Novel approaches for nonlinear evolution equations based on operator splitting

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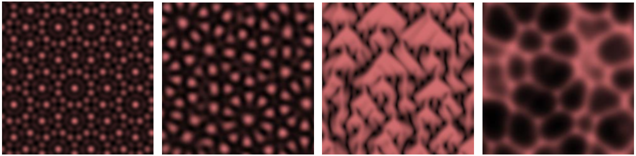

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- Fernando Casas (Castellón, Spain),
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Opening statements

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.

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 (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

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

have similar structures.

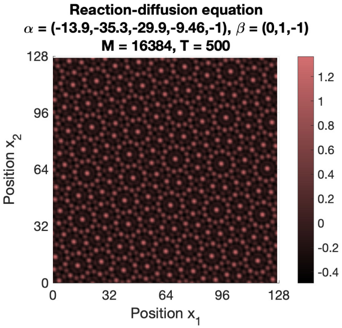
Complex operator splitting methods

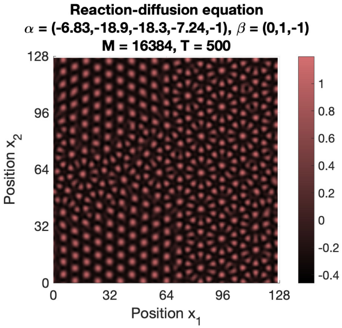
Reaction-diffusion equations
Convergence analysis
Quasicrystalline pattern formation

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.

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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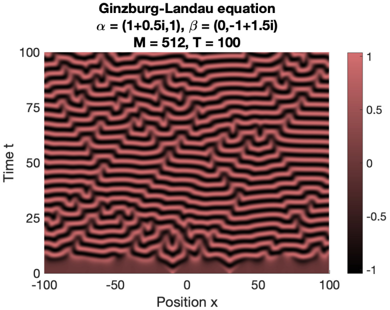
Modified operator splitting methods

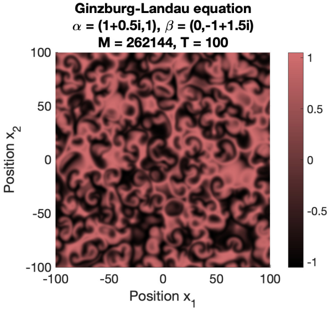
Complex Ginzburg–Landau equations
Invariance principle
Superconductivity

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.

Numerical experiments

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





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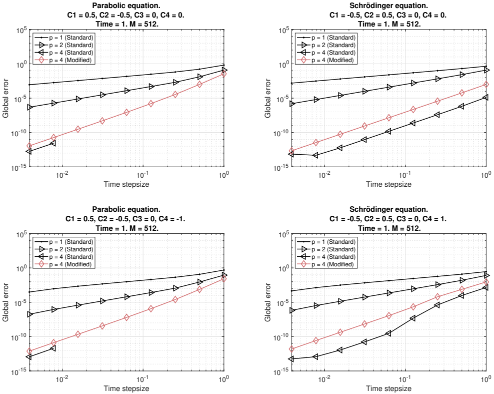
Adaptive modified operator splitting methods

Gross–Pitaevskii equations
Groundstate computation, Time evolution
Bose–Einstein condensation

Numerical experiments

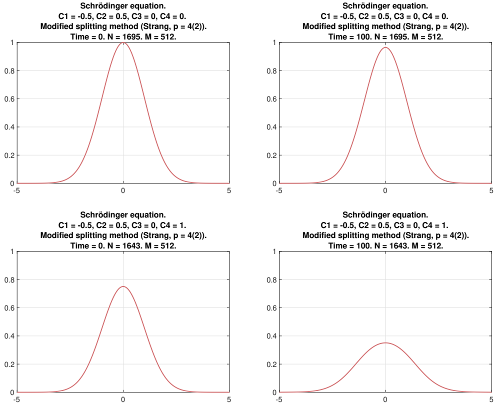
Summary. Design of a stable and efficient fourth-order exponential operator splitting method based on the incorporation of an iterated commutator.



Severe stability issues for a standard fourth-order splitting method applied to linear (up) and nonlinear (down) problems of parabolic type (left).

Numerical experiments

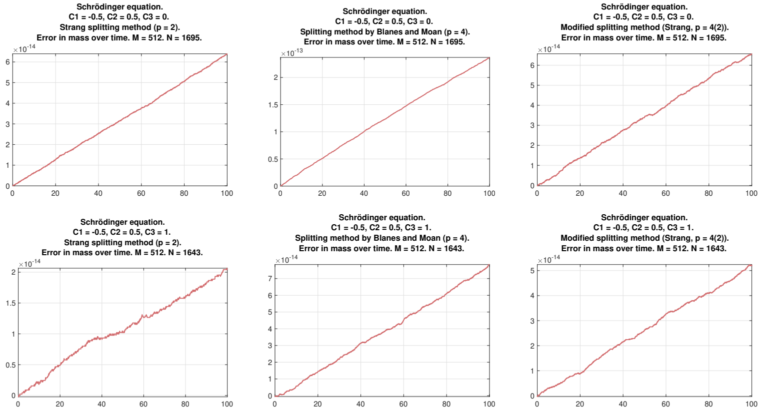
Questions. Favourable behaviour of a fourth-order modified operator splitting method for linear and nonlinear Schrödinger-type equations over longer times? Benefits of a simple local error control based on the second-order Strang splitting method?



Linear (up) versus nonlinear (down) cases.
Solution profiles $\Re(\psi(x,t))$ for initial (left) and final (right) times.

Numerical experiments

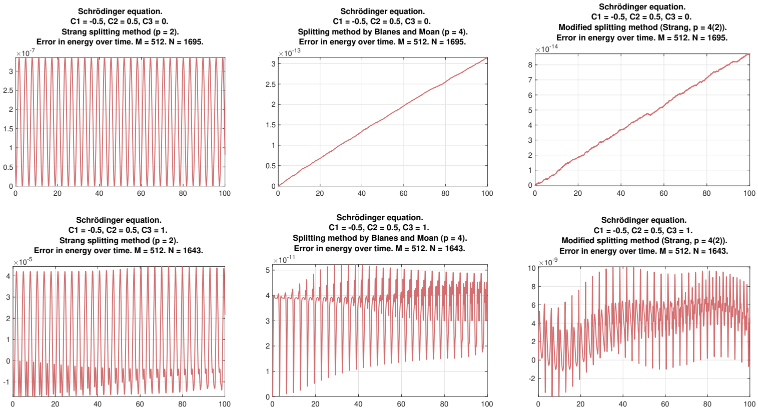
Summary. Mass preservation of a fourth-order modified operator splitting method for linear and nonlinear Schrödinger equations over longer times.



Linear (up) versus nonlinear (down) case. Uniform (left, middle) versus non-uniform (right) time grid.

Numerical experiments

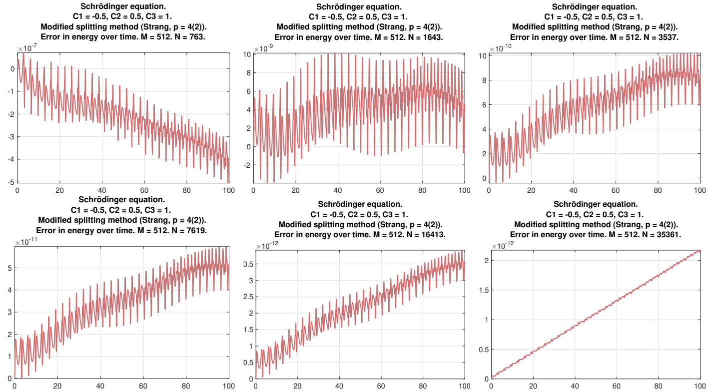
Summary. Energy preservation of a fourth-order modified operator splitting method for linear and nonlinear Schrödinger equations over longer times.



Linear (up) versus nonlinear (down) case. Uniform (left, middle) versus non-uniform (right) time grid.

Numerical experiments

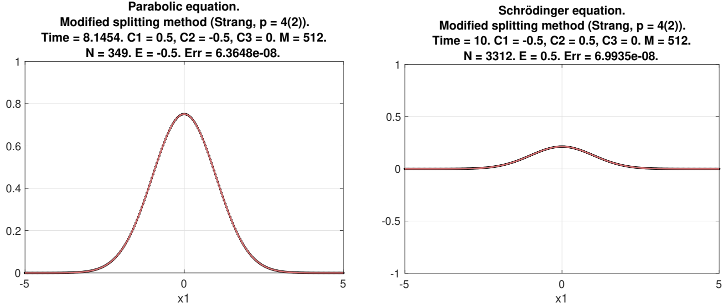
Observation. Improved energy preservation for lower tolerances. Rigorous analysis?



Nonlinear case. Tolerances in $\{10^{-3}, 10^{-4}, 10^{-5}, 10^{-6}, 10^{-7}, 10^{-8}\}$.
Numbers of time steps $(763, 1643, 3537, 7619, 16413, 35361)$ with ratios ≈ 2.15.

Numerical experiments

Summary. Simulation of linear Schrödinger equations. Application of adaptive modified operator splitting methods for groundstate computations (imaginary time method, normalised gradient flow) and time evolution.



Linear case (1d). Evolution of solution profiles $\Re(\psi(x,t))$ in imaginary and real times. Ground state solution given by Hermite basis function. Verify time-dependent solution $\psi(x,t) = \mathrm{e}^{-\mathrm{i}\,\mu\,t}\,\phi(x)$.

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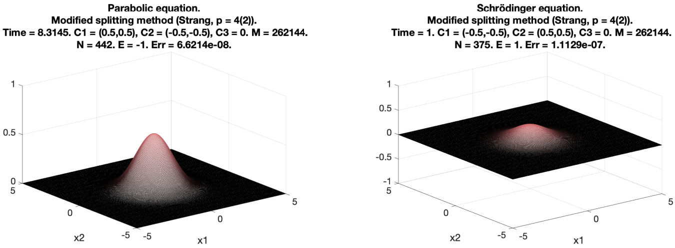
Numerical experiments

Summary. Straightforward extension to higher space dimensions.



Linear case (2d). Evolution of solution profiles $\Re\big(\psi(x,t)\big)$ in imaginary and real times.
Ground state solution given by Hermite basis function. Verify time-dependent solution $\psi(x,t) = \mathrm{e}^{-\mathrm{i}\,\mu\,t}\,\phi(x)$.

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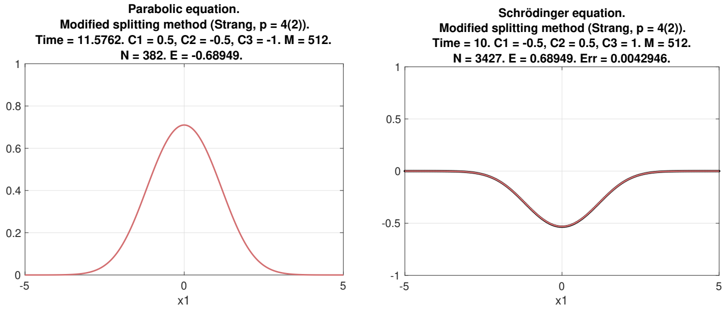
Numerical experiments

Summary. Simulation of Gross-Pitaevskii equations (Bose–Einstein condensates). Application of adaptive modified operator splitting methods for groundstate computations (imaginary time method, normalised gradient flow) and time evolution.



Nonlinear case (1d). Evolution of solution profiles $\Re(\psi(x,t))$ in imaginary and real times.
Verify time-dependent solution $\psi(x,t) = \mathrm{e}^{-\mathrm{i}\mu t}\phi(x)$.

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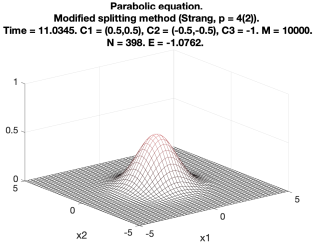
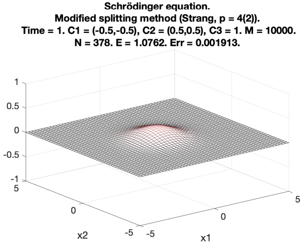
Numerical experiments

Summary. Straightforward extension to higher space dimensions.





Nonlinear case (2d). Evolution of solution profiles $\Re(\psi(x,t))$ in imaginary and real times.

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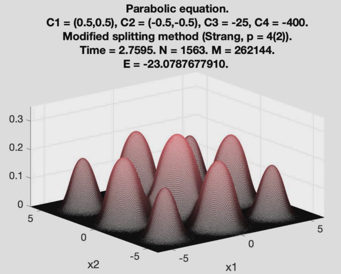
Numerical experiments

Summary. Groundstate computation based on adaptive modified operator splitting method (additional lattice potential, strong nonlinearity). Improvement by stepwise reduction of prescribed tolerances. Initial value given by Thomas–Fermi approximation.



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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.
- Extensions to other classes of nonlinear evolution equations.

Thank you very much!