Favourable space and time discretisations for nonlinear Schrödinger equations

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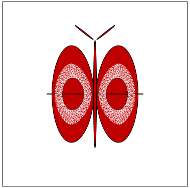

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Collaborators.

- Jochen Abhau (Universität Innsbruck, Austria)
- Winfried Auzinger (Technische Universität Wien, Austria)
- Marco Caliari (Università di Verona, Italy)
- Stéphane Descombes (Université de Nice, France)
- Othmar Koch (Technische Universität Wien, Austria)
- Christof Neuhauser (Universität Innsbruck, Austria)

Many thanks to Gregor Thalhammer.

Theme

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

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

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

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

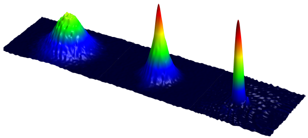
Applications.

- Nonlinear Schrödinger equations (GPS, MCTDHF)
- Parabolic equations (with P. Chartier, S. Descombes, A. Murua)
- Kinetic equations (with L. Pareschi)
- Wave equations (with B. Kaltenbacher)

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.

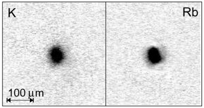
(GRIMM ET AL., Innsbruck)



Bose–Einstein condensation in dilute gases. In 1925 Einstein predicted that at low temperatures particles in a 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. PETHICK, SMITH (2002).

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 $\Psi : \mathbb{R}^d \times [0,\infty) \to \mathbb{C}^J$

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

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

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

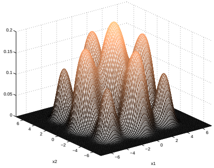
Numerical simulations. Favourable behaviour of time-splitting pseudo-spectral methods confirmed by numerical comparisons. See e.g. contributions by Weizhu Bao and collaborators.

Nonlinear Schrödinger equations – Model problem

Continued study of special problems is still a commendable way towards greater insight. (EBERHARD HOPF, 1902-1983)

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. Ground state solution of GPE in 2D ($\varepsilon = 1 = \omega$, $\kappa = 25$, $\vartheta = 400$, $M = 256 \times 256$).

Semi-classical regime. Computation of time discrete solution for small critical parameter values $0 < \varepsilon \ll 1$. Nonlinear Schrödinger equations of similar form arise in applications from solid state physics. See BAO, JIN, MARKOWICH (2002, 2003).

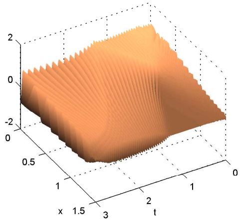
Semi-classical regime

Model problem. Nonlinear Schrödinger equation under classical Wentzel–Kramers–Brillouin (WKB) initial condition

$$\begin{cases} \mathrm{i}\,\partial_t \psi(x,t) = \Big(-\frac{\varepsilon}{2}\,\partial_x^2 + \frac{1}{2\,\varepsilon}\,\omega^2 x^2 + \frac{\vartheta}{\varepsilon}\,\big|\psi(x,t)\big|^2\Big)\,\psi(x,t)\,, \\ \psi(x,0) = \rho_0(x)\,\mathrm{e}^{\frac{\mathrm{i}}{\varepsilon}\sigma_0(x)} = \mathrm{e}^{-x^2}\,\mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon}\ln(\mathrm{e}^x+\mathrm{e}^{-x})}\,, \qquad x \in \mathbb{R}, \quad 0 \le t \le T\,, \end{cases}$$

see also Bao, Jin, Markowich (2003).

Numerical solution. Space and time discretisation of model problem by Fourier pseudo-spectral method and embedded 4(3) splitting pair based on fourth-order time-splitting scheme by Blanes, Moan (2002).



$\Re\psi(x,t)$ for $(\varepsilon,\omega,\vartheta) = (10^{-2},1,1)$
$(x,t) \in [-8,8] \times [0,3]$, $M = 8192$, tol $= 10^{-6}$

Illustration

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 1

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 estimate for local error

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

Adaptive stepsize control. Local error expansion provides theoretical basis of adaptive time stepsize control

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

Local error analysis of high-order splitting methods

Approach based on quadrature formulas. Splitting methods for nonlinear evolution equations. Application to MCTDHF equations in electron dynamics (with O. KOCH).

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

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

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

Approach based on differential equations. Splitting methods for nonlinear evolution equations with critical parameters and application to Schrödinger equations in the semi-classical regime (with S. DESCOMBES).

Theorem (Descombes & Th. 2010b)

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

Convergence analysis of high-order splitting methods

Approach based on quadrature formulas. Convergence estimate for full discretisations based on splitting and pseudo-spectral methods applied to Gross–Pitaevskii equations.

Theorem

$$\left\| \psi_{MN} - \psi(\cdot, t_N) \right\|_{L^2} \leq C \left(\tfrac{1}{M^q} + \tau^p \right).$$

Approach based on differential equations. Convergence estimate for splitting methods applied to linear and nonlinear Schrödinger equations in the semi-classical regime (with S. DESCOMBES).

Theorem (Descombes & Th. 2010a)

$$\| u_N - u(t_N) \|_{L^2} \leq \| u_0 - u(0) \|_{L^2} + C \sum_{n=1}^{N} \frac{\tau_{n-1}^{p+1}}{\varepsilon} \sum_{j=0}^{p} \varepsilon^j \, \| u(0) \|_{H^j} \, .$$

Further details

Further details.

- Discretisations for nonlinear Schrödinger equations
  - Exponential operator splitting methods
  - Fourier and Hermite pseudo-spectral methods
  - Convergence analysis of splitting methods
- Nonlinear Schrödinger equations with critical parameters
  - Exact local error representations for splitting methods
- Adaptivity in space and time
  - Embedded splitting methods, a posteriori error estimators
  - Finite elements versus pseudo-spectral methods

Time-splitting pseudo-spectral methods for nonlinear Schrödinger equations

Calculus of Lie-derivatives

In 1971, I read the beautiful paper of Kato & Fujita on the Navier–Stokes equations and was delighted to find that, properly viewed, it looked like an ODE , and the analysis proceeded in ways familiar for ODEs. (DAN HENRY, 1981)

The calculus of Lie-derivatives is a powerful and magic tool – all at once, the world becomes linear. (M.TH., 2011)

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

Problem. Consider 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

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

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

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

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.

Exponential operator splitting methods

General form. High-order splitting methods are cast into scheme

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

with (real or complex) method coefficients $(a_j, b_j)_{j=1}^{s}$.

Low-order methods. First-order Lie–Trotter splitting method

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

Second-order Strang splitting method

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

Higher-order methods. Higher-order schemes proposed by Blanes and Moan, McLachlan, Suzuki, Yoshida, e.g.

Higher-order splitting methods

Example 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 $\partial_t \psi(x,t) = -\mathrm{i}\,\big(V(x) + \vartheta\,|\psi(x,t)|^2\big)\,\psi(x,t)$ 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 $(\mathcal{F}_m)_{m \in \mathbb{Z}^d}$ form orthonormal basis of $L^2(\Omega)$ and satisfy eigenvalue relation

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

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

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

$$\psi_M(\cdot, t) = \sum_m{}_M\, \psi_m(t)\, \mathcal{F}_m\,,$$

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

Implementation. Realisation by Fast Fourier Techniques.

Hermite pseudo-spectral method

Spectral decomposition. Hermite basis functions $(\mathscr{H}_m)_{m\in\mathbb{N}^d}$ form orthonormal basis of $L^2(\Omega) = L^2(\mathbb{R}^d)$ and satisfy eigenvalue relation

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

$$\big(-\Delta + U_\gamma\big)\,\mathscr{H}_m = \lambda_m\,\mathscr{H}_m\,, \qquad \lambda_m = \sum_{\ell=1}^{d} \gamma_\ell^2\,\big(1+2\,m_\ell\big)\,.$$

Numerical approximation. Truncation of infinite sum and application of Gauss–Hermite quadrature yields approximation

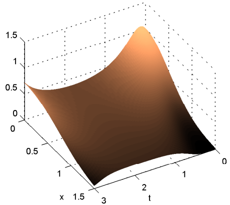
$$\psi_M(\cdot,t) = \sum_m{}_M\,\psi_m(t)\,\mathscr{H}_m\,, \qquad w(x) = \prod_{\ell=1}^{d} \mathrm{e}^{-\frac{1}{2}\gamma_\ell^2 x_\ell^2}\,,$$

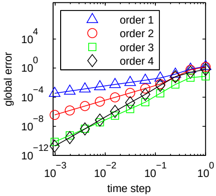
$$\psi_m(t) = \int_\Omega \psi(x,t)\,\mathscr{H}_m(x)\,\mathrm{d}x \approx \sum_k \omega_k\,w(-2\,\xi_k)\,\psi(\xi_k,t)\,\mathscr{H}_m(\xi_k)\,.$$

Implementation. Realisation by matrix × matrix multiplications.

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 (classical) 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).

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.

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. (2010), Lubich (2008), and Th. (2008).
- **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. (2010a, 2010b).

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)

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

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 (classical) 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?

Quadrature formulas

Approach. Alternative local error expansion

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

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. (2011), LUBICH (2008).

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

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

provided that $\|B\|_{X\leftarrow X} \le C_B$, $\left\|\mathrm{e}^{tC}\right\|_{X\leftarrow X} \le \mathrm{e}^{M_C t}$, $C \in \{A, B, A+B\}$. 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

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

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

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

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).

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

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.

Current and future work. Extension to full discretisations for GPS. Study algebraic structure of expansion (with P. Chartier, S. Descombes, A. Murua).

Nonlinear Schrödinger equations with critical parameters

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. (2010a, 2010b). Similar approach utilised for derivation of a posteriori error estimators.

Basic idea. Deduce differential equation for splitting operator

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

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

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

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

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

By variation-of-constants formula obtain representation

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

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

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

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 and application. Generalisation of exact local error representation and application to Schrödinger equations in the semi-classical regime, see DESCOMBES, TH. (2010a, 2010b).

- 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. 2010a)

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

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

$$\mathscr{T} = \sum_{j=0}^{\sigma-1} C_{\sigma-j,j} + \sum_{j=0}^{s-\sigma-1} D_{\sigma+1+j,j}\,, \qquad c_k = \sum_{j=1}^{k} a_j\,, \quad d_k = \sum_{j=1}^{k} b_j\,,$$

$$\mathscr{I}_\pm(L_1, L_2, t) = \int_0^t \mathrm{e}^{\pm tL_1}\, [L_1, L_2]\, \mathrm{e}^{\mp tL_1}\, \mathrm{d}\tau\,,$$

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

Exact local error representation (Nonlinear equations, Lie)

Theorem (Descombes & Th. 2010b)

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

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

Objective. Study exact local error representations for linear and nonlinear Schrödinger equations with critical parameters.

Application to Schrödinger equations

Model problem. Time-dependent nonlinear Schrödinger equation

$$\begin{cases} \mathrm{i}\,\partial_t \psi(x,t) = -\frac{\varepsilon}{2}\,\partial_x^2\,\psi(x,t) + \frac{1}{2\varepsilon}\,\omega^2 x^2\,\psi(x,t) + \frac{\vartheta}{\varepsilon}\,\big|\psi(x,t)\big|^2\,\psi(x,t)\,, \\ \psi(x,0) = \rho_0(x)\,\mathrm{e}^{\frac{\mathrm{i}}{\varepsilon}\sigma_0(x)}\,, \qquad x \in \mathbb{R}\,, \quad 0 \le t \le T\,, \end{cases}$$

involving critical parameter $0 < \varepsilon \ll 1$ under WKB initial condition or regular initial condition (derivatives bounded independent of ε)

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

$$\rho_0(x) = \mathrm{e}^{-(x-\frac{1}{10})^2}\,, \quad \sigma_0(x) = 0\,, \qquad x \in \mathbb{R}\,,$$

see also Bao, Jin, Markowich (2003).

Special cases.

- Linear Schrödinger equation $(\vartheta = 0)$
- Cubic Schrödinger equation $(\omega = 0)$

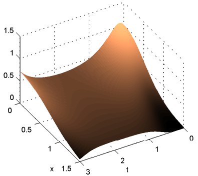
Illustration (Time evolution)

Movie. Space and time discretisation of model problem ($d = 1$, $\varepsilon = 1, 10^{-2}$, $\omega = 1, 2$, $\vartheta = 1$) under WKB initial condition by Fourier pseudo-spectral method and embedded 4(3) splitting pair based on 4th-order scheme by Blanes, Moan (2002) ($x \in [-8, 8]$, $M = 8192$, $t \in [0, 3]$, $\text{tol} = 10^{-6}$, $N = 83, 121, 2178, 3560$). Solution profile $\Re\psi(x, t)$ for $(x, t) \in [0, 1.5] \times [0, 3]$.

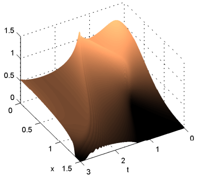
Movie 2

Illustration (Time evolution)

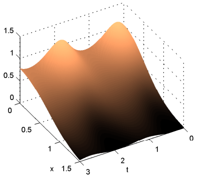
Illustration. Space and time discretisation of model problem ($d = 1$, $\varepsilon = 1, 10^{-2}$, $\omega = 1, 2$, $\vartheta = 1$) under WKB initial condition by Fourier pseudo-spectral method and embedded 4(3) splitting pair based on 4th-order scheme by Blanes, Moan (2002) ($x \in [-8, 8]$, $M = 512, 8192$, $t \in [0, 3]$, $\mathrm{tol} = 10^{-6}$, $N = 104, 141, 2153, 3588$). Solution profile $|\psi(x,t)|^2$, $(x,t) \in [0, 1.5] \times [0, 3]$.



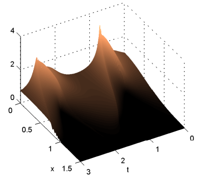
$(\varepsilon, \omega) = (1, 1)$



$(\varepsilon, \omega) = (10^{-2}, 1)$



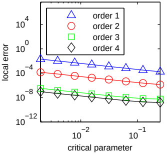
$(\varepsilon, \omega) = (1, 2)$



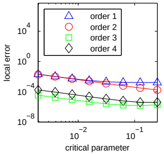
$(\varepsilon, \omega) = (10^{-2}, 2)$

Illustration (Local error versus critical parameter)

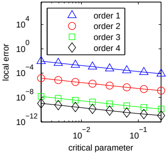
Illustration. Time discretisation of nonlinear Schrödinger equation (GPE, $\omega = 1 = \vartheta$) under WKB ($\partial_x \sigma_0 \neq 0$) and regular ($\sigma_0 = 0$) initial condition by splitting methods of orders $p \leq 4$. Display dependence of local error on critical parameter. Include corresponding results for linear Schrödinger equation ($\vartheta = 0$).



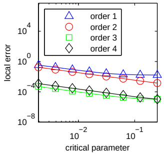
$\vartheta = 1, \partial_x \sigma_0 \neq 0, \tau = \tau_0$



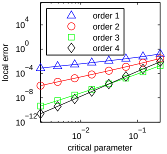
$\vartheta = 1, \sigma_0 = 0, \tau = \tau_0$



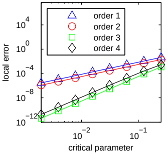
$\vartheta = 0, \partial_x \sigma_0 \neq 0, \tau = \tau_0$



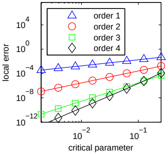
$\vartheta = 0, \sigma_0 = 0, \tau = \tau_0$



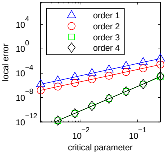
$\vartheta = 1, \partial_x \sigma_0 \neq 0, \tau = \varepsilon$



$\vartheta = 1, \sigma_0 = 0, \tau = \varepsilon$



$\vartheta = 0, \partial_x \sigma_0 \neq 0, \tau = \varepsilon$



$\vartheta = 0, \sigma_0 = 0, \tau = \varepsilon$

Illustration (Local error versus critical parameter)

Illustration. Time discretisation of nonlinear Schrödinger equation (GPE, $\omega = 1 = \vartheta$) under WKB ($\partial_x \sigma_0 \neq 0$) and regular ($\sigma_0 = 0$) initial condition by splitting methods of orders $p \leq 4$. Display dependence $\mathcal{O}(\varepsilon^{\alpha})$ of dominant local error term on critical parameter ε (within chosen range of h/ε). Compare with obtained results for linear Schrödinger equation ($\vartheta = 0$).

$\omega = 1$	$\vartheta = 1$	$\partial_x \sigma_0 \neq 0$	$\tau = \tau_0$	$\alpha \approx -1$
$\omega = 1$	$\vartheta = 1$	$\partial_x \sigma_0 \neq 0$	$\tau = \varepsilon$	$\alpha \approx p$
$\omega = 1$	$\vartheta = 1$	$\sigma_0 = 0$	$\tau = \tau_0$	$\alpha \approx -1$
$\omega = 1$	$\vartheta = 1$	$\sigma_0 = 0$	$\tau = \varepsilon$	$\alpha \approx 2\lfloor (p+1)/2 \rfloor$
$\omega = 1$	$\vartheta = 0$	$\partial_x \sigma_0 \neq 0$	$\tau = \tau_0$	$\alpha = -1$
$\omega = 1$	$\vartheta = 0$	$\partial_x \sigma_0 \neq 0$	$\tau = \varepsilon$	$\alpha = p$
$\omega = 1$	$\vartheta = 0$	$\sigma_0 = 0$	$\tau = \tau_0$	$\alpha = -1$
$\omega = 1$	$\vartheta = 0$	$\sigma_0 = 0$	$\tau = \varepsilon$	$\alpha = 2\lfloor (p+1)/2 \rfloor$

Global error estimate (Linear equations)

Theorem (Descombes & Th. 2010a)

An exponential operator splitting method of (classical) order $p \geq 1$ applied to a linear Schrödinger equation satisfies the error estimate

$$\|u_N - u(t_N)\|_{L^2} \leq \|u_0 - u(0)\|_{L^2} + C \sum_{n=1}^{N} \frac{\tau_{n-1}^{p+1}}{\varepsilon} \sum_{j=0}^{p} \varepsilon^j \, \|u(0)\|_{H^j}$$

with constant depending on $\max\left\{ \left\| \partial_{x_j} U \right\|_{L^\infty} : 0 \leq j \leq 2p \right\}$ *and* $t_N \leq T$.

Classical WKB initial values. If $\varepsilon^j \, \|u(0)\|_{H^j} \leq M_j$, the estimate

$$\|u_N - u(t_N)\|_{L^2} \leq \|u_0 - u(0)\|_{L^2} + C \, \frac{\tau^p}{\varepsilon}$$

follows, where $\tau = \max\{\tau_{n-1} : 1 \leq n \leq N\}$.

Remark. Error estimate in accordance with numerical illustrations.

Local error estimate (Nonlinear equations, Lie)

Linear equations. Lie–Trotter splitting method applied to linear Schrödinger equation satisfies local error estimate

$$\sigma_0 = 0: \qquad \big\|\mathscr{L}_F\big(\tau, u(0)\big)\big\|_{L^2} \leq \big(C_0 + C_1 \tfrac{\tau}{\varepsilon}\big)\, \tau^2 .$$

Theorem (Descombes & Th. 2010b)

The Lie–Trotter splitting method applied to the nonlinear model equation under a regular initial condition (derivatives bounded independent of ε) satisfies the local error estimate

$$\sigma_0 = 0: \qquad \big\|\mathscr{L}_F\big(\tau, u(0)\big)\big\|_{L^2} \leq P\big(\tfrac{\tau}{\varepsilon}\big)\, \tau^2 , \quad P(\xi) = \sum_{j=0}^{3} C_j\, \xi^j .$$

Remark. Error estimate in accordance with numerical illustrations.

Open question. Extension to high-order splitting methods.

Local error estimate (Nonlinear equations, WKB, Lie)

Linear equations. Lie–Trotter splitting method applied to linear Schrödinger equation satisfies local error estimate

$$\partial_x \sigma_0 \neq 0: \qquad \big\| \mathscr{L}_F\big(\tau, u(0)\big) \big\|_{L^2} \leq \big(C_0\, \tau + C_1\, \tfrac{\tau}{\varepsilon} \big)\, \tau\,.$$

Surprising result. For nonlinear model equation, straightforward estimation implies local error bound $\big\| \mathscr{L}_F\big(\tau, u(0)\big) \big\|_{L^2} \leq P\big(\tfrac{\tau}{\varepsilon}\big)$ contrary to numerical observations. Heuristic arguments confirm cancelation of terms involving $\frac{1}{\varepsilon}$ and lead to conjecture in accordance with numerical illustrations.

Conjecture (Classical WKB initial values). If $\varepsilon^j \, \| u(0) \|_{H^j} \leq M_j$, the Lie–Trotter splitting method applied to the nonlinear model equation satisfies the local error estimate

$$\partial_x \sigma_0 \neq 0: \qquad \big\| \mathscr{L}_F\big(\tau, u(0)\big) \big\|_{L^2} \leq Q\big(\tfrac{\tau}{\varepsilon}\big)\, \tau\,, \quad Q(\xi) = \sum_{j=0}^{\infty} C_j\, \xi^j\,.$$

Open questions. Rigorous local error analysis and extension to high-order exponential operator splitting methods.

Adaptivity in space and time

Adaptive time stepsize control

> *A good ODE integrator should exert some adaptive control over its own progress, making frequent changes in its stepsize. Usually the purpose of this adaptive stepsize control is to achieve some predetermined accuracy in the solution with minimum computational effort. Many small steps should tiptoe through treacherous terrain, while a few great strides should speed through smooth uninteresting countryside. The resulting gains in efficiency are not mere tens of percents or factors of two; they can sometimes be factors of ten, a hundred, or more.*
>
> PRESS, FLANNERY, TEUKOLSKY, VETTERLING, *Numerical Recipes in C – The Art of Scientific Computing (1988)*

Adaptive time stepsize control. Local error expansion provides theoretical basis of adaptive time stepsize control. Development of time-step selection algorithms, see SÖDERLIND (2002, 2003, 2006).

Estimation of local error. With W. AUZINGER, O. KOCH.

- Embedded splitting methods
- A posteriori error estimators

Embedded splitting methods

Embedded splitting methods. Construct embedded split-step pairs $p(\hat{p})$ with certain compositions coinciding. Use difference between basic integrator $(a_j, b_j)_{j=1}^{s}$ and error estimator $(\hat{a}_j, \hat{b}_j)_{j=1}^{\hat{s}}$ as estimate for local error

$$\|u_n - \hat{u}_n\|_X \approx \|u_n - u(t_n)\|_X \,,$$

$$u_n = \prod_{j=1}^{s} \mathrm{e}^{a_{s+1-j}\tau_{n-1}D_A}\,\mathrm{e}^{b_{s+1-j}\tau_{n-1}D_B}\,u_{n-1}\,,$$

$$\hat{u}_n = \prod_{j=1}^{\hat{s}} \mathrm{e}^{\hat{a}_{\hat{s}+1-j}\tau_{n-1}D_A}\,\mathrm{e}^{\hat{b}_{\hat{s}+1-j}\tau_{n-1}D_B}\,u_{n-1}\,.$$

Standard stepsize selection. Optimal time stepsize determined through

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

see Hairer, Nørsett, Wanner (2000).

Construction of embedded splitting methods

Example method. Split-step pair of orders 4(3) based on splitting method by Blanes and Moan with (negative) real coefficients appropriate for the time integration of Hamiltonian systems.

Approach. Choose Runge–Kutta–Nyström type method ($p = 4$, $s = 7$) as basic integrator. Compute Gröbner basis of order conditions ($\hat{p} = 3$, $\hat{s} = 7$, $\hat{b}_7 = 0$, $\hat{a}_j = a_j$, $\hat{b}_j = b_j$, $1 \le j \le 4$). Resolve resulting quadratic equation for $\hat{b}_6$ and linear equations for $\hat{a}_j$, $j = 5,6,7$, and $\hat{b}_5$.

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

Dissipative problems. Complex split-step pair of orders 4(3) based on scheme by Yoshida.

A posteriori error estimators (Linear problems, Lie)

Lie–Trotter splitting method for linear evolution equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = F\big(u(t)\big) = \big(A+B\big)\, u(t)\,, \quad \mathscr{S}_F(t) = \mathrm{e}^{tB}\, \mathrm{e}^{tA} \approx \mathscr{E}_F(t) = \mathrm{e}^{t(A+B)}\,, \qquad t \geq 0\,,$$

Differential equation for evolution operator and defect

$$\frac{\mathrm{d}}{\mathrm{d}t}\, \mathscr{E}_F(t) = \big(A+B\big)\, \mathscr{E}_F(t)\,, \qquad t \geq 0\,,$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\, \mathscr{S}_F(t) = \big(A+B\big)\, \mathscr{S}_F(t) + \mathscr{D}(t)\,, \quad \mathscr{D}(t) = \big[\mathscr{S}_F(t), A\big]\,, \qquad t \geq 0\,.$$

Sylvester equation for splitting operator, truncation error, and local error operator

$$\frac{\mathrm{d}}{\mathrm{d}t}\, \mathscr{S}_F(t) = \mathscr{S}_F(t)\, A + B\, \mathscr{S}_F(t)\,, \qquad t \geq 0\,,$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\, \mathscr{E}_F(t) = \mathscr{E}_F(t)\, A + B\, \mathscr{E}_F(t) + \mathscr{T}(t)\,, \quad \mathscr{T}(t) = \big[A, \mathscr{E}_F(t)\big]\,, \qquad t \geq 0\,,$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\, \mathscr{L}_F(t) = \mathscr{L}_F(t)\, A + B\, \mathscr{L}_F(t) - \mathscr{T}(t)\,, \qquad t \geq 0\,.$$

Integral representation for local error operator and quadrature approximation yields a posteriori error estimator

$$\mathscr{L}_F(t) = -\int_0^t \mathrm{e}^{(t-\tau)B}\, \mathscr{T}(\tau)\, \mathrm{e}^{(t-\tau)A}\, \mathrm{d}\tau \approx \int_0^t \mathrm{e}^{(t-\tau)B}\, \mathscr{D}(\tau)\, \mathrm{e}^{(t-\tau)A}\, \mathrm{d}\tau$$

$$\approx \mathscr{P}(t) = \tfrac{1}{2}\, t\, \mathscr{D}(t) = \tfrac{1}{2}\, t\, \big(\mathrm{e}^{tB}\mathrm{e}^{tA} A - A\, \mathrm{e}^{tB}\mathrm{e}^{tA}\big)\,, \qquad t \geq 0\,.$$

A posteriori error estimator (Nonlinear problems, Lie)

Nonlinear problems. Straightforward extension of the a posteriori error estimator $\mathscr{P}(t) = \frac{1}{2}\, t\, \big(\mathrm{e}^{tB}\mathrm{e}^{tA} A - A\,\mathrm{e}^{tB}\mathrm{e}^{tA}\big)$ for linear problems to nonlinear evolution equations (calculus of Lie-derivatives)

$$\mathscr{P}(t,v) = \tfrac{1}{2}\, t \left(D_A\, \mathrm{e}^{tD_A}\, \mathrm{e}^{tD_B}\, v - \mathrm{e}^{tD_A}\, \mathrm{e}^{tD_B}\, D_A v \right), \qquad t \geq 0\,.$$

Application. Specification to nonlinear Schrödinger equation

$$\mathrm{e}^{tD_A}\, \mathrm{e}^{tD_B}\, D_A v = A\, \mathscr{E}_B\big(t, \mathscr{E}_A(t,v)\big)\,,$$

$$D_A\, \mathrm{e}^{tD_A}\, \mathrm{e}^{tD_B}\, v = G'(v)\, A\, v = \partial_2\, \mathscr{E}_B\big(t, \mathscr{E}_A(t,v)\big)\, \partial_2\, \mathscr{E}_A(t,v)\, A\, v\,,$$

$$G(v) = \mathrm{e}^{tD_A}\, \mathrm{e}^{tD_B}\, v = \mathscr{E}_B\big(t, \mathscr{E}_A(t,v)\big)\,, \quad G'(v) = \partial_2\, \mathscr{E}_B\big(t, \mathscr{E}_A(t,v)\big)\, \partial_2\, \mathscr{E}_A(t,v)\,.$$

In particular, specification to single Gross–Pitaevskii equation yields

$$\mathrm{e}^{tD_A}\, \mathrm{e}^{tD_B}\, D_A v = A\, \mathrm{e}^{-\mathrm{i}t\,(V+\vartheta|\mathrm{e}^{tA}v|^2)}\, \mathrm{e}^{tA} v\,, \quad G(v) = \mathrm{e}^{-\mathrm{i}t\,(V+\vartheta|\mathrm{e}^{tA}v|^2)}\, \mathrm{e}^{tA} v\,,$$

$$D_A\, \mathrm{e}^{tD_A}\, \mathrm{e}^{tD_B}\, v = \mathrm{e}^{-\mathrm{i}t\,(V+\vartheta|\mathrm{e}^{tA}v|^2)} \Big(A\mathrm{e}^{tA} v - \mathrm{i}\vartheta t \Big(A\,\mathrm{e}^{tA} v\, |\mathrm{e}^{tA} v|^2 + \overline{A\,\mathrm{e}^{tA} v}\, (\mathrm{e}^{tA} v)^2 \Big)\Big)\,,$$

$$G'(v) = \mathrm{e}^{-\mathrm{i}t\,(V+\vartheta|\mathrm{e}^{tA}v|^2)} \Big(\mathrm{e}^{tA}(\cdot) - \mathrm{i}\vartheta t \big(\mathrm{e}^{tA}(\cdot)\, \overline{\mathrm{e}^{tA} v} + \overline{\mathrm{e}^{tA}(\cdot)}\, \mathrm{e}^{tA} v \big)\, \mathrm{e}^{tA} v \Big)\,.$$

A posteriori error estimator (Nonlinear problems, Lie)

Error estimator. A posteriori error estimator for Lie–Trotter splitting method applied to nonlinear evolution equation

$$\mathscr{P}(t,\cdot) = \tfrac{t}{2}\left(D_A\, \mathrm{e}^{tD_A}\, \mathrm{e}^{tD_B} - \mathrm{e}^{tD_A}\, \mathrm{e}^{tD_B}\, D_A\right) \approx \mathscr{L}(t,\cdot) = \mathscr{S}(t,\cdot) - \mathscr{E}(t,\cdot)\,.$$

Error analysis. Theoretical analysis for linear problems and application to linear Schrödinger equations in AUZINGER, KOCH, TH. (2011). Derivation of following results for Lie–Trotter and Strang splitting method under appropriate regularity requirements on analytical solution.

- A priori estimate $\mathscr{L}(t) = \mathscr{O}\big(t^{p+1}\big)$.
- A posteriori estimator asymptotically correct $\mathscr{P}(t) - \mathscr{L}(t) = \mathscr{O}\big(t^{p+2}\big)$. Improved approximation $\mathscr{S}(t) - \mathscr{P}(t) = \mathscr{E}(t) + \mathscr{O}\big(t^{p+2}\big)$.

Objective. Extension of theoretical results to nonlinear problems.

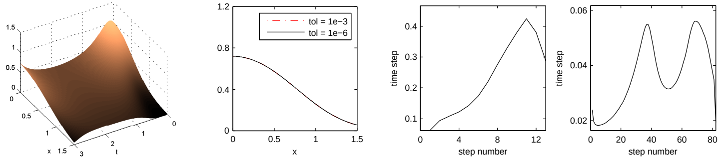
Computational effort (GPE). Two additional applications of A (FFT) required

$$\mathscr{P}(t,v) = \mathrm{e}^{-\mathrm{i}t(V+\vartheta|w|^2)}\left(A\,w - \mathrm{i}\,\vartheta\, t\left(A\,w\,|w|^2 + \overline{A\,w}\,w^2\right)\right) - A\,\mathrm{e}^{-\mathrm{i}t(V+\vartheta|w|^2)}\,w\,, \quad w = \mathrm{e}^{tA}\,v\,.$$

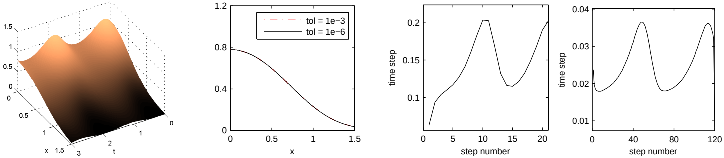
Computational effort comparable with splitting pair Lie (Strang).

Illustration (Reliable time integration)

Illustration. Space and time discretisation of model problem ($d = 1$, $\varepsilon = 1$, $\omega = 1, 2$, $\vartheta = 1$) by Fourier pseudo-spectral method and embedded 4(3) splitting pair based on fourth-order scheme by BLANES, MOAN (2002) ($x \in [-8, 8]$, $M = 512$, $t \in [0, 3]$). Solution profile $|\psi(x, t)|^2$ for $(x, t) \in [0, 1.5] \times [0, 3]$ and generated stepsize sequences for tol $= 10^{-3}$ (left), tol $= 10^{-6}$ (right).



$(\varepsilon, \omega) = (1, 1)$



$(\varepsilon, \omega) = (1, 2)$

Illustration (Reliable time integration, Critical parameter)

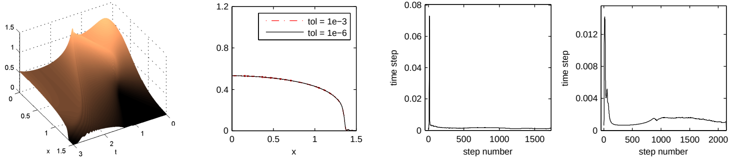
Integration without preparation is frustration. (REVEREND LEON SULLIVAN)

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 $\text{tol} = 10^{-1}, 10^{-2}, 10^{-3}, 10^{-6}$ ($N = 951, 2342, 2452, 3560$).

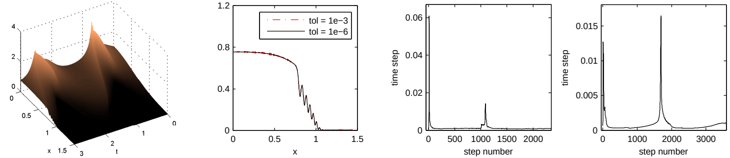
Movie 3

Illustration (Reliable time integration, Critical parameter)

Illustration. Time integration of model problem ($d = 1$, $\varepsilon = 10^{-2}$, $\omega = 1,2$, $\vartheta = 1$) by Fourier pseudo-spectral method and embedded 4(3) splitting pair based on fourth-order splitting scheme by Blanes, Moan (2002) ($x \in [-8,8]$, $M = 8192$, $t \in [0,3]$). Solution profile $|\psi(x,t)|^2$, $(x,t) \in [0,1.5] \times [0,3]$, and generated stepsize sequences for tol $= 10^{-3}$ (left), tol $= 10^{-6}$ (right).



$(\varepsilon,\omega) = (10^{-2},1)$



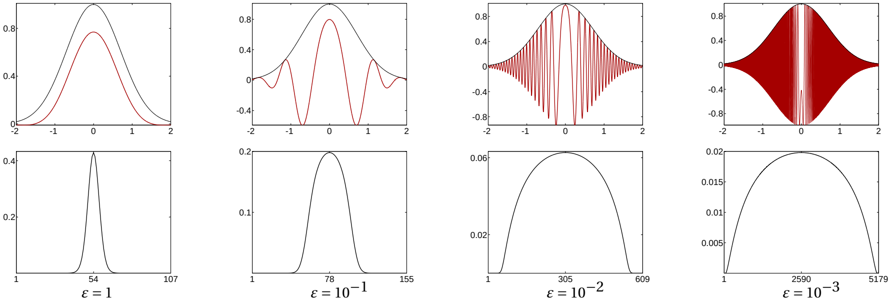
$(\varepsilon,\omega) = (10^{-2},2)$

Illustration (Fourier pseudo-spectral method)

Illustration. Spatial approximation of WKB-type initial condition

$$\psi_0(x) = \rho_0(x)\,\mathrm{e}^{\frac{\mathrm{i}}{\varepsilon}\sigma_0(x)} = \mathrm{e}^{-x^2}\,\mathrm{e}^{-\frac{\mathrm{i}}{\varepsilon}\ln(\mathrm{e}^x+\mathrm{e}^{-x})}\,, \qquad x \in \mathbb{R}\,, \quad 0 \le t \le T\,,$$

by Fourier pseudo-spectral method in dependence of critical parameter. Solution profile $\Re\psi_0$ and Fourier spectral coefficients $|\psi_m| > 10^{-14}$. Observation #coefficients $\propto \frac{1}{\varepsilon}$.



Theoretical background. See Boyd (2011). Approximation error ($d = 1$)

$$\Big|\sum_{m\in\mathbb{Z}} \psi_m(t)\,\mathscr{F}_m - \sum_{-M\le m\le M-1} \widetilde{\psi}_m(t)\,\mathscr{F}_m\Big| \le 2\,|\psi_M(t) - \psi_{-M}(t)| + 4 \sum_{|m|\ge M+1} |\psi_m(t)|.$$

Finite element versus Fourier pseudo-spectral method

Common feature. Approximation of given function by linear combination of basis functions.

Fourier pseudo-spectral method.

- Fourier basis functions supported on entire domain.
- Realisation by Fast Fourier Techniques.
- Periodic boundary conditions imposed.

Finite element method.

- Finite element basis functions locally supported and thus better designed for local adaptation of space grid.
- Numerical solution of (large) linear systems.
- Realisation of different boundary conditions.

Finite element method (Realisation)

Realisation (2D). With JOCHEN ABHAU.

- Utilisation of DEAL.II LIBRARY developed by WOLFGANG BANGERTH and collaborators.
- Piecewise polynomial basis functions (quadratic interpolants) on rectangular grid. Homogeneous Dirichlet boundary conditions.
- Formulate nonlinear Schrödinger equation as real-valued system for $\psi = v + \mathrm{i}\, w$. Linear subproblem $\mathrm{i}\,\partial_t \psi(x,t) = -\varepsilon\,\Delta\psi(x,t)$ becomes $\partial_t v = -\varepsilon\,\Delta w$, $\partial_t w = \varepsilon\,\Delta v$. Employ weak formulation (finite dimensional space $V_h \subset H^1(\Omega)$ with basis (φ_j), use ansatz $v(\cdot,t) = \sum \alpha_j(t)\,\varphi_j$ and $w(\cdot,t) = \sum \beta_k(t)\,\varphi_k$, test resulting system with $\chi \in H^1(\Omega)$)

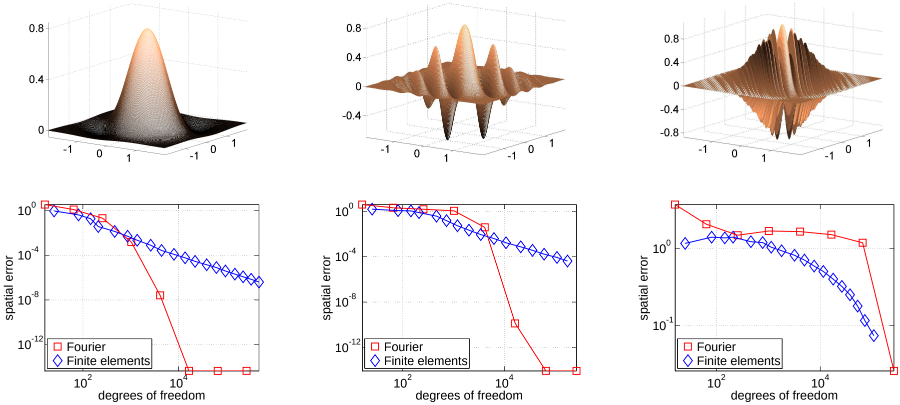
  $$\sum \partial_t \alpha_j(t)\,(\varphi_j \,|\, \chi)_{L^2} = \varepsilon \sum \beta_k(t)\,(\nabla\varphi_k \,|\, \nabla\chi)_{L^2}\,, \sum \partial_t \beta_k(t)\,(\varphi_k \,|\, \chi)_{L^2} = -\varepsilon \sum \alpha_j(t)\,(\nabla\varphi_j \,|\, \nabla\chi)_{L^2}\,,$$

  to obtain $Q\,\partial_t\alpha = \varepsilon\,\widetilde{Q}\beta$, $Q\,\partial_t\beta = -\varepsilon\,\widetilde{Q}\alpha$ ($\chi = \varphi_\ell$, $Q_{k\ell} = (\varphi_k \,|\, \varphi_\ell)_{L^2}$, $\widetilde{Q}_{k\ell} = (\nabla\varphi_k \,|\, \nabla\varphi_\ell)_{L^2}$).
- Local mesh adaptation by standard local a posteriori estimator given in KELLY, GAGO, ZIENKIEWICZ, BABUSKA (1983) on each rectangle K together with Dörfler marking strategy.

  $$\mathrm{error}_K^2(u) = \mathrm{diam}(K) \int_{\partial K} \left[\frac{\partial u}{\partial \vec{n}}\right] \mathrm{d}\sigma\,, \qquad \sum_{K\in\mathcal{K}'} \mathrm{error}_K(u) > c \sum_{K\in\mathcal{K}} \mathrm{error}_K(u)\,.$$

Finite element versus Fourier pseudo-spectral method

Illustration. Spatial approximation of WKB-type initial condition in 2D by Finite element and Fourier pseudo-spectral method in dependence of critical parameter. Solution profile $\Re\psi_0$ and spatial approximation error. Computation time of a couple of days.



$\varepsilon = 1$ $\quad$ $\varepsilon = 10^{-1}$ $\quad$ $\varepsilon = 10^{-2}$

Conclusions

Main focus. Local error behaviour of higher-order exponential operator splitting methods for time integration of nonlinear Schrödinger equations.

Nonlinear Schrödinger equations with non-critical parameters. For time-dependent Gross–Pitaevskii systems with trapping potentials, moderate coupling constants, and non-critical parameter values discouver parameter regions where fascinating physical phenomena arise. Analytical solutions close to ground state remain regular and localised. Dominant linear part well solvable by spectral decomposition. High order of convergence retained for splitting methods. Numerical simulations in 3D feasible.

Nonlinear Schrödinger equations with critical parameters. For nonlinear Schrödinger equations involving critical parameter values fine structures of analytical solution require high resolution in space and time. Adaptivity in space and time desirable.

Conclusions

... methods for stiff problems, we are just beginning to explore them ...

(LAWRENCE SHAMPINE, 1985)

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

Open questions and future work

Open questions and future work. With J. Abhau, W. Auzinger, Ph. Chartier, S. Descombes, O. Koch, A. Murua, L. Pareschi.

- Rigorous error analysis of high-order splitting methods for nonlinear Schrödinger equations with critical parameters.
- Algebraic structures of local error expansions (quadrature formulas, differential equations) for splitting methods applied to evolution equations involving several parts.
- Convergence analysis of full discretisations for nonlinear evolution equations, see also GAUCKLER (2010).
- Spectral methods versus Galerkin methods for nonlinear Schrödinger equations in the semi-classical regime.
- Alternative approaches to obtain efficient local error estimators for adaptive stepsize control.
- Extend approaches to other applications (kinetic equations).

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2. W. Auzinger, O. Koch, and M. Th. *Defect-based local error estimation of splitting methods for evolutionary Schrödinger equations. Part I. The linear case.* Preliminary version available.
3. M. Th. *A convergence analysis of high-order time-splitting pseudo-spectral methods for nonlinear Schrödinger equations.* Preliminary version available.

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

A good numerical method is …

…reliable in demanding moments.

Thank you!