Adaptive space and time discretisations for Gross–Pitaevskii equations

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NUMDIFF-13, Halle, September 2012

FWF
Der Wissenschaftsfonds.

Collaborators

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Theme

Splitting methods. Efficient and accurate time integration of nonlinear evolution equations by adaptive splitting methods

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = F\big(u(t)\big) = A\big(u(t)\big) + B\big(u(t)\big), \quad 0 \le t \le T, \qquad u(0) \text{ given},$$

$$\mathscr{S}_F(t,\cdot) = \prod_{j=1}^{s} \mathrm{e}^{a_{s+1-j}\, tD_A}\, \mathrm{e}^{b_{s+1-j}\, tD_B} \;\approx\; \mathscr{E}_F(t,\cdot) = \mathrm{e}^{tD_F},$$

$$u_n = \mathscr{S}_F(\tau_{n-1}, u_{n-1}) \;\approx\; u(t_n) = \mathscr{E}_F\big(\tau_{n-1}, u(t_{n-1})\big), \quad 1 \le n \le N.$$

Applications.

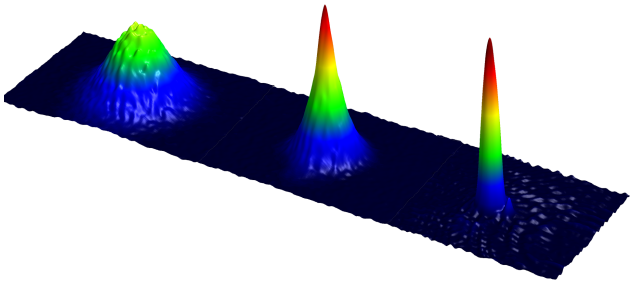
- Nonlinear Schrödinger equations (Time evolution and ground state computation for Gross–Pitaevskii systems)
- Parabolic equations (S. Blanes, F. Casas, P. Chartier, A. Murua)
- Kinetic equations (L. Pareschi)
- Wave equations (B. Kaltenbacher)

Nonlinear Schrödinger equations (Gross–Pitaevskii equations)

Bose–Einstein condensation

In our laboratories temperatures are measured in micro- or nanokelvin ... In this ultracold world ... atoms move at a snail's pace ... and behave like matter waves. Interesting and fascinating new states of quantum matter are formed and investigated in our experiments.

(GRIMM ET AL., Innsbruck)

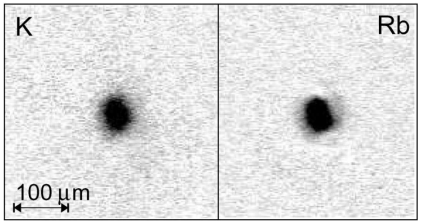


Bose–Einstein condensation in dilute gases. In 1925 Albert Einstein predicted that at (very) low temperatures particles in a (dilute) gas could all reside in the same quantum state. This peculiar gaseous state, a Bose–Einstein condensate, was produced in the laboratory for the first time in 1995 using the powerful laser-cooling methods developed in recent years. These condensates exhibit quantum phenomena on a large scale, and investigating them has become one of the most active areas of research in contemporary physics. See PETHICK, SMITH (2002).

Physical experiments (University of Innsbruck). Realisation of ground state and investigation of time evolution (H.-C. NÄGERL, M. MARK).

Gross–Pitaevskii systems

Physical experiments. Observation of multi-component Bose–Einstein condensates. Realisation of double species ^{87}Rb ^{41}K BEC at LENS, see G. THALHAMMER ET AL. (2008).



Theoretical model. Mathematical description (of certain aspects) by time-dependent Gross–Pitaevskii systems for $\Psi : \mathbb{R}^d \times [0,\infty) \to \mathbb{C}^J$

$$\mathrm{i}\,\hbar\,\partial_t \Psi_j(x,t) = \Big(-\frac{\hbar^2}{2m_j}\Delta + V_j(x) + \hbar^2 \sum_{k=1}^{J} g_{jk}\,|\Psi_k(x,t)|^2 \Big)\,\Psi_j(x,t)\,,$$

$$V_j(x) \approx \sum_{\ell=1}^{d} \Big(\frac{m_j}{2}\,\omega_{j\ell}^2\,(x_\ell - \zeta_{j\ell})^2 + \kappa_{j\ell}\,\big(\sin(q_{j\ell}\,x_\ell)\big)^2 \Big)\,, \quad \|\Psi_j(\cdot,0)\|_{L^2}^2 = N_j\,,$$

$$x \in \mathbb{R}^d\,, \quad 0 \le t \le T\,, \quad 1 \le j \le J\,.$$

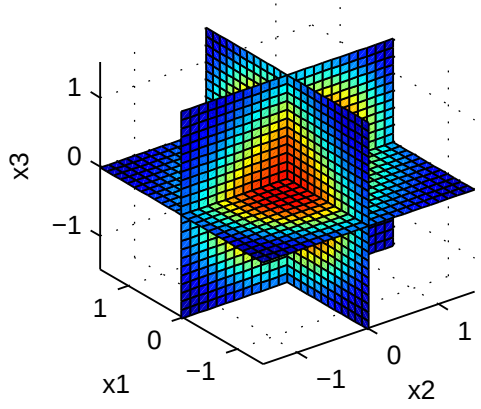
Geometric properties ($J = 1$). Preservation of particle number $\|\Psi(\cdot,t)\|_{L^2}^2$ and energy functional

$$E\big(\Psi(\cdot,t)\big) = \Big(\big(-\tfrac{\hbar}{2m}\Delta + V + \tfrac{1}{2}\,\hbar g\,|\Psi(\cdot,t)|^2 \big)\,\Psi(\cdot,t) \,\Big|\, \Psi(\cdot,t) \Big)_{L^2}.$$

Nonlinear Schrödinger equations – Model problem

Model problem. Consider nonlinear Schrödinger equation for $\psi : \mathbb{R}^d \times [0, T] \to \mathbb{C} : (x, t) \mapsto \psi(x, t)$

$$\begin{cases} \mathrm{i}\,\varepsilon\,\partial_t \psi(x,t) = \left(-\frac{1}{2}\,\varepsilon^2 \Delta + U(x) + \vartheta \left|\psi(x,t)\right|^2 \right) \psi(x,t)\,, \\ \psi(x,0) \text{ given}, \qquad x \in \mathbb{R}^d\,, \quad 0 \le t \le T\,, \end{cases}$$



subject to asymptotic boundary conditions.

Illustration. Solution profile $|\psi|^2$ of GPE in 3D ($\varepsilon = \omega = \vartheta = 1$, $T = 3$, $M = 128^3$, tol $= 10^{-6}$).

Ground state. Solution of special form $\psi(\cdot, t) = \mathrm{e}^{-\mathrm{i}\mu t}\,\varphi$ that minimises energy functional. Useful as reliable reference solution in time integration.

Semi-classical regime. Numerical solution for smaller parameter values $0 < \varepsilon \ll 1$. Problems of similar form arise in applications from solid state physics. See Bao, Jin, Markowich (2002/03).

Time-splitting pseudo-spectral methods for nonlinear Schrödinger equations

Space and time discretisation

Numerical simulations. Favourable behaviour of time-splitting and pseudo-spectral methods for low-dimensional nonlinear Schrödinger equations confirmed by numerical comparisons, see contributions by W. Bao and collaborators.

- **Time evolution.** Discretisation of model problem

$$\mathrm{i}\,\varepsilon\,\partial_t\psi(x,t) = \Big(-\tfrac{1}{2}\,\varepsilon^2\Delta + U(x) + \vartheta\,\big|\psi(x,t)\big|^2\Big)\,\psi(x,t)$$

  by pseudo-spectral method (Fourier, Sine, Hermite, Laguerre) and adaptive splitting method (embedded splitting pairs, a posteriori local error estimators).

- **Ground state computation ($\varepsilon = 1$).** Application of imaginary time method (projection at each artificial time step)

$$\partial_t\psi(x,t) = \Big(\tfrac{1}{2}\,\Delta - U(x) - \vartheta\,\big|\psi(x,t)\big|^2\Big)\,\psi(x,t)\,.$$

  Adaptive splitting method (Lie-Strang pair), pseudo-spectral space discretisation.

Calculus of Lie-derivatives

Formal calculus. Calculus of Lie-derivatives is suggestive of less involved linear case, see for instance HAIRER, LUBICH, WANNER (2002) and SANZ-SERNA, CALVO (1994).

Problem. Rewrite initial-boundary value problem as nonlinear evolution equation on Banach space X involving unbounded nonlinear operator $F : D(F) \subset X \to X$ and employ formal notation for analytical solution

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = F\big(u(t)\big)\,, \quad u(t) = \mathscr{E}_F\big(t, u(0)\big) = \mathrm{e}^{tD_F}\, u(0)\,, \qquad 0 \le t \le T\,.$$

Evolution operator, Lie-derivative. For unbounded nonlinear operator $G : D(G) \subset X \to X$ define

$$\mathrm{e}^{tD_F}\, G\, v = G\big(\mathscr{E}_F(t, v)\big)\,, \quad 0 \le t \le T\,, \qquad D_F\, G\, v = G'(v)\, F(v)\,.$$

Remark. In accordance with $L = \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} \mathrm{e}^{tL}$ it follows

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} \mathrm{e}^{tD_F}\, G\, v &= \frac{\mathrm{d}}{\mathrm{d}t}\Big|_{t=0} G\big(\mathscr{E}_F(t, v)\big) = G'\big(\mathscr{E}_F(t, v)\big)\, F\big(\mathscr{E}_F(t, v)\big)\Big|_{t=0} = G'(v)\, F(v) \\ &= D_F\, G\, v\,.\end{aligned}$$

Exponential operator splitting methods

Aim. For nonlinear evolution equation on Banach space X

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = A\big(u(t)\big) + B\big(u(t)\big), \quad 0 \le t \le T, \qquad u(0) \text{ given},$$

determine approximations at time grid points $0 = t_0 < \cdots < t_N \le T$ with associated stepsizes $\tau_{n-1} = t_n - t_{n-1}$ through recurrence

$$u_n = \mathscr{S}_F(\tau_{n-1}, u_{n-1}) \;\approx\; u(t_n) = \mathscr{E}_F\big(\tau_{n-1}, u(t_{n-1})\big), \qquad 1 \le n \le N.$$

Approach. Splitting methods rely on suitable decomposition of right-hand side and presumption that subproblems

$$\frac{\mathrm{d}}{\mathrm{d}t}\, v(t) = A\big(v(t)\big), \quad v(t) = \mathrm{e}^{tD_A}\, v(0), \qquad 0 \le t \le T,$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\, w(t) = B\big(w(t)\big), \quad w(t) = \mathrm{e}^{tD_B}\, w(0), \qquad 0 \le t \le T,$$

are solvable in accurate and efficient manner.

General form. High-order splitting methods are cast into following form scheme with real (or complex) method coefficients $(a_j, b_j)_{j=1}^{s}$

$$\mathscr{S}_F(t,\cdot) = \prod_{j=1}^{s} \mathrm{e}^{a_{s+1-j}\, tD_A}\, \mathrm{e}^{b_{s+1-j}\, tD_B} \;\approx\; \mathscr{E}_F(t,\cdot) = \mathrm{e}^{tD_F} = \mathrm{e}^{t(D_A+D_B)}.$$

Example methods

Low-order methods. First-order Lie–Trotter splitting method and second-order Strang splitting method

$$\mathscr{S}_F(t,\cdot) = \mathrm{e}^{tD_B}\,\mathrm{e}^{tD_A}\,, \qquad \mathscr{S}_F(t,\cdot) = \mathrm{e}^{\frac{1}{2}tD_A}\,\mathrm{e}^{tD_B}\,\mathrm{e}^{\frac{1}{2}tD_A}\,.$$

Higher-order methods. Symmetric fourth-order splitting method proposed in Blanes, Moan (2002) and embedded third-order splitting method by Koch, Th.

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

Practical realisation (Schrödinger equations)

Spectral decomposition. Numerical solution of first subproblem

$$\frac{\mathrm{d}}{\mathrm{d}t}\, v(t) = A\, v(t)\,, \quad 0 \le t \le T\,, \qquad v(0) \text{ given}\,,$$

involving linear differential operator A (related to Laplacian, eigenrelation $A\mathscr{B}_m = \mu_m \mathscr{B}_m$) relies on spectral decomposition

$$v(t) = \mathrm{e}^{tA} v(0) = \sum_m v_m\, \mathrm{e}^{t\mu_m} \mathscr{B}_m\,, \quad 0 \le t \le T\,, \qquad v(0) = \sum_m v_m \mathscr{B}_m\,.$$

Invariance. Numerical solution of second subproblem

$$\frac{\mathrm{d}}{\mathrm{d}t}\, w(t) = B\big(w(t)\big)\, w(t) = B(w_0)\, w(t)\,, \quad 0 \le t \le T\,, \qquad w(0) = w_0\,,$$

involving (unbounded) nonlinear multiplication operator B (related to potential and nonlinearity) relies on pointwise multiplication

$$\big(w(t)\big)(x) = \big(\mathrm{e}^{tB(w_0)} w_0\big)(x) = \mathrm{e}^{t(B(w_0))(x)} w_0(x)\,, \qquad 0 \le t \le T\,.$$

Explanation. For analytical solution of $\partial_t \psi(x,t) = -\mathrm{i}\left(V(x) + \vartheta\, |\psi(x,t)|^2\right)\psi(x,t)$ it follows

$$\partial_t\, |\psi(x,t)|^2 = \partial_t\big(\overline{\psi(x,t)}\, \psi(x,t)\big) = 2\,\Re\big(\overline{\psi(x,t)}\, \partial_t \psi(x,t)\big) = 2\,\Re\big(-\mathrm{i}\left(V(x) + \vartheta\, |\psi(x,t)|^2\right) |\psi(x,t)|^2\big) = 0\,.$$

Fourier pseudo-spectral method

Spectral decomposition. Let $\Omega = (-a_1, a_1) \times \cdots \times (-a_d, a_d)$ with $a_\ell > 0$ (large) for $1 \le \ell \le d$. Fourier basis functions $(\mathscr{F}_m)_{m \in \mathbb{Z}^d}$ form orthonormal basis of $L^2(\Omega)$ and satisfy eigenvalue relation

$$\psi(\cdot, t) = \sum_m \psi_m(t)\, \mathscr{F}_m\,, \qquad \psi_m(t) = \big(\psi(\cdot, t) \,\big|\, \mathscr{F}_m\big)_{L^2}\,,$$

$$-\Delta \mathscr{F}_m = \lambda_m \mathscr{F}_m\,, \qquad \mathscr{F}_m(x) = \prod_{\ell=1}^{d} \frac{\mathrm{e}^{\mathrm{i}\pi m_\ell \left(\frac{x_\ell}{a_\ell}+1\right)}}{\sqrt{2a_\ell}}\,, \qquad \lambda_m = \sum_{\ell=1}^{d} \frac{\pi^2 m_\ell^2}{a_\ell^2}\,.$$

Numerical approximation. Truncation of infinite sum and application of trapezoid quadrature formula yields approximation

$$\mathscr{Q}_M \psi(\cdot, t) = \sum_{m}{}_M \psi_m(t)\, \mathscr{F}_m\,,$$

$$\psi_m(t) = \int_\Omega \psi(x, t)\, \overline{\mathscr{F}_m(x)}\, \mathrm{d}x \approx \sum_k \omega_k\, \psi(\xi_k, t)\, \overline{\mathscr{F}_m(\xi_k)}\,.$$

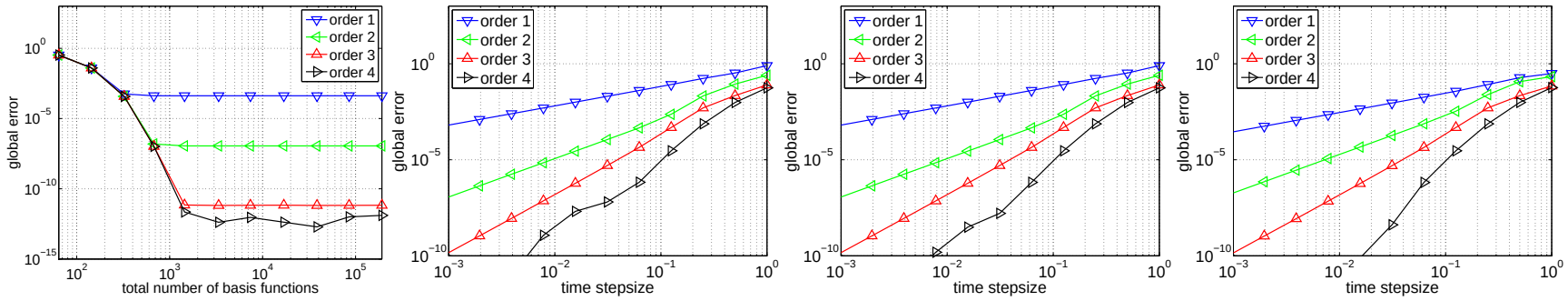
Implementation. Realisation by Fast Fourier Techniques.

Spectral space discretisations. Analogous relations for Sine, Hermite, and generalised Laguerre–Fourier Hermite pseudo-spectral methods.

Stability and convergence analysis

Illustration (Global error, temporal order of convergence)

Illustration. Discretisation of Gross–Pitaevskii equation ($d = 2$, $\varepsilon = \omega = T = 1$) by different pseudo-spectral methods ($M = 256 \times 256$) and time-splitting methods of (nonstiff) orders $p = 1, 2, 3, 4$. Dependence of global error on total number of basis functions ($\vartheta = 0$, dominant error term related to linear part, Fourier, Hermite basis function as exact reference solution, temporal error dominates global error). Numerically observed orders of convergence in time ($\vartheta = 1$, Fourier, Sine, Hermite, smooth initial value, numerical reference solution).



Conjecture. The global error satisfies an estimate of the following form

$$\left\| \widetilde{u}_{nM} - u(t_n) \right\|_{X_0} \leq C \left(\tau^p + M^{-q} \right), \qquad 0 \leq t_n \leq T .$$

Global error estimate (Full discretisations)

Discretisation. Space and time discretisation of nonlinear Schrödinger equations by different pseudo-spectral methods (Fourier, Sine, Hermite) and higher-order variable stepsize time-splitting methods.

Theorem (M.Th., 2012)

Provided that exact solution remains bounded in fractional power space X_β defined by principal linear part for $\beta \geq p$, the global error estimate holds

$$\|\widetilde{u}_{nM} - u(t_n)\|_{X_0} \leq C\left(\tau^p + M^{-q}\right), \qquad 0 \leq t_n \leq T\,.$$

Extension. Extension to Gross–Pitaevskii equations with additional rotation term (Harald Hofstätter).

Approach (Derivation of global error estimate)

Approach. Use decomposition $\widetilde{u}_{nM} - u(t_n) = (\widetilde{u}_{nM} - u_n) + (u_n - u(t_n))$. Employ Lady Winderemere's fan argument to deduce error estimates for the time discrete and fully discrete solution (time-splitting operator $\mathscr{S}_F$, time-splitting pseudo-spectral operator $\mathscr{T}_F$)

$$u_n - u(t_n) = \sum_{j=1}^{n} \Big(\prod_{\ell=j}^{n-1} \mathscr{S}_F(\tau)\, \mathscr{S}_F(\tau)\, u(t_{j-1}) - \prod_{\ell=j}^{n-1} \mathscr{S}_F(\tau)\, \mathscr{E}_F(\tau)\, u(t_{j-1}) \Big),$$

$$\widetilde{u}_{nM} - u_n = (\mathscr{Q}_M - I)\, u_n + \sum_{j=1}^{n} \Big(\prod_{\ell=j}^{n-1} \mathscr{T}_F(\tau)\, \mathscr{T}_F(\tau)\, u_{j-1} - \prod_{\ell=j}^{n-1} \mathscr{T}_F(\tau)\, \mathscr{Q}_M\, \mathscr{S}_F(\tau)\, u_{j-1} \Big).$$

Main tools. Stability estimates and bounds for the defects.

- General setting to include different spectral methods (self-adjoint operator defining principal linear part, associated fractional power spaces).
- Framework of abstract evolution equations and formal calculus of Lie-derivatives (suitable local error expansion).
- Bounds for spectral interpolation error and iterated Lie-commutators in fractional power spaces.

Local error expansion (Time-splitting methods)

Situation. Time integration of nonlinear evolution equations by high-order exponential operator splitting methods

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = F\big(u(t)\big) = A\big(u(t)\big) + B\big(u(t)\big), \quad 0 \le t \le T, \qquad u(0) \text{ given},$$

$$\mathscr{S}_F(t,\cdot) = \prod_{j=1}^{s} \mathrm{e}^{a_{s+1-j}\, tD_A}\, \mathrm{e}^{b_{s+1-j}\, tD_B} \;\approx\; \mathscr{E}_F(t,\cdot) = \mathrm{e}^{tD_F},$$

$$u_n = \mathscr{S}_F(\tau_{n-1}, u_{n-1}) \;\approx\; u(t_n) = \mathscr{E}_F\big(\tau_{n-1}, u(t_{n-1})\big), \quad 1 \le n \le N.$$

Objective. Deduce local error representation for high-order splitting methods that remains suitable for nonlinear evolutions equations involving unbounded operators

$$\mathscr{L}_F(t,v) = \mathscr{S}_F(t,v) - \mathscr{E}_F(t,v) = \mathscr{O}\big(t^{p+1}, \|v\|_D\big).$$

Hope. Requirement $\sup\big\{\|u(t)\|_D : 0 \le t \le T\big\} \le C$ reasonable in connection with nonlinear Schrödinger equations (differentiability of problem data, asymptotic boundary conditions).

Derivation of local error expansions

Standard approaches. Power series expansion of exponential functions, Baker–Campbell–Hausdorff formula.

Alternative approaches.

- **Quadrature formulas.** Optimal error bounds in regard to regularity of analytical solution for evolutionary Schrödinger equations by techniques studied in JAHNKE, LUBICH (2000), KOCH, NEUHAUSER, TH. (2011), LUBICH (2008), and TH. (2008, 2012).

  Main tools.

  - Variation-of-constants formula (Gröbner–Alekseev)
  - Stepwise expansion of e^{tD_B}
  - Quadrature formulas for multiple integrals
  - Bounds for iterated commutators
  - Characterise domains of unbounded operators

- **Differential equations.** Investigation of exact local error representation for evolution equations involving critical parameters exploited in DESCOMBES, DUMONT, LOUVET, MASSOT (2007), DESCOMBES, SCHATZMAN (2002), and DESCOMBES, TH. (2010, 2011).

Local error expansion (Linear equations, Strang)

Situation. Time discretisation of linear evolution equation by splitting method involving two compositions with $a_1 + a_2 = 1$

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = A\, u(t) + B\, u(t)\,, \quad 0 \le t \le T\,, \qquad u(0) \text{ given}\,,$$
$$\mathscr{S}_F(t,\cdot) = \mathrm{e}^{b_2\, t B}\, \mathrm{e}^{a_2\, t A}\, \mathrm{e}^{b_1\, t B}\, \mathrm{e}^{a_1\, t A} \approx \mathscr{E}_F(t,\cdot) = \mathrm{e}^{t(A+B)}\,.$$

Derivation of local error expansion. Expansion of exact solution value by variation-of-constants formula and stepwise expansion of e^{tB} yields

$$\mathscr{L}_F(t,\cdot) = Q_1 - I_1 + Q_2 - I_2 + \mathscr{O}\big(t^3, C_B^3, M_A, M_B, M_{A+B}\big)\,,$$
$$Q_1 = t\,\big(b_1 \mathrm{e}^{(1-a_1)tA} B\, \mathrm{e}^{a_1 tA} + b_2 B\, \mathrm{e}^{tA}\big) \approx I_1 = \int_0^t \mathrm{e}^{(t-\tau_1)A}\, B\, \mathrm{e}^{\tau_1 A}\, \mathrm{d}\tau_1\,,$$
$$Q_2 = \tfrac{1}{2}\, t^2\, \big(b_1^2\, \mathrm{e}^{(1-a_1)tA} B^2 \mathrm{e}^{a_1 tA} + 2\, b_1 b_2 B\, \mathrm{e}^{(1-a_1)tA}\, B\, \mathrm{e}^{a_1 tA} + b_2^2 B^2\, \mathrm{e}^{tA}\big)$$
$$\approx I_2 = \int_0^t \int_0^{\tau_1} \mathrm{e}^{(t-\tau_1)A}\, B\, \mathrm{e}^{(\tau_1-\tau_2)A}\, B\, \mathrm{e}^{\tau_2 A}\, \mathrm{d}\tau_2\, \mathrm{d}\tau_1\,,$$

provided that $\|B\|_{X\leftarrow X} \le C_B$, $\big\|\mathrm{e}^{tC}\big\|_{X\leftarrow X} \le \mathrm{e}^{M_C\, t}$, $C \in \{A, B, A+B\}$. Further Taylor series expansions of integrands (commutators $[A,B]$, $[A,[A,B]]$).

Local error expansion (Linear equations, Strang)

Assumptions. Assume $a_1 + a_2 = 1$ and furthermore

$$\|B\|_{X\leftarrow X} \le C_B\,, \qquad \left\|\mathrm{e}^{tC}\right\|_{X\leftarrow X} \le \mathrm{e}^{M_C t}\,, \quad C \in \{A, B, A+B\}\,,$$
$$\left\|\left[A,B\right]v\right\|_X + \left\|\left[A,\left[A,B\right]\right]v\right\|_X \le C_{\mathrm{ad}}\,\|v\|_D\,.$$

Local error expansion. Exponential operator splitting method involving two compositions (Strang) fulfills local error expansion

$$\begin{aligned}\mathscr{L}_F(t,v) &= \left(\mathrm{e}^{b_2 tB}\,\mathrm{e}^{a_2 tA}\,\mathrm{e}^{b_1 tB}\,\mathrm{e}^{a_1 tA} - \mathrm{e}^{t(A+B)}\right)v \\ &= t\left(b_1+b_2-1\right)\mathrm{e}^{tA}B\,v \\ &\quad - t^2\,\mathrm{e}^{tA}\left(\left(a_1 b_1 + b_2 - \tfrac{1}{2}\right)\left[A,B\right] + \tfrac{1}{2}\left((b_1+b_2)^2-1\right)B^2\right)v \\ &\quad + \mathscr{O}\left(t^3, C_B^3, M_A, M_B, M_{A+B}, C_{\mathrm{ad}}, \|v\|_D\right).\end{aligned}$$

Extension and application to linear Schrödinger equations. Suitable choice $X = L^2(\Omega)$, $D = H^p(\Omega)$, $M_A = M_B = 0$, see Th. (2008).

Local error expansion (Nonlinear equations)

Result. Local error expansion of high-order splitting methods applied to nonlinear evolution equations.

Theorem (Th. 2008, Koch & Neuhauser & Th. 2011, Th. 2012)

The defect operator of an exponential operator splitting method of (classical) order p admits the (formal) expansion

$$\mathscr{L}_F(t,\cdot) = \sum_{k=1}^{p} \sum_{\substack{\mu\in\mathbb{N}^k \\ |\mu|\le p-k}} \frac{1}{\mu!}\, t^{k+|\mu|}\, C_{k\mu} \prod_{\ell=1}^{k} ad_{D_A}^{\mu_\ell}(D_B)\, \mathrm{e}^{tD_A} + R_{p+1}(t,\cdot)\,,$$

$$C_{k\mu} = \sum_{\lambda\in\Lambda_k} \alpha_\lambda \prod_{\ell=1}^{k} b_{\lambda_\ell}\, c_{\lambda_\ell}^{\mu_\ell} - \prod_{\ell=1}^{k} \frac{1}{\mu_\ell+\cdots+\mu_k+k-\ell+1}\,.$$

Remarks. Application to MCTDHF equations in electron dynamics (with O. Koch). Local error expansion suitable for parabolic problems.

Illustrations

Implementation

Realistic models. Physically relevant models for Bose–Einstein condensation involve three-space dimensions

$$\mathrm{i}\,\hbar\,\partial_t \Psi(x,t) = \left(-\frac{\hbar^2}{2m}\Delta + V(x) + \hbar^2 g\,|\Psi(x,t)|^2 \right) \Psi(x,t)\,.$$

Preliminary tests. Employed numerical methods well-suited for computations on GPUs (PYTHON & OPENCL, MATLAB & CUDA) combined with parallelisation techniques. Considerable gain in efficiency (computation time).

Illustrations (Ground state computation, Time evolution)

Movie. Groundstate computation and time evolution of model problem ($d = 2$, $\varepsilon = 1$, $\vartheta = 0,10$) under a harmonic potential ($\omega = 1,2$). Space discretisation by Fourier pseudo-spectral method ($x \in [-8,8] \times [-8,8]$, $M = 200 \times 200$). Artificial time integration by 2(1) pair based on Strang and Lie splitting. Time integration by embedded 4(3) pair based on 4th-order scheme by BLANES, MOAN (2002) ($t \in [0,4]$, $\mathrm{tol} = 10^{-6}$).

Movie
Ground state, Time Evolution, Energy, Time stepsizes (MATLAB)

Illustrations (Ground state computation, Time evolution)

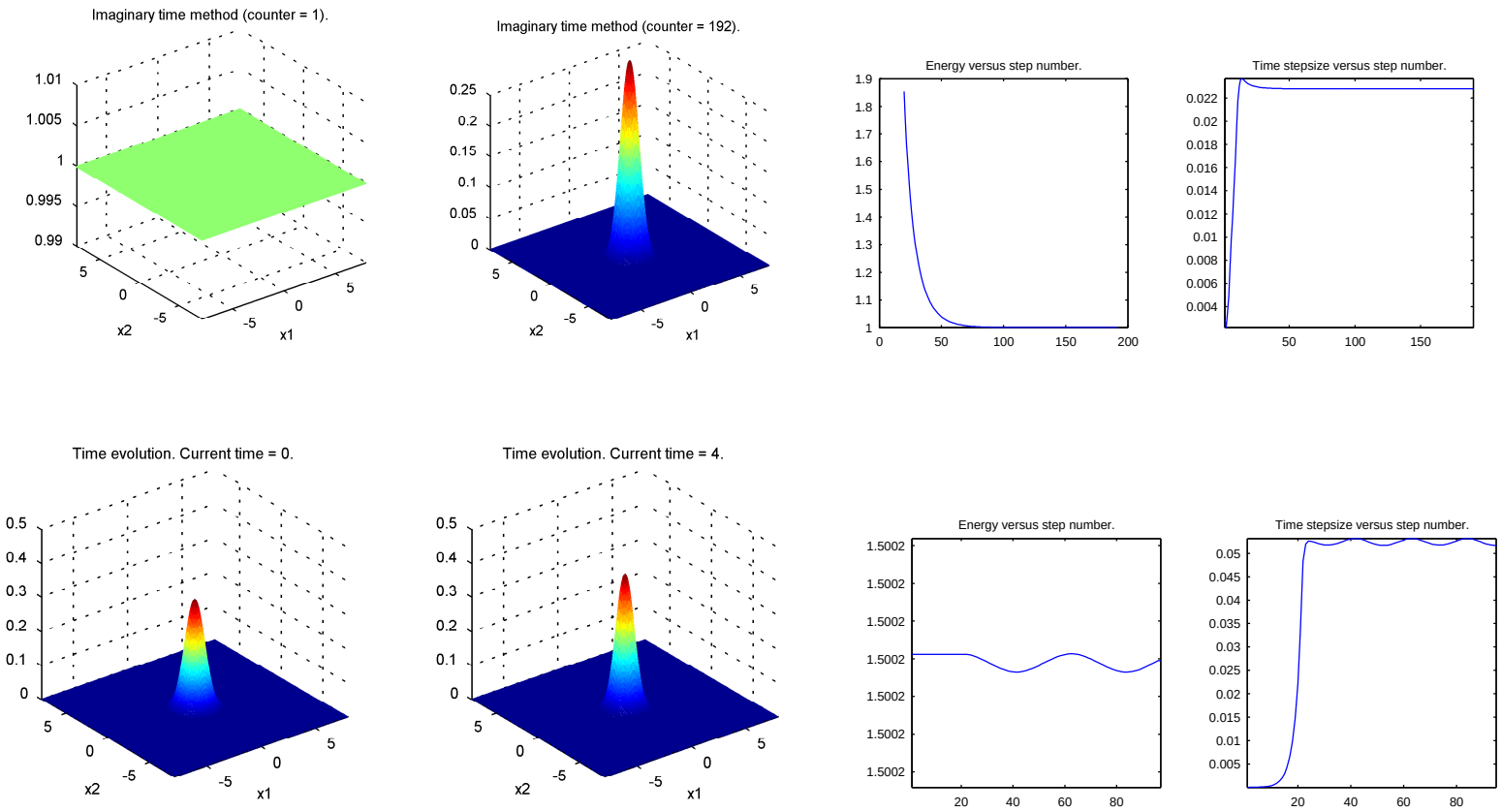


Illustration (GPE with rotation, Time evolution)

Movie. Gross–Pitaevskii equation with additional rotation term (EXAMPLE IN BAO, LI, SHEN, 2009). Movie generated by Harald Hofstätter.

Movie (Rotating condensate)

Illustrations (Smaller parameter, Solution behaviour)

Movie. Space and time discretisation of model problem ($d = 1$, $\varepsilon = 10^{-2}$, $\omega = 1$, $\vartheta = 1$) by Fourier pseudo-spectral method and embedded 4(3) time-splitting pair based on 4th-order scheme by BLANES, MOAN (2002) ($x \in [-8, 8]$, $M = 8192$, $t \in [0, 3]$, $\mathrm{tol} = 10^{-6}$, $N = 2178$).

Movie (Smaller parameter, Solution behaviour)

Illustration (Smaller parameter, Reliable time integration)

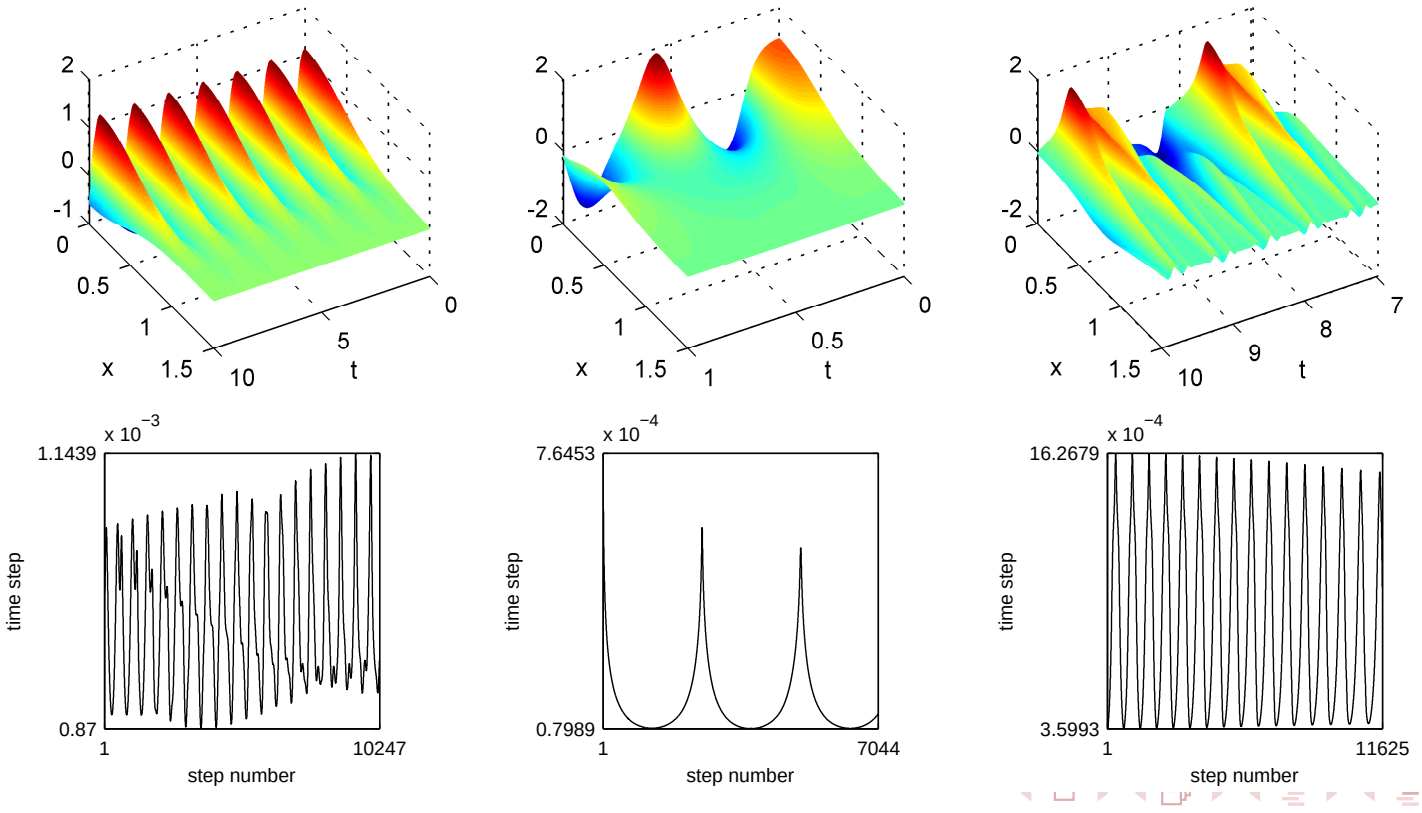
Integration without preparation is frustration. (REVEREND LEON SULLIVAN)

Movie. Time integration of model problem ($d = 1$, $\varepsilon = 10^{-2}$, $\omega = 2$, $\vartheta = 1$) under WKB initial condition by Fourier pseudo-spectral method and embedded 4(3) splitting pair based on 4th-order time-splitting scheme by BLANES, MOAN (2002) ($x \in [-8, 8]$, $M = 8192$, $t \in [0, 3]$). Solution profile $|\psi(x, t)|^2$ for tol $= 10^{-1}, 10^{-2}, 10^{-3}, 10^{-6}$ ($N = 951, 2342, 2452, 3560$).

Movie (Smaller parameter, Reliable time integration)

Illustration (Smaller parameter, Reliable time integration)

Further illustrations. Time integration of model equation ($d = \varepsilon = 1$, $\omega = 5$) by the embedded 4(3) pair (tol $= 10^{-10}$). Solution profiles $\Re\psi$ for $(x,t) \in [0, 1.5] \times [T_0, T]$ and associated time stepsizes. Left: Additional lattice potential with $\kappa = 10$ and defocusing nonlinearity with $\vartheta = 1$ for $t \in [0, 10]$. Middle: Focusing nonlinearity with $\vartheta = -10$ for $t \in [0, 1]$. Right: Defocusing nonlinearity with $\vartheta = 1$ and sharp initial Gaussian with $\gamma = 4$ for $t \in [0, 10]$.



Conclusions

- Theoretical analysis of discretisations for model problems provides insight in regard to more complex applications.
- Adaptivity in time essential for reliable numerical simulations.

Thank you!

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