1} + u^n}{2} \right) \phi^{n+\frac{1}{2}}$$
Besse (2004) works with pure initial value problem, $x \in \mathbb{R}^d$. 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

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

and if

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

then $E_n = E_0$ for every $n$. 
\( T = 320, \quad \Delta t = 0.04. \)
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The scheme is symmetric and conservative in the sense that

\[ N_n = \sum_\ell \frac{\Delta x}{2} (|u_{\ell}^n|^2 + |u_{\ell}^{n+1}|^2) \]

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

are preserved for all time steps.
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)

\[ u(x, t) = p(x, t) + i q(x, t), \quad v = p_x, \quad w = q_x \]

Define

\[ M = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad K = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} p \\ q \\ v \\ w \end{pmatrix} \]

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

Then the NLSE takes the form

\[ MZ_t + KZ_x = \nabla Z S(Z) \]
Multisymplecticity

\( \mathbf{M} \) and \( \mathbf{K} \) define forms

\[
\omega(U, V) = \langle \mathbf{M} U, V \rangle, \quad \kappa(U, V) = \langle \mathbf{K} U, V \rangle
\]

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

\[
\delta_t \omega(U^j_i, V^j_i) + \delta_x \kappa(U^j_i, V^j_i) = 0
\]

\( U^j_i, V^j_i \) being solutions of the discrete variational equations, \( \delta_t, \delta_x \) being approximations to \( \partial_t \) and \( \partial_x \).
Multisymplectic scheme

Centered box scheme of second order

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

\[
Z_{m+1/2}^i = \frac{Z_m^i + Z_{i+1}^m}{2}, \quad Z_{j+1/2}^\ell = \frac{Z_\ell^j + Z_{j+1}^\ell}{2}.
\]

\[
Z_{i+1/2}^{j+1/2} = \frac{Z_{i+1}^{j+1} + Z_i^{j+1} + Z_{i+1}^{j} + Z_i^{j}}{4}
\]
The Ablowitz-Ladik discretization

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

\[ p(x_k, t) \approx P_k(t), \quad q(x_k, t) \approx Q_k(t), \quad k = 1, \ldots, N, \]

\[
\begin{align*}
\frac{d}{dt} P_k &= -\frac{Q_{k+1} - 2Q_k + Q_{k-1}}{\Delta x^2} + \frac{\lambda}{2} (P_k^2 + Q_k^2)(Q_{k-1} + Q_{k+1}) \\
\frac{d}{dt} Q_k &= \frac{P_{k+1} - 2P_k + P_{k-1}}{\Delta x^2} - \frac{\lambda}{2} (P_k^2 + Q_k^2)(P_{k-1} + P_{k+1})
\end{align*}
\]

Noncanonical Hamiltonian system
Ablowitz-Ladik, noncanonical Hamiltonian system

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

\[
H(P, Q) = \frac{1}{\Delta x^2} \sum_{k=1}^{N} (P_k P_{k-1} + Q_k Q_{k-1})
\]

\[
+ \frac{2}{\lambda \Delta x^4} \sum_{k=1}^{N} \log \left(1 - \frac{\lambda}{2} \Delta x^2 (P_k^2 + Q_k^2)\right)
\]

\[
D(P, Q) = \text{diag}(d_k(P, Q)), \quad d_k(P, Q) = 1 - \frac{\lambda}{2} \Delta x^2 (P_k^2 + Q_k^2)
\]
Islas et al. (2001) suggests 3 different ways

1. Introduce phase shift which results in separable Hamiltonian. Apply splitting method.
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2. Design symplectic integrators for special noncanonical structure of the form

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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
- \( \Delta t \) 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

<table>
<thead>
<tr>
<th>Method</th>
<th>Succeeds</th>
<th>Fails</th>
<th>Failure reason</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multisymp (∞)</td>
<td>&lt; 0.2</td>
<td>Never</td>
<td>Drift</td>
</tr>
<tr>
<td>Multisymp (4)</td>
<td>&lt; 0.06</td>
<td>&gt; 0.07</td>
<td>Resonance</td>
</tr>
<tr>
<td>Strang splitting</td>
<td>&lt; 4 \cdot 10^{-4}</td>
<td>&gt; 6 \cdot 10^{-3}</td>
<td>Instability</td>
</tr>
<tr>
<td>Besse method</td>
<td>&lt; 0.008</td>
<td>&gt; 0.01</td>
<td></td>
</tr>
<tr>
<td>ETD4RK</td>
<td>&lt; 0.02</td>
<td>&gt; 0.02</td>
<td>Drift</td>
</tr>
</tbody>
</table>
Time consumption

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

Timings

<table>
<thead>
<tr>
<th>Method</th>
<th>Time</th>
</tr>
</thead>
<tbody>
<tr>
<td>Strang splitting</td>
<td>1.00</td>
</tr>
<tr>
<td>Expint (ETD4RK)</td>
<td>1.37</td>
</tr>
<tr>
<td>Besse scheme</td>
<td>15.12</td>
</tr>
<tr>
<td>Multisymp (0.010)</td>
<td>60.00</td>
</tr>
<tr>
<td>Multisymp (0.025)</td>
<td>79.25</td>
</tr>
<tr>
<td>Multisymp (0.050)</td>
<td>100.25</td>
</tr>
<tr>
<td>Multisymp (0.100)</td>
<td>138.43</td>
</tr>
</tbody>
</table>

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.