Splitting methods for nonlinear evolution equations

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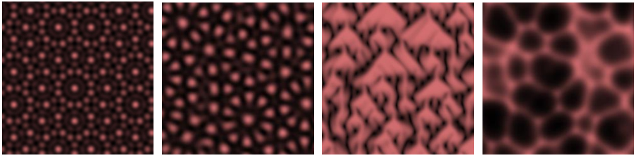

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Website. techmath.uibk.ac.at/mecht/MyHomepage/Publications.html

Opening statements

Time integration methods.

- Exponential operator splitting methods constitute a favourable class of time integration methods for differential equations.
- Numerous contributions demonstrate their substantial advantages over standard approaches regarding reliability and efficiency.
- The preservation of conserved quantities over amplified timeframes justifies the perception as geometric numerical integrators.
- The design, theoretical analysis, and practical implementation for specific applications continues to be an active area of research.

Opening statements

Scope of applications.

- Exponential operator splitting methods are appropriate for a broad variety of relevant applications.
- This includes Hamiltonian systems (classical mechanics) as well as Schrödinger equations (quantum mechanics), where the advantages of geometric numerical integrators become apparent.
- The scope naturally extends to high-order reaction-diffusion systems and complex Ginzburg–Landau-type equations forming beautiful spatio-temporal patterns (biology, chemistry, geology, physics), higher-order damped wave equations (nonlinear acoustics), and kinetic equations (plasma physics).

Class of problems

Class of problems. We focus on partial differential equations that comprise linear combinations of powers of the Laplace operator, space-dependent functions, and nonlinear multiplication operators

$$\begin{cases} \partial_t U(x,t) = \sum_{k=0}^{K} \alpha_k \, \Delta^k U(x,t) + W(x)\, U(x,t) + f\big(U(x,t)\big)\,, \\ U(x,t_0) = U_0(x)\,, \quad (x,t) \in \Omega \times [t_0,T] \subset \mathbb{R}^d \times \mathbb{R}\,. \end{cases}$$

We perform short-term as well as long-term simulations for relevant model problems in $d \in \{1,2,3\}$ space dimensions.

- High-order reaction-diffusion equations (quasicrystals)
- Complex Ginzburg–Landau equations (superconductivity)
- Gross–Pitaevskii equations (Bose–Einstein condensates)

General formulation

General formulation. Setting $u(t) = U(\cdot, t)$ for $t \in [t_0, T]$ and assigning linear differential operators as well as nonlinear multiplication operators

$$\big(A\,v\big)(x) = \sum_{k=0}^{K} \alpha_k\,\Delta^k v(x)\,, \quad \big(B(v)\big)(x) = W(x)\,v(x) + f\big(v(x)\big)\,, \quad x \in \Omega\,,$$

we obtain compact reformulations as nonlinear evolution equations

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\,u(t) = F\big(u(t)\big) = A\,u(t) + B\big(u(t)\big)\,, \\ u(t_0) = u_0\,, \quad t \in [t_0, T]\,, \end{cases}$$

which indicate natural decompositions into two subproblems.

Splitting approach

Splitting approach. Exponential operator splitting methods for nonlinear evolution equations of the form

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = F\big(u(t)\big) = F_1\big(u(t)\big) + F_2\big(u(t)\big)\,, \\ u(t_0) = u_0\,, \quad t \in [t_0, T]\,, \end{cases}$$

rely on the presumption that the numerical approximation of the associated subproblems

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u_1(t) = F_1\big(u_1(t)\big)\,, \quad \frac{\mathrm{d}}{\mathrm{d}t}\, u_2(t) = F_2\big(u_2(t)\big)\,,$$

is significantly simpler compared to the numerical approximation of the original problem.

Side remark. In connection with our model problems, we identify $F_1 = A$ (linear differential operator) and $F_2 = B$ (nonlinear multiplication operator).

Splitting approach

Classical notation. The exact evolution operator associated with the original problem is denoted by

$$\mathscr{E}_{t,F}(u_0) = u(t)\,, \quad t \in [t_0, T]\,,$$

that is, we indicate the dependence on the current time, the defining operator, and the initial state.

Alternative notation. The alternative formal notation

$$\mathrm{e}^{tD_F} u_0 = u(t)\,, \quad t \in [t_0, T]\,,$$

is justified by the calculus of Lie-derivatives. This calculus is most useful with regard to the convergence analysis of complex exponential operator splitting methods and the design of (processed) modified operator splitting methods, since it reveals analogies between linear and nonlinear cases.

Splitting approach

Time-stepping approach. We aim at the computation of numerical approximations at certain time grid points based on a standard time-stepping approach (recurrences for exact and numerical solution values)

$$t_0 < t_1 < \cdots < t_N = T\,, \quad \tau_n = t_{n+1} - t_n\,,$$
$$u_{n+1} = \mathscr{S}_{\tau_n,F}(u_n) \approx u(t_{n+1}) = \mathscr{E}_{\tau_n,F}\big(u(t_n)\big)\,,$$
$$n \in \{0,1,\dots,N-1\}\,.$$

Standard splitting methods. Any standard exponential operator splitting method can be cast into the following form with real coefficients

$$\mathscr{S}_{\tau,F} = \mathscr{E}_{\tau,b_s F_2} \circ \mathscr{E}_{\tau,a_s F_1} \circ \cdots \circ \mathscr{E}_{\tau,b_1 F_2} \circ \mathscr{E}_{\tau,a_1 F_1}\,, \quad \big(a_j, b_j\big)_{j=1}^{s} \in \mathbb{R}^{2s}\,.$$

On firm ground

On firm ground. The excellent behaviour of (optimised) exponential operator splitting methods with respect to stability, accuracy, efficiency, and the preservation of conserved quantities over long timeframes has been confirmed by a variety of contributions.

Selection of comprehensive descriptions and specific studies.

- Open access review of S. Blanes, F. Casas, A. Murua on splitting methods for differential equations is now published online in Acta Numerica 33 (2024).
- Hairer, Lubich, Wanner (2006), McLachlan, Quispel (2002), Sanz-Serna, Calvo (2018).
- Auzinger, Hofstätter, Koch (2019), Bao, Jin, Markowich (2002), Bertoli, Besse, Vilmart (2021), Caliari, Zuccher (2021), Castella, Chartier, Decombes, Vilmart (2009), Chin (1997), Danaila, Protas (2017), Goth (2022), Hansen, Ostermann (2009), Jahnke, Lubich (2000), Kieri (2015), Kozlov, Kvaerno, Owren (2004), Omelyan, Mryglod, Folk (2003), Strang (1968), Trotter (1959), Yoshida (1990).

Alternative approaches

Alternative approaches. Despite the benefits of standard exponential operator splitting methods, it remains an issue of substantial interest to exploit alternative approaches, amongst others,

- to overcome a second-order barrier valid for stable exponential operator splitting methods applied to non-reversible systems,
- to gain additional freedom in the adjustment of the method coefficients for the design of optimised schemes.

The investigation of these fundamental questions reveals surprising findings ...

Alternative approaches

- **Complex operator splitting methods.** The inclusion of complex coefficients permits the design of stable high-order exponential operator splitting methods with specific structural features.
- **Modified operator splitting methods.** Modifications of standard exponential operator splitting methods are expedient for our model problems of complex Ginzburg-Landau type, since the nonlinear multiplication operators F_2 and the iterated commutators

$$\big[D_{F_2}, [D_{F_2}, D_{F_1}]\big] = F_1'' \, F_2 \, F_2 + F_1' \, F_2' \, F_2 + F_2' \, F_2' \, F_1 - F_2'' \, F_1 \, F_2 - 2 \, F_2' \, F_1' \, F_2$$

  have similar structures.
- **Processed operator splitting methods.** The incorporation of processors enhances the benefits of modified operator splitting methods for nonlinear Schrödinger equations (occurrence of resonances).

Complex operator splitting methods

Reaction-diffusion equations
Convergence analysis
Quasicrystalline pattern formation

S. Blanes, F. Casas, C. González, M. Th.
Symmetric-conjugate splitting methods for evolution equations of parabolic type.
Journal of Computational Dynamics 11/1 (2024) 108-134.

Model problem

Model problem. We consider high-order reaction-diffusion equations involving analytic nonlinearities $(K = 4 = \widetilde{K} + 1)$

$$\begin{cases} \partial_t U(x,t) = \sum_{k=0}^{K} \alpha_k \, \Delta^k U(x,t) + \sum_{k=1}^{\widetilde{K}} \beta_k \big(U(x,t)\big)^k, \\ U(x,t_0) = U_0(x), \quad (x,t) \in \Omega \times [t_0,T]. \end{cases}$$

Complex operator splitting methods

Complex operator splitting methods. We apply exponential operator splitting methods involving complex coefficients

$$\mathscr{S}_{\tau,F} = \mathscr{E}_{\tau,b_s F_2} \circ \mathscr{E}_{\tau,a_s F_1} \circ \cdots \circ \mathscr{E}_{\tau,b_1 F_2} \circ \mathscr{E}_{\tau,a_1 F_1}\,, \qquad \big(a_j, b_j\big)_{j=1}^{s} \in \mathbb{C}^{2s}\,.$$

Structural features. Additional structural features are of importance in long-term computations, in particular for linear evolution equations. Specifically, we apply symmetric, symmetric-conjugate, and alternating-conjugate schemes

$$\big(b_1, a_2, b_2, \dots, a_r, b_r, a_{r+1}, b_r, a_r, \dots, b_2, a_2, b_1, 0\big)\,,$$

$$\big(\overline{b_1}, \overline{a_2}, \overline{b_2}, \dots, \overline{a_r}, \overline{b_r}, a_{r+1}, b_r, a_r, \dots, b_2, a_2, b_1, 0\big)\,,$$

$$\big(b_1, a_2, b_2, \dots, a_r, b_r, a_{r+1}, \overline{b_r}, \overline{a_r}, \dots, \overline{b_2}, \overline{a_2}, \overline{b_1},$$
$$\overline{b_1}, \overline{a_2}, \overline{b_2}, \dots, \overline{a_r}, \overline{b_r}, a_{r+1}, b_r, a_r, \dots, b_2, a_2, b_1, 0)\,.$$

Stability analysis

Stability analysis (Hilbert space setting, Fourier).

- In view of the decisive linear subproblem involving powers of the Laplacian, it suffices to consider the principal contributions

$$a_j\, A_K = a_j\, \alpha_K\, \Delta^K\,, \quad a_j, \alpha_K \in \mathbb{C}\,, \quad j \in \{1, \dots, s\}\,.$$

- For simplicity, we consider the Lebesgue space $\big(L^2(\Omega, \mathbb{C}), \|\cdot\|_{L^2}\big)$ with bounded domain $\Omega = [-\pi, \pi]^d$ as underlying function space.
- A complete orthonormal system is given by the family of Fourier functions $(\mathscr{F}_m)_{m \in \mathbb{Z}^d}$, which forms a set of eigenfunctions such that

$$\frac{\mathrm{d}}{\mathrm{d}x}\,\mathrm{e}^{\mathrm{i}\mu x} = \mathrm{i}\mu\,\mathrm{e}^{\mathrm{i}\mu x}\,, \quad a_j\, A_K\, \mathscr{F}_m = a_j\, \alpha_K\, \big(-\lambda_m\big)^K \mathscr{F}_m\,,$$

$$\lambda_m = |m|^2 = \sum_{\ell=1}^{d} m_\ell^2\,, \quad m = (m_1, \dots, m_d) \in \mathbb{Z}^d\,.$$

Stability analysis

Stability analysis (Hilbert space setting, Fourier). By Fourier series representations and Parseval's identity, we obtain $(\tau_n, \lambda_m \geq 0)$

$$a_j \, A_K \, \mathscr{F}_m = a_j \, \alpha_K \, (-\lambda_m)^K \mathscr{F}_m \, ,$$

$$\mathscr{E}_{\tau_n, a_j A_K} \mathscr{F}_m = \mathrm{e}^{\tau_n \, a_j \, \alpha_K \, (-\lambda_m)^K} \mathscr{F}_m \, ,$$

$$v(t_n) = \sum_{m \in \mathbb{Z}^d} v_m(t_n) \, \mathscr{F}_m \, , \quad \|v(t_n)\|_{L^2}^2 = \sum_{m \in \mathbb{Z}^d} |v_m(t_n)|^2 \, ,$$

$$\mathscr{E}_{\tau_n, a_j A_K} \, v(t_n) = \sum_{m \in \mathbb{Z}^d} \mathrm{e}^{\tau_n \, a_j \, \alpha_K \, (-\lambda_m)^K} \, v_m(t_n) \, \mathscr{F}_m \, ,$$

$$\|\mathscr{E}_{\tau_n, a_j A_K} \, v(t_n)\|_{L^2}^2 = \sum_{m \in \mathbb{Z}^d} \left| \mathrm{e}^{\tau_n \, a_j \, \alpha_K \, (-\lambda_m)^K} \right|^2 |v_m(t_n)|^2 = \sum_{m \in \mathbb{Z}^d} \mathrm{e}^{(-1)^K \, \Re(a_j \, \alpha_K) \, 2 \, \tau_n \, \lambda_m^K} \, |v_m(t_n)|^2 \, .$$

Boundedness is ensured under the condition $(\lambda_m \to \infty$ as $|m| \to \infty)$

$$\mathrm{e}^{(-1)^K \, \Re(a_j \, \alpha_K) \, \tau_n \, \lambda_m^K} \leq 1 \, , \quad m \in \mathbb{Z}^d \, .$$

Stability analysis

Stability analysis. For complex exponential operator splitting methods, the following stability conditions hold

$$(-1)^K \Re\big(a_j\,\alpha_K\big) = (-1)^K \Big(\Re(a_j)\,\Re(\alpha_K) - \Im(a_j)\,\Im(\alpha_K)\Big) \leq 0\,, \quad j \in \{1,\dots,s\}\,.$$

These conditions apply to high-order reaction-diffusion equations $(K=4)$ and complex Ginzburg–Landau equations $(K=1)$.

Convergence analysis (Analytical framework)

Theorem (Reaction-diffusion and Ginzburg–Landau equations). Assume that

- the evolution equation comprises a sectorial operator $A : D(A) \subseteq X \to X$ generating an analytic semigroup $(\mathscr{E}_{t,A})_{t \in [t_0,T]}$ on a Banach space and a nonlinear operator $B : D(B) \subseteq X \to X$,
- the coefficients of the complex exponential operator splitting method fulfill the classical order conditions for some integer $p \in \mathbb{N}_{\geq 1}$,
- the stability bounds $\|\mathscr{E}_{t,a_j A}\|_{X \leftarrow X} \leq \mathrm{e}^{C_1 t}$ hold for $t \in [t_0, T]$ and $j \in \{1, \dots, s\}$,
- the iterated commutators arising in the local error expansion $\|\mathrm{ad}_A^\ell(B)\|_{X \leftarrow D} \leq C_2$ for $\ell \in \{0, 1, \dots, p\}$ and the solution values $\|u(t)\|_D \leq C_3$ remain bounded with respect to the norm of a suitably restricted subspace.

Then the following global error estimate is valid

$$\|u_n - u(t_n)\|_X \leq C\Big(\|u_0 - u(t_0)\|_X + \tau_{\max}^p\Big), \quad n \in \{1, \dots, N\}.$$

Side remarks.

- Analogous statements for nonlinear Schrödinger equations (framework of strongly continuous groups).
- Generalisations to full discretisations based on spectral space discretisations combined with time-splitting methods (Hilbert space setting).

Numerical experiments

Focus.

- Complex exponential operator splitting methods ($p \in \{4,6\}$)
- High-order reaction-diffusion equations (analytic nonlinearities)
- Short-term integration (stability, global error, efficiency, 3d)
- Long-term integration (solution profile, pattern formation, 2d)

Verification.

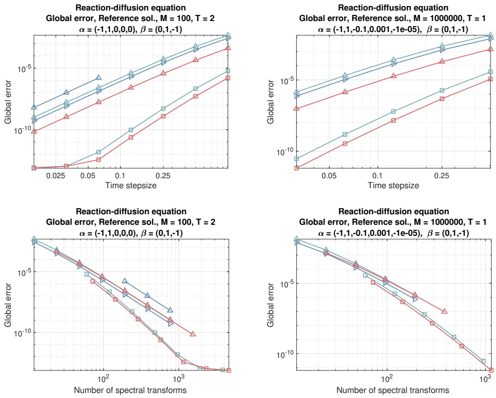
- The performed numerical experiments confirm the theoretical stability and global error analysis.

Numerical experiments

- Yoshida splitting (real, symmetric, p = 4, s = 4)
- Yoshida splitting (complex, symmetric, p = 4, s = 4)
- Complex splitting (symmetric-conj, p = 4, s = 4)
- Complex splitting (symmetric-conj, p = 6, s = 16)
- Complex splitting (alternating-conj, p = 4, s = 7)
- Complex splitting (alternating-conj, p = 6, s = 19)

Numerical experiments

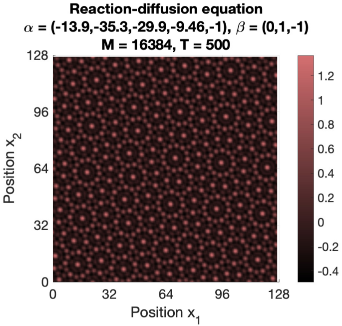
Summary. Design of stable and efficient sixth-order exponential operator splitting methods based on the incorporation of complex coefficients.

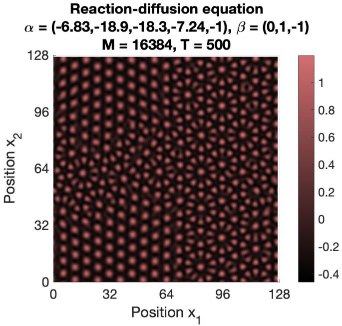


Left/Right: Stability issues for real splittings (1d/3d). Up: Order. Down: Cost.

Numerical experiments

Summary. Application of complex exponential operator splitting methods in long-term computations for the simulation of quasicrystalline pattern formation.





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Modified operator splitting methods

Complex Ginzburg–Landau equations
Invariance principle
Superconductivity

S. Blanes, F. Casas, C. González, M. Th.
Generalisation of splitting methods based on modified potentials to nonlinear evolution equations of parabolic and Schrödinger type.
Computer Physics Communications 295 (2024) 109007.

Basic idea

Basic idea. An educated guess leads us to the novel class of modified operator splitting methods for nonlinear evolution equations. In essence, we exploit a formal generalisation of the linear case based on the calculus of Lie derivatives

$$\big[B,[B,A]\big] = B^2 A - 2\,B\,A\,B + A\,B^2\,,$$
$$\big[D_{F_2},[D_{F_2},D_{F_1}]\big] = F_1''\,F_2\,F_2 + F_1'\,F_2'\,F_2 + F_2'\,F_2'\,F_1 - F_2''\,F_1\,F_2 - 2\,F_2'\,F_1'\,F_2\,.$$

Focus. We focus on the extension of Chin's fourth-order modified potential operator splitting method to Ginzburg–Landau equations.

Side remark. For linear operators F_1, F_2, we indeed obtain

$$F_j' = F_j\,,\quad F_j'' = 0\,,\quad \big[D_{F_2},[D_{F_2},D_{F_1}]\big] = F_1\,F_2\,F_2 + F_2\,F_2\,F_1 - 2\,F_2\,F_1\,F_2\,.$$

Linear case

Linear ordinary differential equations. Our starting point are (large) systems of linear ordinary differential equations defined by square matrices

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = A\, u(t) + B\, u(t)\,, \quad t \in [0, T]\,, \quad A, B \in \mathbb{C}^{M \times M}\,.$$

The solution values at the final time are given by the matrix exponential

$$u(T) = \mathrm{e}^{T(A+B)}\, u(0) = \left(\mathrm{e}^{\tau(A+B)}\right)^N u(0)\,, \quad \tau = \frac{T}{N}\,, \quad N \in \mathbb{N}\,.$$

Linear case

Operator splitting methods.

- Standard exponential operator splitting methods are built on several compositions of the factors $\mathrm{e}^{a\tau A}$, $\mathrm{e}^{b\tau B}$ with real coefficients $a, b \in \mathbb{R}$.
- Modified potential operator splitting methods are built on

$$\mathrm{e}^{a\tau A}, \quad \mathrm{e}^{b\tau B + c\tau^3 [B,[B,A]]}, \quad \big[B,[B,A]\big] = B^2 A - 2\,BAB + AB^2,$$

with real coefficients $a, b, c \in \mathbb{R}$ (positivity $a, b \geq 0$ desirable).

The underlying idea of this approach is to overcome a second-order barrier that is valid for standard stable exponential operator splitting methods when applied to non-reversible systems and to gain additional freedom in the adjustment of the method coefficients for the design of optimised schemes.

Linear case

Linear partial differential equations. The advantages of modified potential operator splitting methods become apparent in the context of ground and excited state computations for linear Schrödinger equations based on an imaginary time propagation. In this setting, the arising operators A and B correspond to the Laplacian and a potential, and hence the iterated commutator reduces to a multiplication operator, which is defined by the gradient of the potential

$$B \sim V, \quad \big[B,[B,A]\big] \sim \nabla V.$$

This explains the common notion force-gradient operator splitting method or modified potential operator splitting method.

In Chin's words (1997). *The basic idea is to incorporate an additional higher order composite operator so that the implementation of one algorithm requires only one evaluation of the force and one evaluation of the force and its gradient*

$$\mathscr{S}_{\tau,F} = \mathrm{e}^{\frac{1}{6}\tau B}\,\mathrm{e}^{\frac{1}{2}\tau A}\,\mathrm{e}^{\frac{2}{3}\tau B - \frac{1}{72}\tau^3 [B,[B,A]]}\,\mathrm{e}^{\frac{1}{2}\tau A}\,\mathrm{e}^{\frac{1}{6}\tau B}.$$

Nonlinear case

Nonlinear partial differential equations. Our guideline for the extension to nonlinear evolution equations is provided by the formal calculus of Lie derivatives.

- The nonlinear operators F_1, F_2 take the roles of the matrices A, B.
- The matrix exponential

$$\mathrm{e}^{b\tau B + c\tau^3 [B,[B,A]]}, \quad \big[B,[B,A]\big] = B^2 A - 2\,B\,A\,B + A\,B^2\,,$$

  is replaced by the evolution operator associated with the nonlinear evolution equation involving the iterated commutator

$$\frac{\mathrm{d}}{\mathrm{d}t}\,u(t) = b\,F_2\big(u(t)\big) + c\,\tau_n^2\,G\big(u(t)\big), \quad t \in [t_n, t_n + \tau_n]\,,$$
$$G = F_1''\,F_2\,F_2 + F_1'\,F_2'\,F_2 + F_2'\,F_2'\,F_1 - F_2''\,F_1\,F_2 - 2\,F_2'\,F_1'\,F_2\,.$$

Nonlinear case

- As a consequence, the extension of Chin's fourth-order scheme

$$\mathscr{S}_{\tau,F} = \mathrm{e}^{\frac{1}{6}\tau B}\, \mathrm{e}^{\frac{1}{2}\tau A}\, \mathrm{e}^{\frac{2}{3}\tau B - \frac{1}{72}\tau^3 [B,[B,A]]}\, \mathrm{e}^{\frac{1}{2}\tau A}\, \mathrm{e}^{\frac{1}{6}\tau B}$$

to (general) nonlinear evolution equations is (formally) given by

$$\mathscr{S}_{\tau,F} = \mathscr{E}_{\tau,\frac{1}{6}F_2} \circ \mathscr{E}_{\tau,\frac{1}{2}F_1} \circ \mathscr{E}_{\tau,\frac{2}{3}F_2 - \frac{1}{72}\tau^2 G} \circ \mathscr{E}_{\tau,\frac{1}{2}F_1} \circ \mathscr{E}_{\tau,\frac{1}{6}F_2}\,.$$

Specification

Specification. We specify the extension of Chin's fourth-order scheme for our general model problem of complex Ginzburg–Landau-type

$$\partial_t U(x,t) = \alpha_1 \, \Delta U(x,t) + \alpha_0 \, U(x,t) + \beta_1 V(x) \, U(x,t) + \beta_2 \left| U(x,t) \right|^2 U(x,t) \, .$$

As special cases, it includes reaction-diffusion equations (real constants) and time-dependent Gross–Pitaevskii equations (purely imaginary constants).

Specification

Iterated commutator. For the general model problem based on the complex Ginzburg–Landau-type equation, the iterated commutator is given by

$$\begin{aligned}
G &= G_1 + G_2 + G_3 + G_4\,,\\
G_1(v) &= 4\,\Re(\beta_1)\,\beta_2\left(-\Re(\alpha_2)\,|v|^2\,v + 2\,\alpha_1\,|\nabla v|^2\,v + \mathrm{i}\,\Im(\alpha_1)\,\overline{\Delta v}\,v^2 + \alpha_1\,\nabla v\cdot\nabla v\,\overline{v}\right)V\,,\\
G_2(v) &= 2\left(\alpha_1\,\beta_1^2\,\nabla V + 4\,\alpha_1\,\Re(\beta_1)\,\beta_2\,\nabla v\,\overline{v} + \left(3\,\alpha_1\,\beta_1 + \alpha_1\,\overline{\beta_1} - 2\,\overline{\alpha_1}\,\overline{\beta_1}\right)\beta_2\,\overline{\nabla v}\,v\right)\cdot\nabla V\,v\,,\\
G_3(v) &= -2\left(\mathrm{i}\,\alpha_1\,\Im(\beta_1) + \overline{\alpha_1}\,\overline{\beta_1}\right)\beta_2\,\Delta V\,|v|^2\,v + 2\,\alpha_1\left(2\,\beta_2^2 + 3\,|\beta_2|^2\right)\nabla v\cdot\nabla v\,\overline{v}^2\,v\,,\\
G_4(v) &= 4\left(2\,\alpha_1\,\beta_2^2 + 3\,\alpha_1\,|\beta_2|^2 - 2\,\overline{\alpha_1}\,|\beta_2|^2\right)|\nabla v|^2\,|v|^2\,v + 2\left(2\,\alpha_1\,\beta_2^2 + \alpha_1\,|\beta_2|^2\right.\\
&\qquad \left.-2\,\overline{\alpha_1}\,|\beta_2|^2\right)\overline{\nabla v}\cdot\overline{\nabla v}\,v^3 + 8\,\mathrm{i}\,\Im(\alpha_1)\,|\beta_2|^2\,\Re\left(\Delta v\,\overline{v}\right)|v|^2\,v\,.
\end{aligned}$$

The simplification for reaction-diffusion equations with (normalised) real constants is

$$G(v) = 2\left(\nabla V\cdot\nabla V - \Delta V\,v^2 + 6\,\nabla V\cdot\nabla v\,v + 6\left(V + 2\,v^2\right)\nabla v\cdot\nabla v\right)v\,.$$

The simplification for GPEs with (normalised) purely imaginary constants is

$$G(v) = -2\,\mathrm{i}\left(\nabla V\cdot\nabla V - 2\left(|v|^2\,\Delta V + |v|^2\left(2\,\Re(\overline{v}\,\Delta v) + 3\,\nabla\overline{v}\cdot\nabla v\right) + \Re\left(\overline{v}^2\,\nabla v\cdot\nabla v\right)\right)\right)v\,.$$

Invariance principle

Invariance principle.

- A fundamental invariance principle holds for standard exponential operator splitting methods applied to nonlinear Schrödinger equations (Gross–Pitaevskii equations).
- It (magically) extends to modified operator splitting methods.

Theorem. The exact solution to the nonlinear subproblem comprising the iterated commutator

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = \mathrm{i}\Big(f_1\big(u(t)\big) + \tau_n^2\, f_2\big(u(t)\big)\Big)\, u(t)\,, \\ u(t_n) = u_n\,, \qquad t \in [t_n, t_n + \tau_n]\,, \end{cases}$$

satisfies the invariance principle

$$f_1\big(u(t)\big) + \tau_n^2\, f_2\big(u(t)\big) = f_1(u_n) + \tau_n^2\, f_2(u_n)\,, \qquad t \in [t_n, t_n + \tau_n]\,.$$

Proof. Verify the identity

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(f_1\big(u(t)\big) + \tau_n^2\, f_2\big(u(t)\big)\Big) = 0\,, \qquad t \in [t_n, t_n + \tau_n]\,.$$

Invariance principle

Summary. The realisation of the modified operator splitting method

$$u_{n+1} = \left(\mathscr{E}_{\tau,\frac{1}{6}F_2} \circ \mathscr{E}_{\tau,\frac{1}{2}F_1} \circ \mathscr{E}_{\tau,\frac{2}{3}F_2-\frac{1}{72}\tau^2 G} \circ \mathscr{E}_{\tau,\frac{1}{2}F_1} \circ \mathscr{E}_{\tau,\frac{1}{6}F_2}\right) u_n\,,$$
$$n \in \{0,1,\dots,N-1\}\,,$$

applied to Gross–Pitaevskii equations involves the time integration of linear Schrödinger equations (fast Fourier techniques)

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = \mathrm{i}\, a\, \Delta u(t)\,, \qquad t \in [t_n, t_n+\tau_n]\,,$$

and pointwise evaluations of solution representations of the form

$$\mathscr{E}_{\tau_n, bF_2 + c\tau_n^2 G}(u_n) = \mathrm{e}^{\mathrm{i}\,\tau_n (b f_1(u_n) + c\tau_n^2 f_2(u_n))}\, u_n\,, \qquad \tau_n \in \mathbb{R}\,.$$

Due to the invariance principle, the time integration of nonlinear problems reduces to the time integration of linear subproblems.

Numerical experiments

Focus.

- Fourth-order modified operator splitting method (in comparison with complex exponential operator splitting methods)
- Complex Ginzburg–Landau equations and related evolution equations of parabolic and Schrödinger type (Gross–Pitaevskii)
- Short-term integration (stability, global error, efficiency, 3d)
- Long-term integration (solution profile, 2d)

Verification.

- The performed numerical experiments confirm the validity of the invariance principle for modified operator splitting methods as well as the theoretical stability and global error analysis for complex exponential operator splitting methods.

Numerical experiments

Practical aspects.

- Even though the formula for the iterated commutator is lengthy, the implementation of modified operator splitting methods is straightforward.
- The application of the second-order Strang splitting method to the nonlinear subproblem $\big(u' = bF_2(u) + c\tau^2 G(u)\big)$ and the knowledge of the exact solution $\big(u' = bF_2(u)\big)$ improves stability and efficiency.
- The correct implementation of higher-order complex exponential operator splitting methods for evolution equations involving non-analytic nonlinearities is a subtle issue and requires suitable reformulations as systems for $(u, \overline{u})$. Otherwise, significant order reductions are encountered!

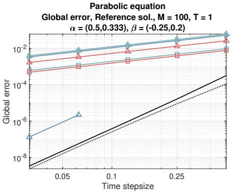
Numerical experiments

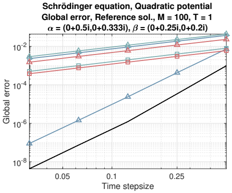
- Yoshida splitting (real, symmetric, p = 4, s = 4)
- Yoshida splitting (complex, symmetric, p = 4, s = 4)
- Complex splitting (symmetric-conj, p = 4, s = 4)
- Complex splitting (symmetric-conj, p = 6, s = 16)
- Complex splitting (alternating-conj, p = 4, s = 7)
- Complex splitting (alternating-conj, p = 6, s = 19)
- Modified splitting (real, p = 4, s = 3)
- Modified splitting (Strang, RKM)

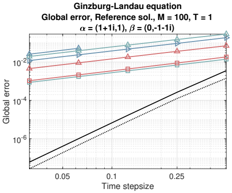
Numerical experiments

Observations.

- The modified operator splitting method remains stable and retains order four.
- When applied to non-reversible systems, the fourth-order Yoshida splitting method involving negative coefficients suffers from severe instabilities.
- A naive implementation of higher-order real or complex exponential operator splitting methods for complex Ginzburg–Landau-type equations involving non-analytic nonlinearities leads to significant order reductions.

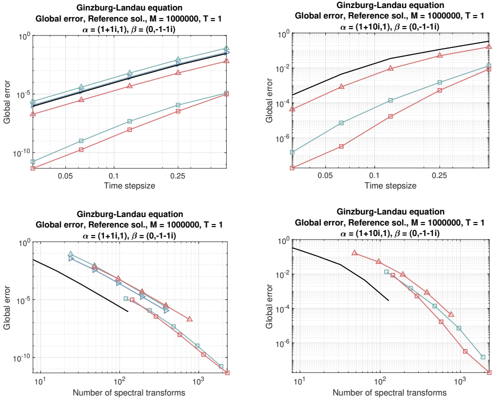






Numerical experiments

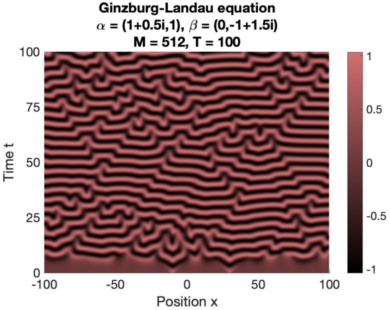
Summary. Design and practical implementation of stable and efficient fourth-order operator splitting methods for complex Ginzburg–Landau-type equations based on the incorporation of iterated commutators.

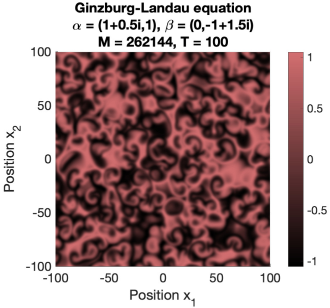


Left/Right: Stability issues for complex splittings ($\alpha_1 \in \{1+\mathrm{i}, 1+10\mathrm{i}\}$). Up: Order. Down: Cost.

Numerical experiments

Summary. Application of modified operator splitting methods in long-term computations for the simulation of nonlinear waves.





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Final conclusions and future work

Final conclusions and future work

Summary. Our theoretical results and numerical experiments confirm the benefits of complex exponential operator splitting methods for reaction-diffusion equations and of modified operator splitting methods for complex Ginzburg–Landau-type equations.

General perspective. Our investigations range from the design of time integration methods and their theoretical analysis to implementation aspects for relevant applications.

Final conclusions and future work

Future work to complete the picture.

- Rigorous convergence analysis of modified operator splitting methods applied to Ginzburg–Landau-type equations.
- Implementation of modified operator splitting methods for high-order reaction-diffusion equations describing quasicrystals.
- Thorough investigation and design of (processed) modified operator splitting methods in the context of resonances.

Thank you very much!

Stability analysis – Special case

Stability analysis. For complex exponential operator splitting methods, the following stability conditions hold

$$(-1)^K \Re\big(a_j\, \alpha_K\big) = (-1)^K \Big(\Re(a_j)\,\Re(\alpha_K) - \Im(a_j)\,\Im(\alpha_K)\Big) \leq 0\,, \quad j \in \{1,\dots,s\}\,.$$

These conditions apply to high-order reaction-diffusion equations $(K=4)$ and complex Ginzburg–Landau equations $(K=1)$.

Side remark. For exponential operator splitting methods involving real coefficients $(a_j)_{j=1}^s$, the following simplifications are valid

$$\Im(a_j) = 0\,, \quad j \in \{1,\dots,s\} \quad \Longrightarrow \quad (-1)^K \Re(a_j)\,\Re(\alpha_K) \leq 0\,, \quad j \in \{1,\dots,s\}\,.$$

For well-posed reaction-diffusion equations such that $(-1)^K \Re(\alpha_K) \leq 0$, this yields the stability conditions (second-order barrier)

$$a_j = \Re(a_j) \geq 0\,, \quad j \in \{1,\dots,s\}\,.$$

Due to $\Re(\alpha_K) = 0$, stability is ensured for Schrödinger equations.

Processed (modified) splitting methods

Nonlinear Schrödinger equations
Observation of resonances

Processed methods

Basic idea. We raise the order and enhance the efficiency of a time integration method when applied with constant time stepsizes

$$u_n = \mathscr{S}_{\tau,F}^{n}(u_0)$$

by incorporating a processor (corrector)

$$\begin{aligned} u_n &= \Big(\big(\mathscr{P}_{\tau,F}^{-1} \circ \mathscr{S}_{\tau,F} \circ \mathscr{P}_{\tau,F}\big) \circ \cdots \circ \big(\mathscr{P}_{\tau,F}^{-1} \circ \mathscr{S}_{\tau,F} \circ \mathscr{P}_{\tau,F}\big) \Big)(u_0) \\ &= \big(\mathscr{P}_{\tau,F}^{-1} \circ \mathscr{S}_{\tau,F}^{n} \circ \mathscr{P}_{\tau,F}\big)(u_0)\,. \end{aligned}$$

Processed methods

Special setting. Processing techniques permit the design of higher-order exponential operator splitting methods involving low numbers of stages. We observe favourable performances for nonlinear Schrödinger equations in long-term computations (occurrence of resonances).

Example. A fourth-order processed modified operator splitting method involving a single stage is given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = A\, u(t) + B\big(u(t)\big)\,, \quad t \in [t_0, T]\,,$$

$$\mathscr{S}_{\tau,F} = \mathscr{E}_{\tau,\frac{1}{2}A} \circ \mathscr{E}_{\tau,B-\frac{1}{24}\tau^2 G} \circ \mathscr{E}_{\tau,\frac{1}{2}A}\,,$$

$$\mathscr{P} : (\tilde{a}_4, \tilde{b}_3, \tilde{a}_3, \tilde{b}_2, \tilde{a}_2, \tilde{b}_1)\,, \quad \mathscr{P}^{-1} : -(\tilde{b}_1, \tilde{a}_2, \tilde{b}_2, \tilde{a}_3, \tilde{b}_3, \tilde{a}_4)\,, \quad \tilde{a}_3 = \tilde{a}_2\,.$$

Numerical experiments

Focus.

- We apply standard and (processed) modified operator splitting methods for the time integration of nonlinear Schrödinger equations over longer timeframes.
- For various choices of the constant time stepsizes, we determine the errors in energy at the final time.

Numerical experiments

- Lie splitting (real, p = 1, s = 1)
- Strang splitting (real, symmetric, p = 2, s = 2)
- Yoshida splitting (real, symmetric, p = 4, s = 4)
- Modified splitting (real, p = 4, s = 3)
- Processed modified splitting (real, p = 4, s = 1)

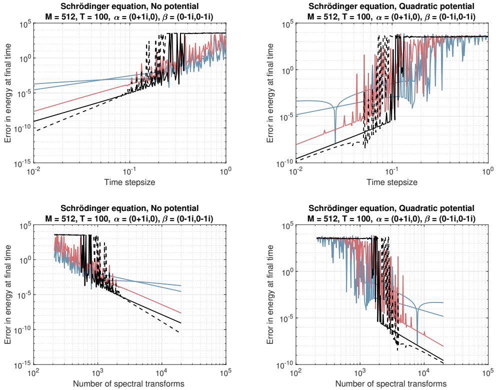
Numerical experiments

Observations.

- For smaller / larger time stepsizes, the errors in energy at the final time are smooth / erratic (phenomenon of resonances).
- This behaviour can be understood for simplified test cases such as linear differential equations defined by Pauli matrices, where explicit representations of the exact and numerical solutions are known.
- The analysis of nonlinear cases is a highly complex problem.
- Refinements of the space discretisations as well as the sizes of potentials and nonlinearities effect the occurrence of resonances.
- The stated fourth-order processed modified operator splitting method performs in a favourable manner. This justifies the thorough investigation of this class of methods.

Numerical experiments

Summary. Design and practical implementation of stable and efficient operator splitting methods for the long-term integration of nonlinear Schrödinger equations based on the incorporation of iterated commutators and processors.



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