Reliable and efficient numerical methods based on operator splitting and applications to optimal control of Gross–Pitaevskii equations

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- Barbara Kaltenbacher (Klagenfurt, Austria),
- José Antonio Carrillo (Oxford, United Kingdom),
- Hanns-Christoph Nägerl, Manuele Landini (Innsbruck, Austria).

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

Main reference (Optimal control)

Main reference (Optimal control). M. Hintermüller, D. Marahrens, P. Markowich, Ch. Sparber. *Optimal bilinear control of Gross–Pitaevskii equations.* SIAM Journal on Control and Optimization (2013).

- Formulation of optimal control problem
- Proof of well-posedness and existence of optimal control
- Derivation of first-order optimality system

Main inspiration (Quantum systems)

Main inspiration (Quantum systems). Experimental realisation and manipulation of Bose–Einstein condensates by Hanns-Christoph Nägerl and his team.

> *Hanns-Christoph Nägerl's research centers on experimental quantum many-body physics with systems of ultracold atoms and molecules. A central goal is to "quantum engineer" novel states of matter using the toolbox of quantum atom optics. At temperatures in the nanokelvin range, quantum mechanics dominates the individual and collective properties of the particles, giving rise to novel phases for quantum matter and to non-trivial phase transitions between the different quantum phases. Using advanced techniques such as laser cooling, Bose-Einstein condensation, and coherent laser control, Nägerl's group investigates e.g. the properties of highly correlated many-body states that are generated when the particles are confined to periodic potentials or to lower dimensions.*

www.uibk.ac.at/en/sp-physik/forschung/forschungsgruppen/experimental-physics/strongly-correlated-quantum-matter

Optimal control problem

Bilinear optimal control problem. The basic aim is to minimise an objective functional

$$J(\alpha) \to \text{minimal}$$

under the condition that the time evolution of a parameter-dependent quantum state

$$\psi = \psi(\alpha)$$

is governed by a Gross–Pitaevskii equation.

Typically, the considered objective functionals comprise

- the physical quantities to be minimised (observables, target states),
- the physical work for the desired outcome (time derivatives of energy functionals, integrals of certain powers up to fixed control times), and
- penalisation terms (integrals of time derivatives of control parameters).

Fundamental model (Gross–Pitaevskii equation)

Fundamental model. The time-dependent Gross–Pitaevskii equation

$$\mathrm{i}\hbar\,\partial_t\psi(x,t) = -\frac{\hbar^2}{2m}\,\Delta\psi(x,t) + W(x,t)\,\psi(x,t) + N\,g\,f\big(|\psi(x,t)|^2\big)\,\psi(x,t)$$

for the macroscopic wave function $\psi : \mathbb{R}^d \times [t_0,T] \to \mathbb{C} : (x,t) \mapsto \psi(x,t)$ involves physical parameters (particle mass and number), an external space-time-dependent potential, and a nonlinear term.

- The characteristic scattering length describes repulsive / attractive interparticle collisions and defines the coupling constant $g = \frac{4\pi\hbar^2 a}{m}$.
- Commonly, cubic $\big(f(x) = x\big)$ and quintic $\big(f(x) = x^2\big)$ nonlinearities or generalisations $\big(f(x) = x^\sigma$ with $\sigma \in (0,2]$ for $d = 3\big)$ are considered.
- Typically, the real-valued potential $W(x,t) = U(x) + \alpha(t)\,V(x)$ comprises a trapping potential (harmonic confinement) and a control potential (intensity and spatial profile of the external laser field, Gaussian-like, lattice, additional kicks).

Our approach (Specific setting)

Specific setting. The numerical solution of the optimal control problem involves a sequence of initial value problems for nonlinear Schrödinger equations with space-time-dependent potentials.

Our approach. Apply higher-order geometric numerical integrators based on commutator-free Magnus-type and operator splitting methods to obtain reliable and efficient numerical approximations.

Our approach (General setting)

General setting. The considered problems can be cast into the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\,u(t) = F\big(t, u(t)\big) = F_1\big(t, u(t)\big) + F_2\big(t, u(t)\big).$$

Our approach. Consider different classes of nonlinear evolution equations with a similar structure of the defining operators.

- Commutator-free Magnus-type integrators permit a reduction to autonomous problems (high-order approximations by evaluation at certain intermediate times and composition)

$$\frac{\mathrm{d}}{\mathrm{d}t}\,u(t) = F\big(t_*, u(t)\big) = F_1\big(t_*, u(t)\big) + F_2\big(t_*, u(t)\big).$$

- Operator splitting methods permit a reduction to subproblems of a simpler structure (high-order approximations by certain method coefficients scaling the time increment and composition)

$$\frac{\mathrm{d}}{\mathrm{d}t}\,u(t) = F_1\big(t_*, u(t)\big), \quad \frac{\mathrm{d}}{\mathrm{d}t}\,u(t) = F_2\big(t_*, u(t)\big).$$

Operator splitting methods in a nutshell

Time-dependent Gross–Pitaevskii equations and related problems
Standard and novel classes of splitting methods

Time integration methods

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.

Scope of applications

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 systems (multi-species Bose–Einstein condensates)

We obtain compact reformulations as nonlinear evolution equations 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.

Classical notation. The exact evolution operator is denoted by (indicate dependence on current time, defining operator, and initial state)

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

Standard splitting methods

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

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

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.

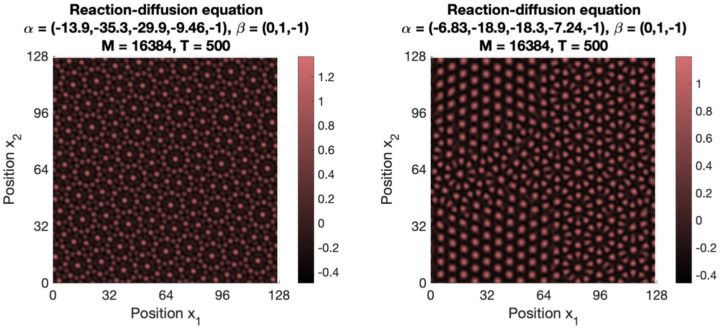
Complex operator splitting methods

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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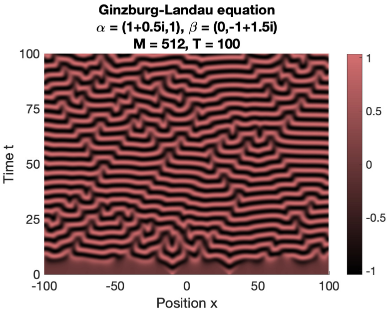
Modified operator splitting methods

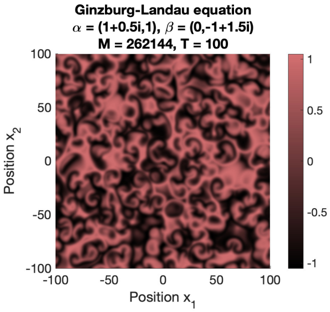
Complex Ginzburg–Landau equations
Invariance principle
Superconductivity

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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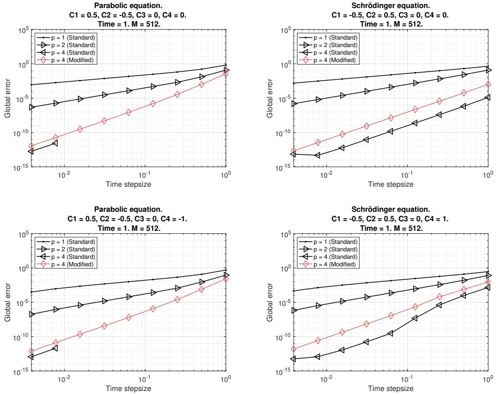
Adaptive modified operator splitting methods

Systems of coupled Gross–Pitaevskii equations
Groundstate computation, Time evolution
Multi-species Bose–Einstein condensates

Numerical experiments

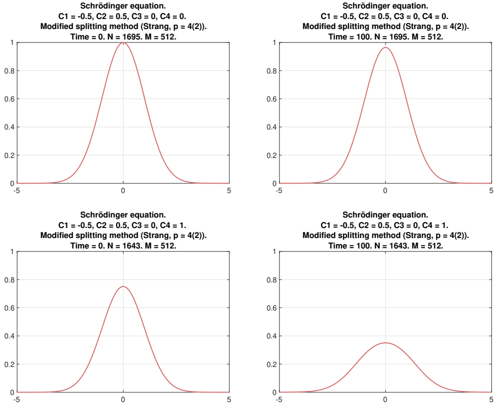
Summary. Design of a stable and efficient fourth-order exponential operator splitting method based on the incorporation of an iterated commutator.



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

Numerical experiments

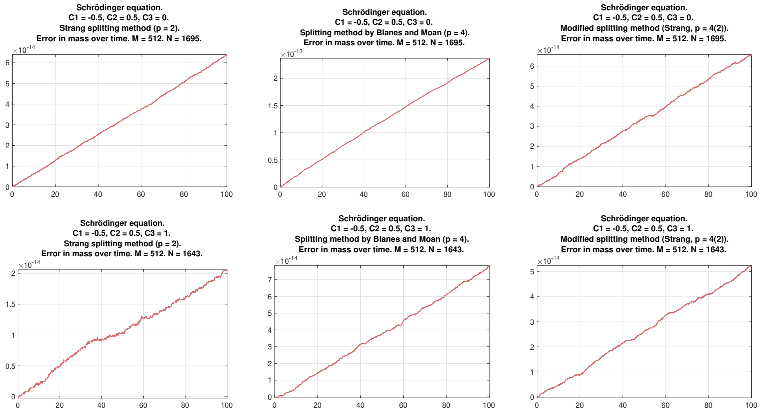
Questions. Favourable behaviour of a fourth-order modified operator splitting method for linear and nonlinear Schrödinger-type equations over longer times? Benefits of a simple local error control based on the second-order Strang splitting method?



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

Numerical experiments

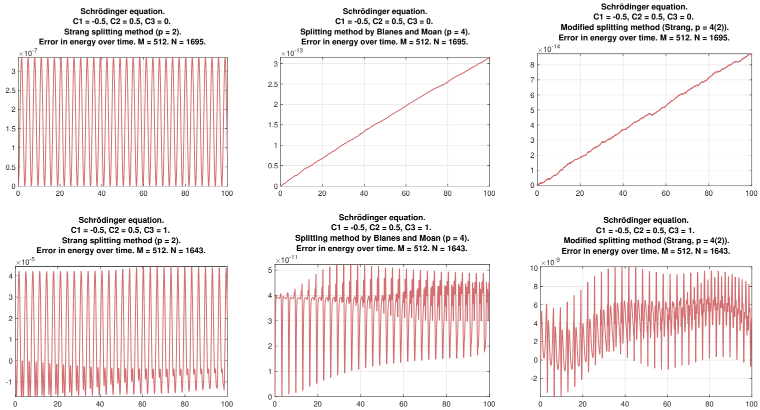
Summary. Mass preservation of a fourth-order modified operator splitting method for linear and nonlinear Schrödinger equations over longer times.



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

Numerical experiments

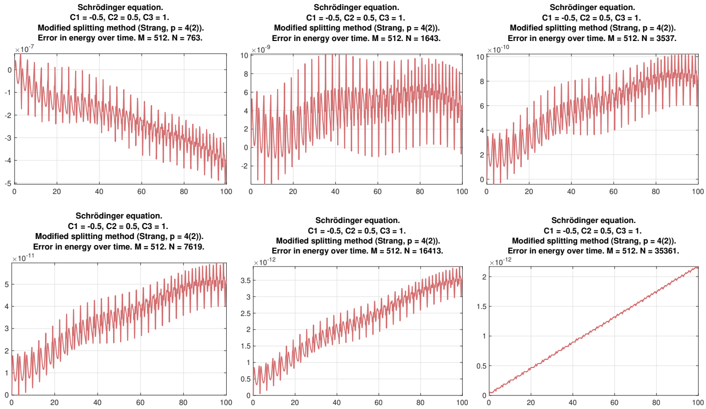
Summary. Energy preservation of a fourth-order modified operator splitting method for linear and nonlinear Schrödinger equations over longer times.



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

Numerical experiments

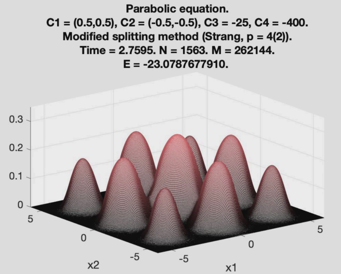
Observation. Improved energy preservation for lower tolerances. Rigorous analysis?



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. 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

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

Summary. Our theoretical results and numerical experiments confirm the benefits of complex splitting methods for reaction-diffusion equations and (adaptive) modified splitting methods for Ginzburg–Landau-type equations and systems of Gross–Pitaevskii equations.

On the way towards the numerical approximation of quantum control systems, we gain new insight, but also take some mountain trails ...

Thank you very much!

Optimal control problem

Optimal control problem. The first-order optimality conditions read as (for notational simplicity, set $d = \sigma = 1$)

$$\frac{\mathrm{d}}{\mathrm{d}t}\Big(\alpha'(t)\,\big(\gamma_1\,\big(V\,\psi(\cdot,t)\big|\psi(\cdot,t)\big)_{L^2}^2+\gamma_2\big)\Big)=\tfrac{1}{2}\,\Re\big(V\,\psi(\cdot,t)\big|\varphi(\cdot,t)\big)_{L^2}\,,$$

$$\mathrm{i}\,\partial_t\psi(x,t)=-\tfrac{1}{2}\,\partial_{xx}\,\psi(x,t)+\big(U(x)+\alpha(t)\,V(x)\big)\,\psi(x,t)+\vartheta\,|\psi(x,t)|^2\,\psi(x,t)\,,$$

$$\mathrm{i}\,\partial_t\varphi(x,t)=-\tfrac{1}{2}\,\partial_{xx}\,\varphi(x,t)+\big(U(x)+\alpha(t)\,V(x)\big)\,\varphi(x,t)+2\,\vartheta\,|\psi(x,t)|^2\,\varphi(x,t)$$
$$+\,\vartheta\,\big(\psi(x,t)\big)^2\,\varphi(x,t)+4\,\gamma_1\,\alpha'(t)^2\,\big(V\,\psi(\cdot,t)\big|\psi(\cdot,t)\big)_{L^2}\,V(x)\,\psi(x,t)\,,$$

$$\alpha(0)\,,\psi(x,0)\ \text{ given}\,,$$

$$\alpha'(T)=0\,,\quad \varphi(x,T)=4\,\mathrm{i}\,\big(\psi(\cdot,T)\big|A_0\psi(\cdot,T)\big)_{L^2}\,A_0\psi(x,T)\,.$$