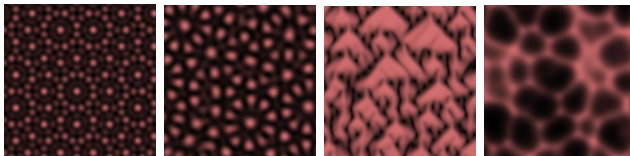


Splitting methods for nonlinear evolution equations

Mechthild Thalhammer
Leopold-Franzens-Universität Innsbruck, Austria



Conference on the Numerical Solution of
Differential and Differential-Algebraic Equations
Numdiff-17, Halle, Germany, September 2024

Acknowledgements

Acknowledgements. The contents of this talk are based on recent and current investigations in collaboration with

- Sergio Blanes (Valencia, Spain),
- Fernando Casas (Castellón, Spain),
- Cesáreo González (Valladolid, Spain).

Additional inspiration comes from joint research activities with

- Barbara Kaltenbacher (Klagenfurt, Austria),
- José Antonio Carrillo (Oxford, United Kingdom).

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.

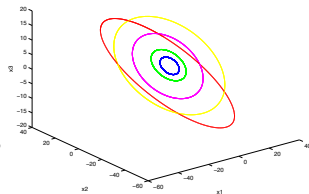
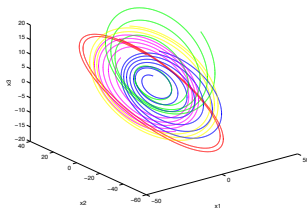
- Exponential operator splitting methods are appropriate for a broad variety of **relevant applications**.
- This includes **Hamiltonian systems** (classical mechanics) as well as **Schrödinger equations** (quantum mechanics), where the advantages of geometric numerical integrators become apparent.
- 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).

Intermezzo: Thanks for the excursion to the planetarium! :-)

Splitting methods are appropriate for the simulation of Hamiltonian systems such as the **outer solar system** (Lecture notes 2012/13 based on the monograph **Geometric Numerical Integration** by Lubich, Hairer, Wanner, 2006).

(ii) Numerische Lösung des Äußeren Sonnensystems (Sechskörperproblem) mittels verschiedener Einschrittverfahren, vgl. Buch (Abbildung 2.4).

- Explizites Eulerverfahren
(Spiralen nach außen, Schlechte Erhaltung der Hamiltonfunktion)
- Symplektische Eulerverfahren (Lie-Trotter-Splittingverfahren), Störmer-Verlet-Verfahren (Strang-Splittingverfahren)
(Zufriedenstellende Resultate)



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**

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

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

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

we obtain compact reformulations as nonlinear evolution equations

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

which indicate natural decompositions into two subproblems.

Splitting approach

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

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

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

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

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

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

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

Alternative notation. The alternative **formal notation**

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

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)

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

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

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

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** 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**

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

have **similar structures**.

- **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 ($K = 4 = \tilde{K} + 1$)

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

Complex operator splitting methods

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

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

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

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

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

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

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

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

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

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

Stability analysis

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

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

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

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

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

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

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

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

Stability analysis

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

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

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 $A: D(A) \subseteq X \rightarrow X$ generating an analytic semigroup $(\mathcal{E}_{t,A})_{t \in [t_0, T]}$ on a Banach space and a nonlinear operator $B: D(B) \subseteq X \rightarrow X$,
- 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 $\|\mathcal{E}_{t,a_j A}\|_{X \leftarrow X} \leq e^{C_1 t}$ hold for $t \in [t_0, T]$ and $j \in \{1, \dots, s\}$,
- the iterated commutators arising in the local error expansion $\|\text{ad}_A^\ell(B)\|_{X \leftarrow D} \leq C_2$ 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

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

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.

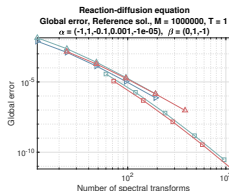
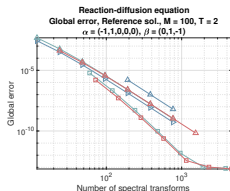
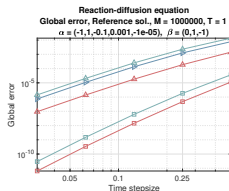
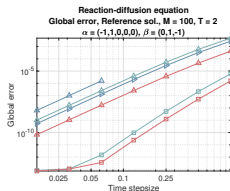
- The performed numerical experiments confirm the theoretical **stability** and **global error analysis**.

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

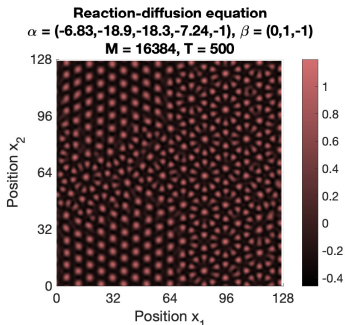
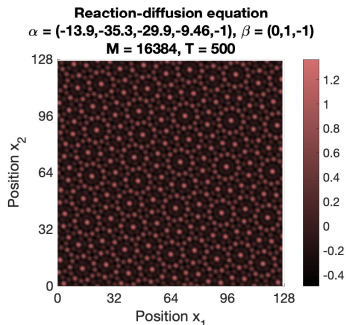
Summary. Design of **stable** and **efficient** sixth-order exponential operator splitting methods based on the incorporation of **complex coefficients**.



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**.



techmath.uibk.ac.at/mecht/MyHomepage/Research/Movie2024Quasicrystal1.m4v
techmath.uibk.ac.at/mecht/MyHomepage/Research/Movie2024Quasicrystal2.m4v

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

$$[B, [B, A]] = B^2 A - 2BAB + AB^2,$$

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

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

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

Linear case

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

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

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

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

Linear case

Operator splitting methods.

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

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

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**

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

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***

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

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

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

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

$$\begin{aligned} \frac{d}{dt} u(t) &= bF_2(u(t)) + c\tau_n^2 G(u(t)), \quad t \in [t_n, t_n + \tau_n], \\ G &= F_1'' F_2 F_2 + F_1' F_2' F_2 + F_2' F_2' F_1 - F_2'' F_1 F_2 - 2F_2' F_1' F_2. \end{aligned}$$

Nonlinear case

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

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

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

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

Specification

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

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

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

$$G = G_1 + G_2 + G_3 + G_4,$$

$$G_1(v) = 4\Re(\beta_1)\beta_2(-\Re(\alpha_2)|v|^2v + 2\alpha_1|\nabla v|^2v + i\Im(\alpha_1)\overline{\Delta v}v^2 + \alpha_1\nabla v \cdot \nabla v\bar{v})V,$$

$$G_2(v) = 2\left(\alpha_1\beta_1^2\nabla V + 4\alpha_1\Re(\beta_1)\beta_2\nabla v\bar{v} + (3\alpha_1\beta_1 + \alpha_1\bar{\beta}_1 - 2\bar{\alpha}_1\bar{\beta}_1)\beta_2\overline{\nabla v}v\right) \cdot \nabla Vv,$$

$$G_3(v) = -2(i\alpha_1\Im(\beta_1) + \bar{\alpha}_1\bar{\beta}_1)\beta_2\Delta V|v|^2v + 2\alpha_1(2\beta_2^2 + 3|\beta_2|^2)\nabla v \cdot \nabla v\bar{v}^2v,$$

$$G_4(v) = 4(2\alpha_1\beta_2^2 + 3\alpha_1|\beta_2|^2 - 2\bar{\alpha}_1|\beta_2|^2)|\nabla v|^2|v|^2v + 2(2\alpha_1\beta_2^2 + \alpha_1|\beta_2|^2 - 2\bar{\alpha}_1|\beta_2|^2)\overline{\nabla v} \cdot \overline{\nabla v}v^3 + 8i\Im(\alpha_1)|\beta_2|^2\Re(\Delta v\bar{v})|v|^2v.$$

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

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

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

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

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**

$$\begin{cases} \frac{d}{dt} u(t) = i \left(f_1(u(t)) + \tau_n^2 f_2(u(t)) \right) u(t), \\ u(t_n) = u_n, \quad t \in [t_n, t_n + \tau_n], \end{cases}$$

satisfies the invariance principle

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

Proof. Verify the identity

$$\frac{d}{dt} \left(f_1(u(t)) + \tau_n^2 f_2(u(t)) \right) = 0, \quad t \in [t_n, t_n + \tau_n].$$

Invariance principle

Summary. The **realisation** of the **modified** operator splitting method

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

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

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

and **pointwise evaluations** of **solution representations** of the form

$$\mathcal{E}_{\tau_n, bF_2 + c\tau_n^2 G}(u_n) = e^{i\tau_n(bf_1(u_n) + c\tau_n^2 f_2(u_n))} u_n, \quad \tau_n \in \mathbb{R}.$$

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** ($u' = bF_2(u) + c\tau^2 G(u)$) and the knowledge of the **exact solution** ($u' = bF_2(u)$) 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, \bar{u}) . Otherwise, **significant order reductions** are encountered!

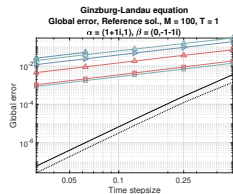
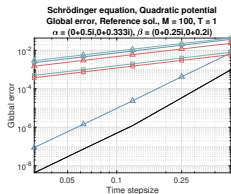
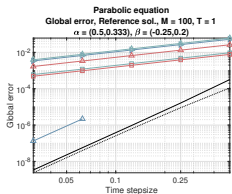
Numerical experiments

-  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

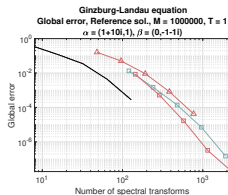
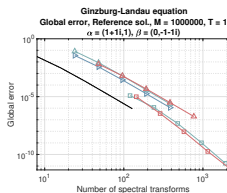
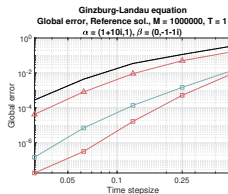
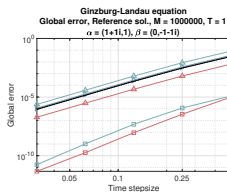
Observations.

- 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

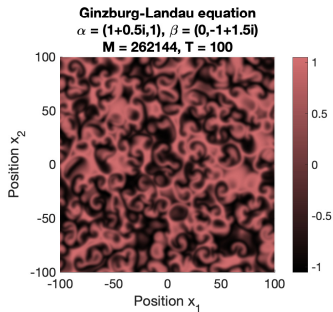
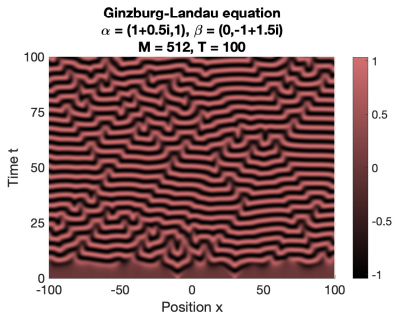
Summary. Design and practical implementation of stable and efficient fourth-order operator splitting methods for complex Ginzburg–Landau-type equations based on the incorporation of iterated commutators.



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

Numerical experiments

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



techmath.uibk.ac.at/mecht/MyHomepage/Research/Movie2024GinzburgLandau1.m4v
techmath.uibk.ac.at/mecht/MyHomepage/Research/Movie2024GinzburgLandau2.m4v

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

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

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

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

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

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

by incorporating a **processor** (corrector)

$$\begin{aligned} u_n &= \left((\mathcal{P}_{\tau,F}^{-1} \circ \mathcal{S}_{\tau,F} \circ \mathcal{P}_{\tau,F}) \circ \dots \circ (\mathcal{P}_{\tau,F}^{-1} \circ \mathcal{S}_{\tau,F} \circ \mathcal{P}_{\tau,F}) \right) (u_0) \\ &= (\mathcal{P}_{\tau,F}^{-1} \circ \mathcal{S}_{\tau,F}^n \circ \mathcal{P}_{\tau,F}) (u_0). \end{aligned}$$

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

$$\begin{aligned} \frac{d}{dt} u(t) &= A u(t) + B(u(t)), \quad t \in [t_0, T], \\ \mathcal{S}_{\tau, F} &= \mathcal{E}_{\tau, \frac{1}{2}A} \circ \mathcal{E}_{\tau, B - \frac{1}{24}\tau^2 G} \circ \mathcal{E}_{\tau, \frac{1}{2}A}, \\ \mathcal{P} &: (\tilde{a}_4, \tilde{b}_3, \tilde{a}_3, \tilde{b}_2, \tilde{a}_2, \tilde{b}_1), \quad \mathcal{P}^{-1} : -(\tilde{b}_1, \tilde{a}_2, \tilde{b}_2, \tilde{a}_3, \tilde{b}_3, \tilde{a}_4), \quad \tilde{a}_3 = \tilde{a}_2. \end{aligned}$$

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, $p = 4$, $s = 1$)

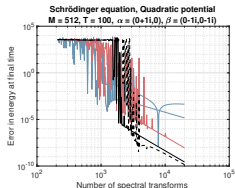
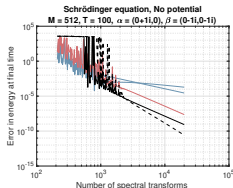
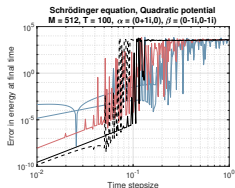
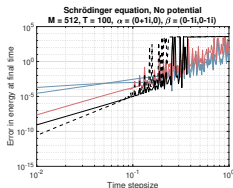
Numerical experiments

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.



techmath.uibk.ac.at/mecht/MyHomepage/Research/Movie2024Resonances2.m4v
techmath.uibk.ac.at/mecht/MyHomepage/Research/Movie2024Resonances3.m4v