Adaptive Full Discretization of Gross–Pitaevskii Equations with Rotation Term

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Nonlin. Evolution Equations

Consider

$$\dot{u} = F(u), \quad F(u) = Au + B(u),$$

A . . . linear differential operator,

$B(u)$ . . . nonlinear operator, generally unbounded.

- Cubic NLS — Semi–discretization.
- Cubic NLS with rotation term —
  Full discretization Laguerre–Fourier–[Hermite].
- Embedded error estimators.
- Defect based error estimators.

Error Estimators

We consider two classes of error estimators:

- Embedded splitting formulae:
  - Reuse compositions to construct pairs of different orders.
  - Real coefficients for Schrödinger equations.
  - Complex coefficients for parabolic problems.
- Defect correction:
  - Form defect of splitting solution.
  - Backsolve for the estimator using a generalized (nonlinear!) Sylvester equation.
  - Hermite quadrature for integral solution representation (Gröbner–Alexeev Lemma).

Lie Calculus

$\varphi_F^t(\psi_0)$ ... flow of $\quad \dot{\psi} = F(\psi), \quad \psi(0) = \psi_0.$

Lie derivative D_F

$$(D_F G)(\psi) := \frac{d}{dt}\Big|_{t=0} G(\varphi_F^t(\psi)) = G'(\psi)F(\psi).$$

$$\big(\exp(tD_F)G\big)(\psi) := G(\varphi_F^t(\psi)).$$

Commutator

$$[D_A, D_B] := D_A D_B - D_B D_A = D_{[B,A]}.$$

Define recursively iterated commutators

$$\mathrm{ad}^0_{D_A}(D_B)u := D_B u, \qquad \mathrm{ad}^j_{D_A}(D_B)u := [D_A, \mathrm{ad}^{j-1}_{D_A}(D_B)](u).$$

Higher-Order Splittings

$$u_{n+1} = \mathcal{S}(h, u_n) := \prod_{j=1}^{s} \mathrm{e}^{a_{s+1-j}\, hD_A}\, \mathrm{e}^{b_{s+1-j}\, hD_B}\, u_n, \qquad n = 0, 1, \ldots$$

Theorem: The local error of the splitting operator admits the expansion

$$\mathrm{e}^{hD_{A+B}} v - \mathcal{S}(h, v) \sim \sum_{k=1}^{p} \sum_{\substack{\mu \in \mathbb{N}^k \\ |\mu| \leq p-k}} \frac{1}{\mu!}\, h^{k+|\mu|}\, C_{k\mu} \prod_{\ell=1}^{k} \mathrm{ad}_{D_A}^{\mu_\ell}(D_B)\, \mathrm{e}^{hD_A}\, v.$$

$C_{k\mu}$ . . . computable constants.

The remainder term can be proven separately to be of higher order.

NLS

Cubic nonlinear Schrödinger equation (NLS)

$$\mathrm{i}\,\partial_t \psi(x,t) = -\frac{1}{2}\Delta\psi(x,t) + \beta|\psi(x,t)|^2\psi(x,t), \qquad x \in \mathbb{R}^3.$$

Theorem: Consider order p splitting for NLS,
let $\|\,\psi(t)\|_{H^k} \le M_k,\ k \in \mathbb{N}$.

- $\left\|\,\psi_n - \psi(t_n)\right\|_{L^2} \le C\,h^p\,, \qquad C = C(M_{2p}).$
- $\left\|\,\psi_n - \psi(t_n)\right\|_{H^1} \le C\,h^{p-1}\,, \qquad C = C(M_{2p-1}).$
- $\left\|\,\psi_n - \psi(t_n)\right\|_{H^2} \le C\,h^{p-2}\,, \qquad C = C(M_{2p-2}).$

Proof: First H^2, then H^2-conditional stability in H^1 and L^2, respectively.

Embedded Splittings

We use *embedded pairs* of splitting formulae for estimating the local error:

j	a_j	j	b_j
1	0	1,7	0.0829844064174052
2,7	0.245298957184271	2,6	0.3963098014983680
3,6	0.604872665711080	3,5	-0.0390563049223486
4,5	$1/2-(a_2+a_3)$	4	$1-2\,(b_1+b_2+b_3)$

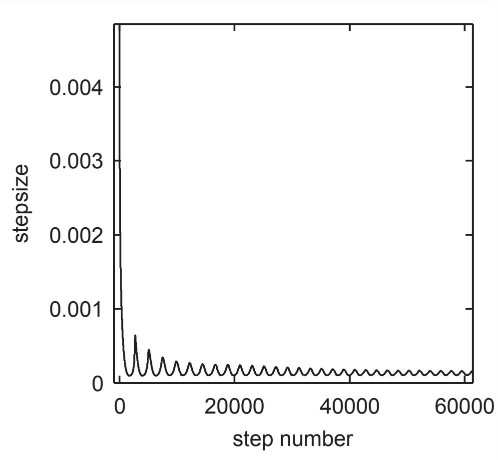
j	$\hat{a}_j$	j	$\hat{b}_j$
1	a_1	1	b_1
2	a_2	2	b_2
3	a_3	3	b_3
4	a_4	4	b_4
5	0.3752162693236828	5	0.4463374354420499
6	1.4878666594737946	6	-0.0060995324486253
7	-1.3630829287974774	7	0

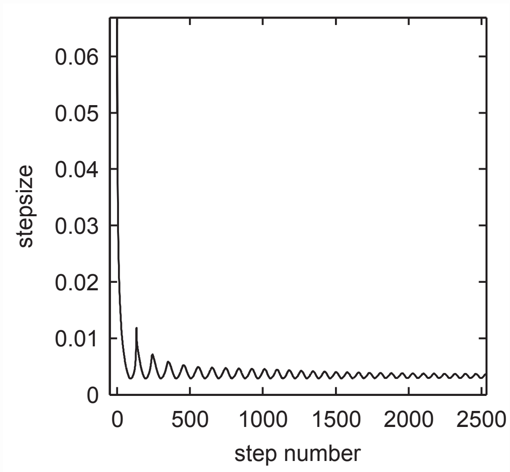
Embedded Splittings (2)

Cubic NLS with blow-up solution:

$$\mathrm{i}\,\partial_t \psi(x,t) = -\frac{1}{2}\Delta\psi(x,t) - 2|\psi(x,t)|^2\psi(x,t), \qquad x \in \mathbb{R}^2.$$

Time-stepping for pairs 2(1) (left) and 4(3) (right):





Defect Based Estimate

We consider the linear case,

$$\dot{u} = Au + Bu, \qquad u(0) = u_0.$$

Lie–Trotter and Strang splitting, we present Lie–Trotter:

$$u(t) = \mathcal{E}(t)u_0 = \mathrm{e}^{t(A+B)}u_0 \approx \mathrm{e}^{tA}\mathrm{e}^{tB}u_0 = \mathcal{S}(t)u_0.$$

The exact flow satisfies

$$\dot{\mathcal{E}}(t) = A\mathcal{E}(t) + B\mathcal{E}(t).$$

The splitting flow satisfies Sylvester equation

$$\dot{\mathcal{S}}(t) = A\mathcal{S}(t) + \mathcal{S}(t)B.$$

Defect Based Estimate (2)

Defect and truncation error of splitting flow:

$$\begin{aligned}\mathcal{D}(t) &= \dot{\mathcal{S}}(t) - A\mathcal{S}(t) - B\mathcal{S}(t) = [\mathcal{S}(t), B],\\ \mathcal{T}(t) &= \dot{\mathcal{E}}(t) - A\mathcal{E}(t) - \mathcal{E}(t)B = [B, \mathcal{E}(t)].\end{aligned}$$

Local error $\mathcal{L}(t) = \mathcal{S}(t) - \mathcal{E}(t)$:

$$\begin{aligned}\dot{\mathcal{L}}(t) &= A\mathcal{L}(t) + \mathcal{L}(t)B - \mathcal{T}(t)\\ &\approx A\mathcal{L}(t) + \mathcal{L}(t)B + \mathcal{D}(t).\end{aligned}$$

Solve Sylvester VOC equation for estimate $\mathcal{P} \approx \mathcal{L}$:

$$\int_0^h \mathrm{e}^{(h-s)A}\mathcal{D}(s)\mathrm{e}^{(h-s)B}\,ds \approx \frac{h}{2}\mathcal{D}(h) = \mathcal{P}(h).$$

Schrödinger Equations

Linear Schrödinger equation

$$\mathrm{i}\,\partial_t \psi(x,t) = -\tfrac{1}{2}\,\Delta\,\psi(x,t) + V(x)\,\psi(x,t)\,, \quad x \in \mathbb{R}^3\,.$$

Theorem: Let $\mathcal{L}$ be the local error, $\mathcal{P}$ its estimate. Then for the Lie–Trotter splitting,

- For $V \in C^2,\ \|\psi_0\|_{H^1} \le M_1$,

$$\|\mathcal{L}(h)\psi_0\|_{L^2} \le Ch^2, \qquad C = C(M_1).$$

- For $V \in C^4,\ \|\psi_0\|_{H^2} \le M_2$,

$$\|(\mathcal{P} - \mathcal{L})(h)\psi_0\|_{L^2} \le Ch^3, \qquad C = C(M_2).$$

Full Discretization

Cubic NLS with *rotation term* in 2D:

$$\begin{aligned} \mathrm{i}\partial_t \psi(x,y,t) &= -\frac{1}{2}\Delta\psi(x,y,t) + \frac{\gamma^2}{2}(x^2+y^2)\psi(x,y,t) + \cdots \\ &\quad + \mathrm{i}\Omega(x\partial_y - y\partial_x)\psi(x,y,t) + V(x,y)\psi(x,y,t) + \cdots \\ &\quad + \beta|\psi(x,y,t)|^2\psi(x,y,t), \quad (x,y)\in\mathbb{R}^2,\ t>0. \end{aligned}$$

Spatial discretization in cylindrical coordinates: Laguerre(r)–Fourier(θ)–[Hermite(z)].

Theorem: Consider splitting of order p for full discretization. If $\psi \in H_{2p}$, then

$$\|\psi_{n,M} - \psi(t_n)\|_{L^2} \le C\left(\|\psi_{0,M} - \psi(0)\|_{L^2} + M^{-q} + (\Delta t)^p\right),$$

where $q > 0$ and M^d . . . # of basis functions, $d = 2, 3$.

Nonlinear Defect Estimate

Define defect

$$
\begin{aligned}
\mathcal{D}(t) &= \partial_t \mathcal{S}(t,\psi_0) - A\mathcal{S}(t,\psi_0) - B(\mathcal{S}(t,\psi_0)) \\
&= \partial_2 \mathcal{S}(t,\psi_0)\cdot B(\psi_0) - B(\mathcal{S}(t,\psi_0)) \\
&= \mathcal{S}(t, B(\psi_0)) - B(\mathcal{S}(t,\psi_0)) + O(t^2).
\end{aligned}
$$

Error estimate: Generalized Gröbner–Alexeev Lemma.

Quadrature $\rightsquigarrow \mathcal{P}(h) = \frac{h}{2}\mathcal{D}(h)$.

Asymptotically correct in nonlinear semi-discrete and fully-discrete setting!

Numerical example (1)

For $\Omega = \gamma = V = 0$ and $\beta = -1$ in 1D
(512 Fourier modes, spatial error negligible),

an exact solution is

$$\psi(x,t) = \frac{2\mathrm{e}^{\frac{3}{2}\mathrm{i}t - \mathrm{i}x}}{\cosh(2t + 2x)}.$$

k	Δt	err	p	err_{est}	p_{est}
8	3.9062×10^{-3}	1.5560×10^{-4}	2.00	1.1997×10^{-6}	3.03
9	1.9531×10^{-3}	3.8906×10^{-5}	2.00	1.4902×10^{-7}	3.01
10	9.7656×10^{-4}	9.7267×10^{-6}	2.00	1.8597×10^{-8}	3.00
11	4.8828×10^{-4}	2.4317×10^{-6}	2.00	2.3237×10^{-9}	3.00
12	2.4414×10^{-4}	6.0792×10^{-7}	2.00	2.9044×10^{-10}	3.00
13	1.2207×10^{-4}	1.5198×10^{-7}	2.00	3.6304×10^{-11}	3.00

Numerical example (2)

2D example: $V = 0.4\,y^2,\ \Omega = 0.5,\ \beta = 100,\ \gamma = 0.8.$

The movie shows $|\psi|^2$ for

$$\psi_0(x,y) = \frac{x + \mathrm{i}y}{\sqrt{\pi}} \mathrm{e}^{-\frac{x^2+y^2}{2}}.$$

100 Laguerre, 128 Fourier, Strang splitting ($\Delta t = 0.02$).

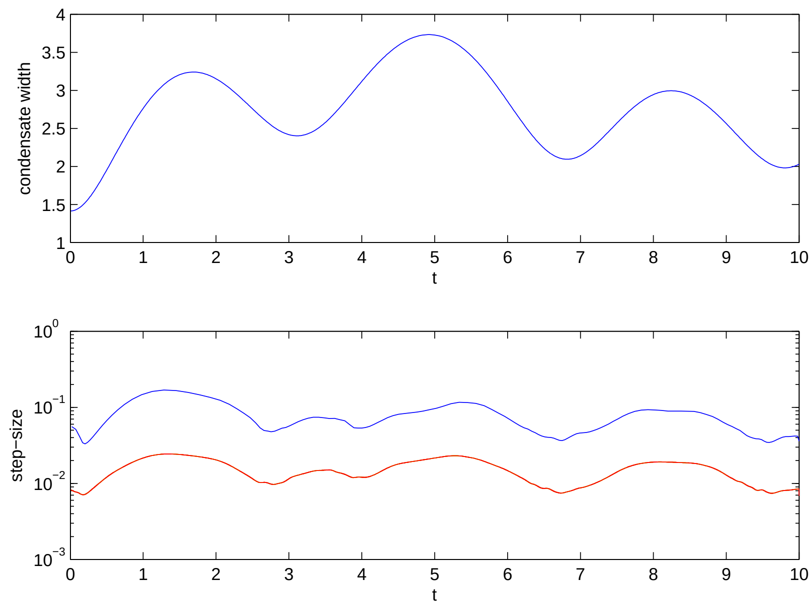
[density_fourier_laguerre_strang.avi]

Numerical example (3)

We plot the functional “condensate width”,

$$\sigma_r^2 = \sigma_x^2 + \sigma_y^2, \quad \sigma_\alpha^2 = \int_{\mathbb{R}^2} \alpha^2 |\psi(x,y,t)|^2 \, d(x,y).$$

Plot of width and step-sizes for embedded 4(3) and defect based Lie–Trotter (tolerance $= 10^{-3}$):



Extensions

- Lie splitting

$$\dot{u} = Au + Bu + Cu.$$

Design and analysis similar to the case $C = 0$.

- Strang splitting: Set $C = A$, further expansion,

$$\mathcal{D}(h) = \left[\mathrm{e}^{hA}\mathrm{e}^{hB}, A + B\right] \mathrm{e}^{hA} = O(h^2).$$

Use third-order Hermite quadrature
$\rightsquigarrow$ asymptotically correct local error estimator

$$\tilde{\varepsilon}_Q(h) = \frac{h}{3}\mathcal{D}(h) = \varepsilon(h) + O(h^4).$$

(error analysis uses higher order commutators).

Outlook

- Extension of defect–based approach to higher-order splittings (in progress) (suitable quadrature).
- Construction of higher–order (complex) embedded splitting methods is a highly nontrivial optimization problem.
- Defect based approach may be iterated to obtain higher-order approximation. Convergence?
- Comparisons of error estimators.
- Alternative spatial discretizations — FEM.

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