Adaptive integration methods for time-dependent Gross–Pitaevskii equations: Theoretical and practical aspects

Mechthild Thalhammer
Leopold–Franzens Universität Innsbruck, Austria

Workshop on
Confined Quantum Systems: Modeling, Analysis and Computation
Wolfgang Pauli Institute, Vienna, February 2013

Theme

Splitting methods. Efficient time integration of nonlinear evolution equations by exponential operator splitting methods

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

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

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

Applications.

- Nonlinear Schrödinger equations (GPS, MCTDHF)
  (with W. Auzinger & H. Hofstätter & O. Koch, Ph. Chartier & F. Mehats, S. Descombes)
- Parabolic equations (Ground state computation by artificial time integration)
- Wave equations (with B. Kaltenbacher)

Objectives

Local error representations. Specification and inspection of local error representations for high-order splitting methods

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

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

Convergence analysis. Derivation of convergence result relies on stability bounds and estimates for local error

$$\big\| u_N - u(t_N) \big\|_X \leq C \left(\big\| u_0 - u(0) \big\|_X + \sum_{n=1}^{N} \tau_{n-1}^{p+1} \right).$$

Extension to full discretisations based on time-splitting pseudo-spectral methods

$$\big\| u_{NM} - u(t_N) \big\|_X \leq C \left(\big\| u_0 - u(0) \big\|_X + \tau_{\max}^{p} + M^{-q} \right).$$

References. DESCOMBES, TH. (2010, 2012), TH. (2008, 2012)

Objectives

Adaptive stepsize control. Standard strategy for adaptive time stepsize control

$$\tau_{\text{optimal}} = \tau \cdot \min\left(\alpha_{\max}, \max\left(\alpha_{\min}, \sqrt[p+1]{\alpha \cdot \frac{\text{tol}}{\text{err}_{\text{local}}}}\right)\right).$$

Construction and analysis of local error estimators for higher-order splitting methods.

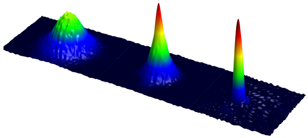
- Embedded splitting methods
- Asymptotically correct a posteriori local error estimators

References. AUZINGER, KOCH, TH. (2012), KOCH, NEUHAUSER, TH. (2013)

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)

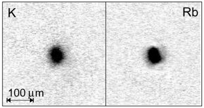


Bose–Einstein condensation in dilute gases. In 1925 Albert Einstein predicted that at (very) low temperatures particles in a (dilute) gas could all reside in the same quantum state. This peculiar gaseous state, a Bose–Einstein condensate, was produced in the laboratory for the first time in 1995 using 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 $\Psi : \mathbb{R}^d \times [0,\infty) \to \mathbb{C}^J$

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

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

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

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

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

Nonlinear Schrödinger equations – Model problem

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

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

subject to asymptotic boundary conditions.

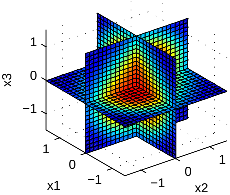


Illustration. Solution profile $|\psi|^2$ of GPE in 3D ($\varepsilon = \omega = \vartheta = 1,\ T = 3,\ M = 128^3$, tol $= 10^{-6}$).

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)

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

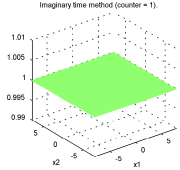
  Adaptive splitting method (Lie-Strang pair), pseudo-spectral space discretisation.

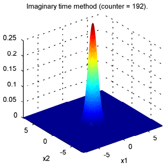
Illustrations (Ground state computation, Time evolution)

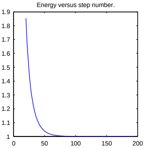
Movie. Groundstate computation and time evolution of model problem ($d = 2$, $\varepsilon = 1$, $\vartheta = 0, 10$) under a harmonic potential ($\omega = 1, 2$). Space discretisation by Fourier pseudo-spectral method ($x \in [-8, 8] \times [-8, 8]$, $M = 200 \times 200$). Artificial time integration 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) ($t \in [0, 4]$, tol $= 10^{-6}$).

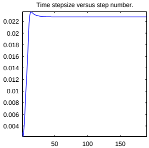
Movie
Ground state, Time Evolution, Energy, Time stepsizes (MATLAB)

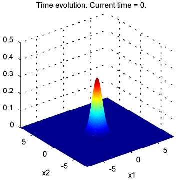
Illustrations (Ground state computation, Time evolution)

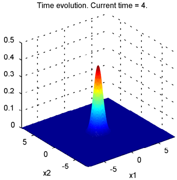


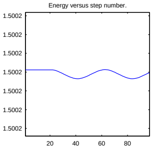


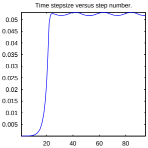












Exponential operator splitting methods

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 $\tau_{n-1} = t_n - t_{n-1}$ for $1 \le n \le N$ through recurrence

$$u_n = \mathscr{S}_F(\tau_{n-1}, u_{n-1}) \;\approx\; u(t_n) = \mathscr{E}_F\big(\tau_{n-1}, u(t_{n-1})\big) = \mathrm{e}^{\tau_{n-1} D_F}\, u(t_{n-1})\,.$$

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 (Koch, Th.) for time stepsize control.

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 $\partial_t \psi(x,t) = -\mathrm{i}\,\big(V(x) + \vartheta\,|\psi(x,t)|^2\big)\,\psi(x,t)$ it follows

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

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 $1 \leq \ell \leq d$. Fourier basis functions $(\mathscr{F}_m)_{m \in \mathbb{Z}^d}$ form orthonormal basis of $L^2(\Omega)$ and satisfy eigenvalue relation

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

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

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.

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)

Convergence analysis

Objective

Mein Verzicht auf das Restglied war leichtsinnig. (W. ROMBERG, 1979)

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

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

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

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

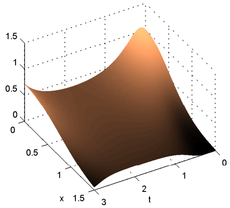
Objective. Deduce local error representation for high-order splitting methods that remains suitable for nonlinear evolutions equations involving unbounded operators and critical parameters

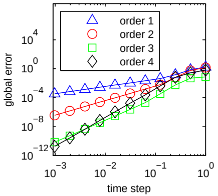
$$\mathscr{L}_F(t,v) = \mathscr{S}_F(t,v) - \mathscr{E}_F(t,v) = \mathscr{O}\big(t^{p+1}, \|v\|_D\big)\,.$$

Hope. Requirement $\sup\big\{\|u(t)\|_D : 0 \leq t \leq T\big\} \leq C$ (or $\varepsilon^j \big\|\partial_x^j u(0)\big\|_X \leq C$) reasonable in connection with nonlinear Schrödinger equations.

Illustration (Order of convergence)

Illustration. Space and time discretisation of Gross–Pitaevskii equation ($\varepsilon = 1$, $\omega = 1$, $\vartheta = 1$, $T = 1$) by Fourier pseudo-spectral method ($M = 256$) and different splitting methods of (nonstiff) orders $p \leq 4$. Numerically observed orders of convergence.





Numerical comparisons. Numerical comparisons (accuracy, efficiency, long-term behaviour) of higher-order time-splitting Fourier/Hermite pseudo-spectral methods (2D), see CALIARI, NEUHAUSER, TH. (2009).

Derivation of local error expansions

Standard approaches.

- Expansion of exponential functions
- Baker–Campbell–Hausdorff formula

Alternative approaches.

- **Quadrature formulas.** Optimal error bounds regarding regularity of analytical solution for evolutionary Schrödinger equations by techniques studied in JAHNKE, LUBICH (2000), KOCH, NEUHAUSER, TH. (2013), LUBICH (2008), and TH. (2008, 2012).
- **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, 2012).

Baker–Campbell–Hausdorff formula

Baker–Campbell–Hausdorff formula. BCH formula implies

$$\mathrm{e}^{tL}\,\mathrm{e}^{tK} = \mathrm{e}^{tS(t)}, \qquad S(t) = K + L - \tfrac{1}{2}\,t\,[K,L] + \mathscr{O}\left(t^2\right).$$

Local error expansion. For exponential operator splitting methods involving two compositions (Lie, Strang)

$$\mathscr{S}_F(t,\cdot) = \mathrm{e}^{tS(t)} = \mathrm{e}^{a_1 tD_A}\,\mathrm{e}^{b_1 tD_B}\,\mathrm{e}^{a_2 tD_A}\,\mathrm{e}^{b_2 tD_B} \approx \mathscr{E}_F(t,\cdot) = \mathrm{e}^{t(D_A+D_B)}$$

above relation yields expansion (order conditions)

$$\begin{aligned} D_A + D_B \approx S(t) &= (a_1 + a_2)\,D_A + (b_1 + b_2)\,D_B \\ &\quad + \tfrac{1}{2}\,t\left(b_2(a_2 + a_1) + b_1(a_1 - a_2)\right)\left[D_A, D_B\right] + \mathscr{O}\left(t^2\right), \end{aligned}$$

where $[D_A, D_B]\,v = D_A\,D_B\,v - D_B\,D_A\,v = B'(v)\,A(v) - A'(v)\,B(v)$.

Difficulties. Justify approach for unbounded nonlinear operators? Capture precise form of remainder to obtain optimal regularity requirements on analytical solution? Employ alternative approaches ...

Order conditions (Lie, Strang)

Order conditions. For bounded nonlinear operators requirement $\mathscr{L}_F(t,\cdot) = \mathscr{O}\big(t^{p+1}\big)$ for $p = 1,2$ implies (nonstiff) order conditions

$$a_1 + a_2 = 1\,, \qquad b_1 + b_2 = 1\,, \qquad (p=1)$$
$$(1-a_1)\,b_1 = \tfrac{1}{2}\,. \qquad (p=2)$$

Examples. Retain first-order Lie–Trotter splitting

$$s = 1\,, \qquad a_1 = 1\,, \quad b_1 = 1\,,$$
$$s = 2\,, \qquad a_1 = 0\,, \quad a_2 = 1\,, \quad b_1 = 1\,, \quad b_2 = 0\,,$$

and second-order Strang splitting

$$s = 2\,, \qquad a_1 = \tfrac{1}{2} = a_2\,, \quad b_1 = 1\,, \quad b_2 = 0\,,$$
$$s = 2\,, \qquad a_1 = 0\,, \quad a_2 = 1\,, \quad b_1 = \tfrac{1}{2} = b_2\,.$$

Question. Order reduction of splitting methods when applied to equations involving unbounded operators and critical parameters?

Approach based on quadrature formulas

Quadrature formulas

Approach. Alternative local error expansion

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

provides optimal error estimates regarding regularity of analytical solution for (non)linear evolutionary Schrödinger equations with (un)bounded potentials.

- **Linear equations.** See also JAHNKE, LUBICH (2000), NEUHAUSER, TH. (2009), TH. (2008).
- **Nonlinear equations.** See also GAUCKLER (2010), KOCH, NEUHAUSER, TH. (2013), LUBICH (2008), TH (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

Local error expansion (Linear equations, Strang)

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

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

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

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

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

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

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

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

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).

Drawback. Numerical illustrations show that approach not optimal with respect to critical parameter ($B = U/\varepsilon$).

Local error expansion (Nonlinear equations)

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

Theorem (Koch & Neuhauser & Th. 2013, Th. 2008, Th. 2012)

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

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

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

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

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 (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

$$\|u_{NM} - u(t_N)\|_{X_0} \leq C\Big(\|u_0 - u(0)\|_{X_0} + \tau_{\max}^{p} + M^{-q}\Big).$$

Extension. Extension to Gross–Pitaevskii equations with additional rotation term (with O. KOCH & H. HOFSTÄTTER).

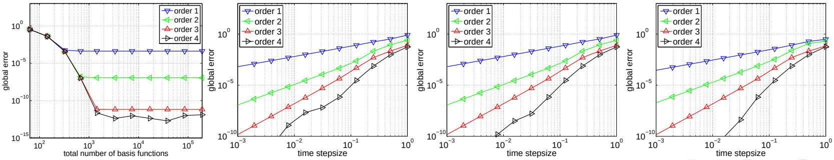
Global error estimate (Full discretisations)

Theorem (Th. 2012)

Global error estimate for sufficiently smooth solutions

$$\|u_{NM} - u(t_N)\|_{X_0} \leq C\Big(\|u_0 - u(0)\|_{X_0} + \tau_{\max}^{p} + M^{-q}\Big).$$

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).



Approach based on differential equations

Differential equations

Approach. Derivation of exact local error representation for splitting methods applied to linear and nonlinear equations involving critical parameters, see Descombes, Schatzman (2002) and Descombes, Th. (2010, 2012). Similar approach utilised for derivation of a posteriori error estimators.

Basic idea. Deduce differential equation for splitting operator

$$\mathscr{S}_F(t,\cdot) = \prod_{j=1}^{s} \mathrm{e}^{a_{s+1-j}\, t D_A}\, \mathrm{e}^{b_{s+1-j}\, t D_B}$$

closely related to differential equation for evolution operator

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\mathscr{E}_F(t,\cdot) = (D_A + D_B)\,\mathscr{E}_F(t,\cdot)\,, \quad 0 \le t \le T\,, \qquad \mathscr{E}_F(0,\cdot) = I\,.$$

Main tools. Variation-of-constants formula, iterated commutators.

Exact local error representation (Linear equations, Lie)

Situation. Time integration of linear evolution equation by first-order Lie–Trotter splitting $\mathscr{S}_F(t) = \mathrm{e}^{tB}\,\mathrm{e}^{tA}$.

Derivation of exact local error representation. Consider initial value problem for evolution operator

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{E}_F(t) = (A+B)\,\mathscr{E}_F(t)\,, \quad 0 \leq t \leq T\,, \qquad \mathscr{E}_F(0) = I\,.$$

Rewrite time derivative of splitting operator as

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{S}_F(t) = B\,\mathscr{S}_F(t) + \mathrm{e}^{tB}A\,\mathrm{e}^{tA} = (A+B)\,\mathscr{S}_F(t) + \big[\mathrm{e}^{tB}, A\big]\,\mathrm{e}^{tA}$$

and obtain initial value problem for splitting operator

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathscr{S}_F(t) = (A+B)\,\mathscr{S}_F(t) + \mathscr{R}(t)\,, \quad 0 \leq t \leq T\,, \qquad \mathscr{S}_F(0) = I\,.$$

By variation-of-constants formula obtain representation

$$\mathscr{L}_F(t,\cdot) = \int_0^t \mathscr{E}_F(t-\tau)\,\mathscr{R}(\tau)\,\mathrm{d}\tau\,, \quad \mathscr{R}(t) = \big[\mathrm{e}^{tB}, A\big]\,\mathrm{e}^{tA}\,, \qquad 0 \leq t \leq T\,.$$

Exact local error representation (Linear equations, Lie)

Expansion of remainder. Consider remainder

$$\mathscr{R}(t) = \tfrac{\mathrm{d}}{\mathrm{d}t}\,\mathscr{S}_F(t) - (A+B)\,\mathscr{S}_F(t) = \big[\mathrm{e}^{tB}, A\big]\,\mathrm{e}^{tA}\,.$$

Rewrite time derivative of $r(t) = \big[\mathrm{e}^{tB}, A\big] = \mathrm{e}^{tB} A - A\,\mathrm{e}^{tB}$ as

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\,r(t) = B\,\mathrm{e}^{tB} A - A\,B\,\mathrm{e}^{tB} = B\,r(t) + \big(B\,A - A\,B\big)\mathrm{e}^{tB}\,,$$

which yields initial value problem for commutator

$$\tfrac{\mathrm{d}}{\mathrm{d}t}\,r(t) = B\,r(t) + \big[B, A\big]\,\mathrm{e}^{tB}\,, \quad 0 \le t \le T\,, \qquad r(0) = 0\,.$$

By variation-of-constants formula obtain representation

$$r(t) = \big[\mathrm{e}^{tB}, A\big] = \int_0^t \mathrm{e}^{\tau B}\,\big[B, A\big]\,\mathrm{e}^{(t-\tau)B}\,\mathrm{d}\tau\,, \qquad 0 \le t \le T\,.$$

Exact local error representation (Linear equations, Lie)

Local error representation. Above considerations imply exact local error representation

$$\mathscr{L}_F\big(\tau_{n-1}, u(t_{n-1})\big) = \int_0^{\tau_{n-1}} \int_0^{\sigma_1} \mathscr{E}_F(\tau_{n-1} - \sigma_1)\, \mathrm{e}^{\sigma_2 B}\, [B, A]\, \mathrm{e}^{-\sigma_2 B}\, \mathscr{S}_F(\sigma_1)\, u(t_{n-1})\, \mathrm{d}\sigma_2\, \mathrm{d}\sigma_1\,.$$

Provided that bound $\|\mathscr{E}_F(\tau_{n-1} - \sigma_1)\, \mathrm{e}^{\sigma_2 B}\, [B, A]\, \mathrm{e}^{-\sigma_2 B}\, \mathscr{S}_F(\sigma_1)\, u(t_{n-1})\|_X \leq C\, \|u(t_{n-1})\|_D$ holds, local error estimate $\|\mathscr{L}_F(\tau_{n-1}, u(t_{n-1}))\|_X \leq C\, \tau_{n-1}^2$ follows.

Generalisation. Generalisation of exact local error representation, see Descombes, Th. (2010, 2012).

- High-order splitting methods for linear evolution equations.
- Lie–Trotter splitting method for nonlinear evolution equations.

Exact local error representation (Linear equations)

Theorem (Descombes & Th. 2010)

$$\mathscr{L}_F(t) = \prod_{j=1}^{s} \mathrm{e}^{b_j tB}\,\mathrm{e}^{a_j tA} - \mathrm{e}^{t(A+B)} = \int_0^t \mathscr{E}_F(t-\tau)\,\mathscr{R}(\tau)\,\mathrm{d}\tau\,, \qquad t \geq 0\,,$$

$$\mathscr{R} = \prod_{j=\sigma+1}^{s} \mathrm{e}^{b_j tB}\,\mathrm{e}^{a_j tA}\,\mathscr{T} \prod_{j=1}^{\sigma} \mathrm{e}^{b_j tB}\,\mathrm{e}^{a_j tA}\,, \qquad \sigma = \tfrac{1}{2}\begin{cases} s\,, & s \text{ even}\,,\\ s+1\,, & s \text{ odd}\,,\end{cases}$$

$$\mathscr{T} = \sum_{j=0}^{\sigma-1} C_{\sigma-j,j} + \sum_{j=0}^{s-\sigma-1} D_{\sigma+1+j,j}\,, \qquad \mathscr{I}_{\pm}(L_1,L_2,t) = \int_0^t \mathrm{e}^{\pm tL_1}\,[L_1,L_2]\,\mathrm{e}^{\mp tL_1}\,\mathrm{d}\tau\,,$$

$$\begin{aligned}
C_{k,0} &= c_k\,\mathscr{I}_{+}(B_k,A) + d_{k-1}\,\mathscr{I}_{+}(A_k,B) + d_{k-1}\mathscr{I}_{+}\big(B_k,\mathscr{I}_{+}(A_k,B)\big)\,,\\
C_{k,j} &= C_{k,j-1} + \mathscr{I}_{+}(A_{k+j},C_{k,j-1}) + \mathscr{I}_{+}(B_{k+j},C_{k,j-1})\\
&\quad + \mathscr{I}_{+}\big(B_{k+j},\mathscr{I}_{+}(A_{k+j},C_{k,j-1})\big)\,, \quad 1 \leq k \leq \sigma\,,\ 0 \leq j \leq \sigma-1\,,\\
D_{k,0} &= c_k\,\mathscr{I}_{-}(B_k,A) - c_k\,\mathscr{I}_{-}\big(A_k,\mathscr{I}_{-}(B_k,A)\big) + d_{k-1}\,\mathscr{I}_{-}(A_k,B)\,,\\
D_{k,j} &= D_{k,j-1} - \mathscr{I}_{-}(A_{k-j},D_{k,j-1}) - \mathscr{I}_{-}(B_{k-j},D_{k,j-1})\\
&\quad + \mathscr{I}_{-}\big(A_{k-j},\mathscr{I}_{-}(B_{k-j},D_{k,j-1})\big)\,, \quad \sigma+1 \leq k \leq s\,,\ 0 \leq j \leq s-\sigma-1\,.
\end{aligned}$$

Alternative representation. Related approach exploited in the context of a posteriori local error estimators for high-order splitting methods (with W. Auzinger, O. Koch).

Exact local error representation (Nonlinear equations, Lie)

Theorem (Descombes & Th. 2012)

The defect operator of the first-order Lie–Trotter splitting method admits the (formal) integral representation

$$\begin{aligned}\mathscr{L}_F(t,\cdot) &= \int_0^t \int_0^{\tau_1} \mathrm{e}^{\tau_1 D_A}\,\mathrm{e}^{\tau_2 D_B}\,[D_A, D_B]\,\mathrm{e}^{(\tau_1-\tau_2) D_B}\,\mathrm{e}^{(t-\tau_1) D_F}\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1\\ &= \int_0^t \int_0^{\tau_1} \partial_2 \mathscr{E}_F\big(t-\tau_1, \mathscr{S}_F(\tau_1,\cdot)\big)\,\partial_2 \mathscr{E}_B\big(\tau_1-\tau_2, \mathscr{E}_A(\tau_1,\cdot)\big)\\ &\qquad \times [B,A]\Big(\mathscr{E}_B\big(\tau_2, \mathscr{E}_A(\tau_1,\cdot)\big)\Big)\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1\,, \qquad 0 \le t \le T\,.\end{aligned}$$

Remark. Formal extension of linear case

$$\mathscr{L}_F(t,\cdot) = \int_0^t \int_0^{\tau_1} \mathrm{e}^{(t-\tau_1)(A+B)}\,\mathrm{e}^{(\tau_1-\tau_2) B}\,[B,A]\,\mathrm{e}^{\tau_2 B}\,\mathrm{e}^{\tau_1 A}\,\mathrm{d}\tau_2\,\mathrm{d}\tau_1\,.$$

Current work. Extend approach to higher-order splitting methods and prove asymptotical correctness of a posteriori local error estimators (with W. Auzinger, H. Hofstätter, O. Koch).

Application (Problems with critical parameters)

Application. Error analysis of splitting methods for Schrödinger equations involving critical parameters $0 < \varepsilon \ll 1$

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

see DESCOMBES, TH. (2010, 2012).

- High-order splitting methods for linear evolution equations.

$$\text{Local error} = \mathscr{O}\Big(\tfrac{\tau^{p+1}}{\varepsilon}\Big)\,.$$

- Lie–Trotter splitting method for nonlinear evolution equations.

$$\text{Smooth initial value:} \quad \text{Local error} = C\big(\tfrac{\tau}{\varepsilon}\big)\,\tau^2\,,$$
$$\text{WKB initial value:} \quad \text{Local error} = C\big(\tfrac{\tau}{\varepsilon}\big)\,\tau\,.$$

Remark. Difficult task to adjust time stepsize in suitable manner. Reliable and efficient time integration of Schrödinger equations with critical parameters based on adaptive time stepsize control.

Illustrations (Adaptive time integration)

Illustration

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

$$\begin{cases} \mathrm{i}\,\varepsilon\,\partial_t \psi(x,t) = \Big(-\tfrac{1}{2}\,\varepsilon^2 \Delta + U(x) + \vartheta \,\big|\psi(x,t)\big|^2\Big)\,\psi(x,t)\,, \\ \psi(x,0) = \rho_0(x)\,\mathrm{e}^{\mathrm{i}\sigma_0(x)} \text{ given}, \qquad x \in \mathbb{R}^d, \quad 0 \le t \le T\,, \end{cases}$$

involving critical parameter $0 < \varepsilon \ll 1$ under harmonic potential (scaling ω) and WKB initial condition

$$\rho_0(x) = \mathrm{e}^{-x^2}, \quad \sigma_0(x) = -\ln\big(\mathrm{e}^{x} + \mathrm{e}^{-x}\big), \qquad x \in \mathbb{R},$$

see also Bao, Jin, Markowich (2003).

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)

Situation. Time integration of model problem ($\vartheta = 1$) by splitting methods with constant time stepsizes.

Illustration. Model problem with $\varepsilon = 10^{-2}$ and $\omega = 1$ (columns 1 and 2) or $\omega = 2$ (columns 3 and 4), respectively. Comparison of the solution profiles $|\psi(x,t)|^2$ for $x \in [0, 1.5]$ at time $t = 3$, computed by the first-order Lie–Trotter (p = 1) and a fourth-order splitting method proposed by BLANES & MOAN (p = 4). Time stepsize $h = \varepsilon/20$ (columns 1 and 3) or $h = \varepsilon/50$ (columns 2 and 4), respectively, for $p = 1$. Time stepsize $h = \varepsilon/20$ for $p = 4$.

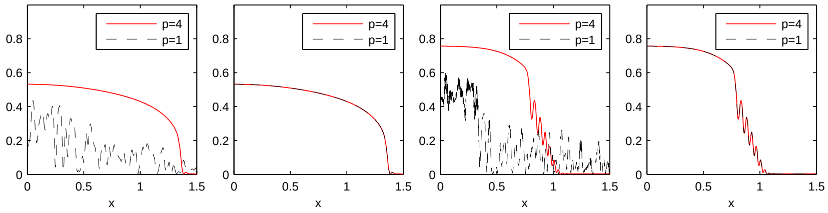


Illustration (Smaller parameter, Reliable time integration)

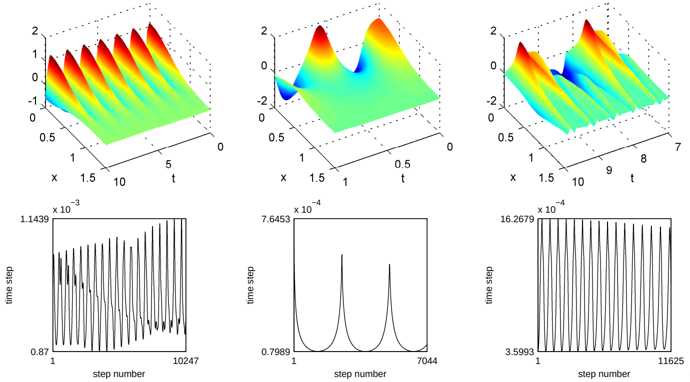
Integration without preparation is frustration. (REVEREND LEON SULLIVAN)

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 and future work

Conclusions.

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

Future work.

- Asymptotical correctness of higher-order a posteriori local error estimators for nonlinear Schrödinger equations.
- Convergence analysis of higher-order time-splitting pseudo-spectral methods for nonlinear Schrödinger equations involving small parameters $\mathrm{i}u' = Au + \frac{1}{\varepsilon} B(u)$.
- Convergence analysis of multi-revolution compositon methods combined with time-splitting pseudo-spectral methods for Schrödinger equations $\mathrm{i}u' = \frac{1}{\varepsilon} Au + B(u)$.

Thank you!

References

Publications.

1. W. Auzinger, O. Koch, and M. Th. *Defect-based local error estimators for splitting methods, with application to Schrödinger equations. Part I. The linear case.* J. Comput. Appl. Math. 236 (2012) 2643–2659.
2. M. Caliari, Ch. Neuhauser, and M. Th. *High-order time-splitting Hermite and Fourier spectral methods for the Gross–Pitaevskii equation.* J. Comput. Phys. 228 (2009) 822–832.
3. M. Caliari, A. Ostermann, S. Rainer, and M. Th. *A minimisation approach for computing the ground state of Gross–Pitaevskii systems.* J. Comput. Phys. 228 (2009), 349–360.
4. S. Descombes and M. Th. *An exact local error representation of exponential operator splitting methods for evolutionary problems and applications to linear Schrödinger equations in the semi-classical regime.* BIT 50 (2010) 729–749.
5. S. Descombes, M. Th. *The Lie–Trotter splitting for nonlinear evolutionary problems with critical parameters. A compact local error representation and application to nonlinear Schrödinger equations in the semi-classical regime.* IMA J. Numer. Anal. (2012) doi:10.1093/imanum/drs021.
6. O. Koch, Ch. Neuhauser, and M. Th. *Error analysis of high-order splitting methods for nonlinear evolutionary Schrödinger equations and application to the MCTDHF equations in electron dynamics.* M2AN, to appear.
7. O. Koch, Ch. Neuhauser, and M. Th. *Embedded exponential operator splitting methods for the time integration of nonlinear evolution equations.* Appl. Numer. Math. 63 (2013) 14–24.
8. Ch. Neuhauser and M. Th. *On the convergence of splitting methods for linear evolutionary Schrödinger equations involving an unbounded potential.* BIT 49 (2009) 199–215.
9. M. Th. *High-order exponential operator splitting methods for time-dependent Schrödinger equations.* SIAM J. Numer. Anal. 46/4 (2008) 2022–2038.
10. M. Th. *Convergence analysis of high-order time-splitting pseudo-spectral methods for nonlinear Schrödinger equations.* SIAM J. Numer. Anal. 50/6 (2012) 3231–3258.
11. M. Th. and J. Abhau. *A numerical study of adaptive space and time discretisations for Gross–Pitaevskii equations.* J. Comp. Phys. 231 (2012) 6665–6681.

References

Submitted manuscripts.

1. H. Hofstätter, O. Koch, and M. Th. *Convergence of split-step generalized-Laguerre–Fourier–Hermite methods for Gross–Pitaevskii equations with rotation term.*
2. W. Auzinger, O. Koch, and M. Th. *Defect-based local error estimators for splitting methods, with application to Schrödinger equations. Part II. Higher-order methods for linear problems.*

Lecture note. *Time-splitting spectral methods for nonlinear Schrödinger equations.*