Modified operator splitting methods for nonlinear evolution equations of parabolic and Schrödinger type

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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.
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Nonlinear evolution equations

Nonlinear evolution equations

General formulation. We consider nonlinear evolution equations that permit a natural decomposition into two subproblems

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = F_1\big(u(t)\big) + F_2\big(u(t)\big)\,, \\ u(0) = u_0\,, \qquad t \in [0, T]\,. \end{cases}$$

Nonlinear evolution equations

Nonlinear Schrödinger equation. We consider the time-dependent Gross–Pitaevskii equation (GPE) describing a Bose–Einstein condensate

$$\begin{cases} \mathrm{i}\,\partial_t \Psi(x,t) = -\Delta\Psi(x,t) + V(x)\,\Psi(x,t) + \vartheta\,|\Psi(x,t)|^2\,\Psi(x,t)\,, \\ \Psi(x,0) = \Psi_0(x)\,, \quad (x,t) \in \Omega \times [0,T]\,. \end{cases}$$

General formulation. We obtain the above formulation by setting

$$u(t) = \Psi(\cdot,t)\,, \quad t \in [0,T]\,,$$

and assigning for regular complex-valued functions $v:\Omega \to \mathbb{C}$ the linear differential and nonlinear multiplication operators

$$\begin{gathered} \big(F_1(v)\big)(x) = c\,\Delta\, v(x)\,, \quad c = \mathrm{i}\,, \\ \big(F_2(v)\big)(x) = \overline{c}\,\big(V(x) + \vartheta\,|v(x)|^2\big)\,v(x)\,, \quad \overline{c} = -\mathrm{i}\,, \\ x \in \Omega\,. \end{gathered}$$

Nonlinear evolution equations

Nonlinear parabolic equation. By analogy to the GPE, we consider

$$\begin{cases} \partial_t U(x,t) = \Delta U(x,t) + V(x)\, U(x,t) + \vartheta\, |U(x,t)|^2\, U(x,t)\,, \\ U(x,0) = U_0(x)\,, \quad (x,t) \in \Omega \times [0,T]\,. \end{cases}$$

General formulation. We obtain the above formulation by setting

$$u(t) = U(\cdot,t)\,, \quad t \in [0,T]\,,$$

and assigning for regular real-valued functions $v : \Omega \to \mathbb{R}$ the linear differential and nonlinear multiplication operators

$$\begin{gathered} \big(F_1(v)\big)(x) = c\,\Delta\, v(x)\,, \quad c = 1\,, \\ \big(F_2(v)\big)(x) = \overline{c}\,\big(V(x) + \vartheta\,|v(x)|^2\big)\, v(x)\,, \quad \overline{c} = 1\,, \\ x \in \Omega\,. \end{gathered}$$

Operator splitting methods

Operator splitting methods

Standard approach. Standard operator splitting methods 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. The excellent behaviour of (optimised) splitting methods (stability, accuracy, preservation of conserved quantities) has been confirmed by a variety of contributions.

Operator splitting methods

Alternative approach. We propose a favourable alternative to standard operator splitting methods for settings, where the operator F_2 and the iterated commutator

$$G_2(v) = F_1''(v)\,F_2(v)\,F_2(v) + F_1'(v)\,F_2'(v)\,F_2(v) + F_2'(v)\,F_2'(v)\,F_1(v) \\ - F_2''(v)\,F_1(v)\,F_2(v) - 2\,F_2'(v)\,F_1'(v)\,F_2(v)$$

have a similar structure.

Scope of applications.

- **Model problems.** Relevant applications include the time evolution and imaginary time propagation of GPEs.
- **Extensions.** The approach applies to complex Ginzburg–Landau equations and high-order semilinear parabolic equations (quasicrystalline patterns).

Fundamental means

Basic idea

Basic idea. An educated guess leads us to the class of modified operator splitting methods. In essence, we exploit a formal generalisation of the linear case by the calculus of Lie derivatives.

Specification. For simplicity, we focus on the extension of Chin's fourth-order modified potential operator splitting method (1997) to nonlinear evolution equations.

Linear case

Linear ordinary differential equations. Our starting point is a (large) system of linear ordinary differential equations (defined by non-commuting square matrices)

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

The corresponding solution value at the final time is given by the matrix exponential, that is

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

Linear case

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

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

suitably chosen real coefficients $b, c \in \mathbb{R}$.

The underlying idea of this alternative approach is to gain freedom in the adjustment of the method coefficients and, amongst others, to overcome an order barrier that is valid for standard splitting methods.

Linear case

Linear partial differential equations. Advantages of modified potential operator splitting methods become apparent in the context of the imaginary time propagation of linear Schrödinger equations. In this setting, the operators A and B correspond to the Laplacian and a potential, and hence the iterated commutator

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

reduces to a multiplication operator, which is defined by the gradient of the potential.

- In Chin's words: 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*.
- This explains the common notion *force-gradient operator splitting method* or *modified potential operator splitting method*.

Nonlinear case

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

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

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

is replaced by the solution to the nonlinear evolution equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = b\,F_2\big(u(t)\big) + c\,\tau^2\, G_2\big(u(t)\big), \quad t \in [0,\tau],$$

involving the iterated commutator

$$\begin{aligned} G_2(v) = {} & F_1''(v)\,F_2(v)\,F_2(v) + F_1'(v)\,F_2'(v)\,F_2(v) + F_2'(v)\,F_2'(v)\,F_1(v) \\ & - F_2''(v)\,F_1(v)\,F_2(v) - 2\,F_2'(v)\,F_1'(v)\,F_2(v)\,. \end{aligned}$$

Nonlinear case

- Denoting the exact evolution operators associated with the two subproblems by

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u_j(t) = \alpha F_j\big(u_j(t)\big), \quad \mathscr{E}_{\tau,\alpha F_j}\big(u_j(t_n)\big) = u_j(t_n+\tau),$$

the extension of Chin's scheme

$$u_{n+1} = \mathrm{e}^{\frac{1}{6}\tau B}\,\mathrm{e}^{\frac{1}{2}\tau A}\,\mathrm{e}^{\frac{2}{3}\tau B - \frac{1}{72}\tau^3 [B,[B,A]]}\,\mathrm{e}^{\frac{1}{2}\tau A}\,\mathrm{e}^{\frac{1}{6}\tau B}\, u_n \approx u(t_{n+1}),$$
$$n \in \{0,1,\dots,N-1\}.$$

to the nonlinear case reads as

$$u_{n+1} = \big(\mathscr{E}_{\tau,\frac{1}{6}F_2} \circ \mathscr{E}_{\tau,\frac{1}{2}F_1} \circ \mathscr{E}_{\tau,\frac{2}{3}F_2 - \frac{1}{72}\tau^2 G_2} \circ \mathscr{E}_{\tau,\frac{1}{2}F_1} \circ \mathscr{E}_{\tau,\frac{1}{6}F_2}\big)\, u_n \approx u(t_{n+1}),$$
$$n \in \{0,1,\dots,N-1\}.$$

Nonlinear case

- For the model problems of parabolic and Schrödinger type, the iterated commutators are given by multiplication operators involving first- and second-order space derivatives of the potential and the current solution value

$$G_2(v) = 2\big((\nabla V)^T(\nabla V) + \vartheta\,\widetilde{G}_2(v)\big)\,v\,,$$
$$\widetilde{G}_2(v) = -\Delta V\,v^2 + 6\,(\nabla V)^T(\nabla v)\,v + 6\big(V + 2\,\vartheta\,v^2\big)\,(\nabla v)^T(\nabla v)\,,$$

$$G_2(v) = -2\,\mathrm{i}\Big((\nabla V)^T(\nabla V) - 2\,\vartheta\big(\widetilde{G}_{21}(v) + \vartheta\,\widetilde{G}_{22}(v)\big)\Big)\,v\,,$$
$$\widetilde{G}_{21}(v) = |v|^2\,\Delta V\,,$$
$$\widetilde{G}_{22}(v) = |v|^2\,\big(2\,\Re(\bar{v}\,\Delta v) + 3\,(\nabla\bar{v})^T(\nabla v)\big) + \Re\big(\bar{v}^2\,(\nabla v)^T(\nabla v)\big)\,.$$

Invariance principle

Invariance principle

Schrödinger case. A fundamental invariance principle that holds for standard operator splitting methods applied to the GPE (magically) extends to modified operator splitting methods.

Theorem. The solution to the nonlinear subproblem

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = -\mathrm{i}\, f\big(u(t)\big)\, u(t)\,, \\ u(0) = u_0\,, \quad t \in [0,\tau]\,, \end{cases}$$

satisfies the invariance principle

$$f\big(u(t)\big) = f(u_0)\,, \quad t \in [0,\tau]\,.$$

Invariance principle

Sketch of the proof. Exploit the structure of the components

$$f(v) = \beta_1 f_1(v) + \beta_2 \tau^2 f_2(v),$$
$$F_2(v) = \overline{c}\, f_1(v)\, v, \quad G_2(v) = \overline{c}\, f_2(v)\, v,$$
$$f_1(v) = V + \vartheta\, g_1(v), \quad f_2(v) = 2\,(\nabla V)^T (\nabla V) - 4\,\vartheta\, g_6(v),$$
$$g_1(v) = |v|^2, \quad g_2(v) = \Re(\bar{v}\,\Delta v),$$
$$g_3(v) = (\nabla \bar{v})^T (\nabla v), \quad g_4(v) = \Re\big(\bar{v}^2\,(\nabla v)^T (\nabla v)\big),$$
$$g_5(v) = \vartheta\,\big(2\,g_2(v) + 3\,g_3(v)\big), \quad g_6(v) = g_1(v)\,\big(\Delta V + g_5(v)\big) + \vartheta\, g_4(v),$$

and confirm the identity

$$\frac{\mathrm{d}}{\mathrm{d}t}\, f\big(u(t)\big) = 0, \quad t \in [0, \tau].$$

Invariance principle

Summary. The realisation of the modified operator splitting method

$$u_{n+1} = \left(\mathscr{E}_{\tau,\frac{1}{6}F_2} \circ \mathscr{E}_{\tau,\frac{1}{2}F_1} \circ \mathscr{E}_{\tau,\frac{2}{3}F_2-\frac{1}{72}\tau^2 G_2} \circ \mathscr{E}_{\tau,\frac{1}{2}F_1} \circ \mathscr{E}_{\tau,\frac{1}{6}F_2}\right) u_n\,, \quad n \in \{0,1,\dots,N-1\}\,,$$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = \mathrm{i}\,\alpha\,\Delta u(t)\,, \quad t \in [t_n, t_n+\tau]\,, \quad \mathscr{E}_{\tau,\alpha F_1}\big(u(t_n)\big) = u(t_n+\tau)\,,$$

and the pointwise evaluation of the solution representation

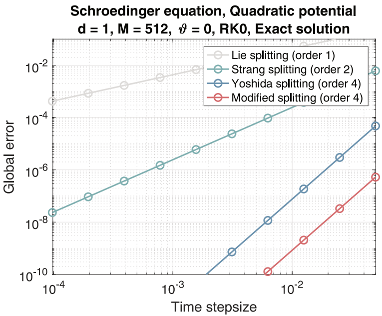
$$\mathscr{E}_{\tau,\beta_1 F_2+\beta_2\tau^2 G_2}(u_0) = \mathrm{e}^{-\mathrm{i}\,\tau(\beta_1 f_1(u_0)+\beta_2\tau^2 f_2(u_0))}\, u_0\,, \quad \tau \in \mathbb{R}\,.$$

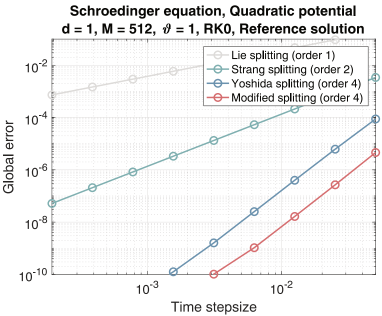
Numerical experiments

Numerical experiments

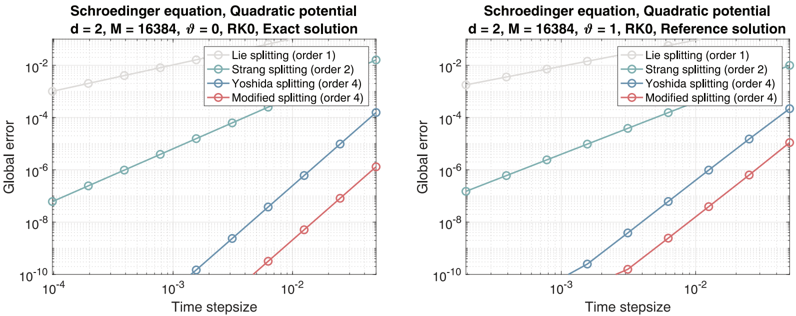
- Time integration of the Gross–Pitaevskii equation involving a quadratic potential by standard operator splitting methods and the novel modified operator splitting method.
- Global errors versus time stepsizes in space dimensions $d \in \{1,2,3\}$.
- Nonlinear $(\vartheta = 1)$ versus simplified linear $(\vartheta = 0)$ case.
- Due to the validity of the invariance principle, the application of an explicit Runge–Kutta method is not needed (RK0).

Numerical experiments

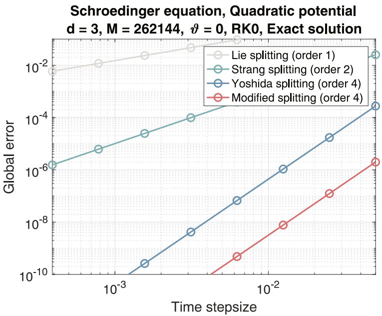


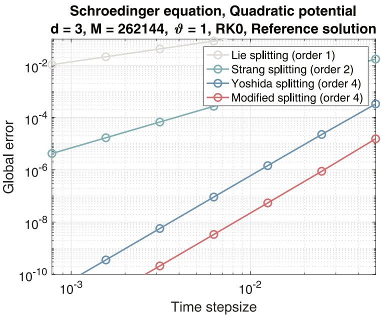


Numerical experiments



Numerical experiments

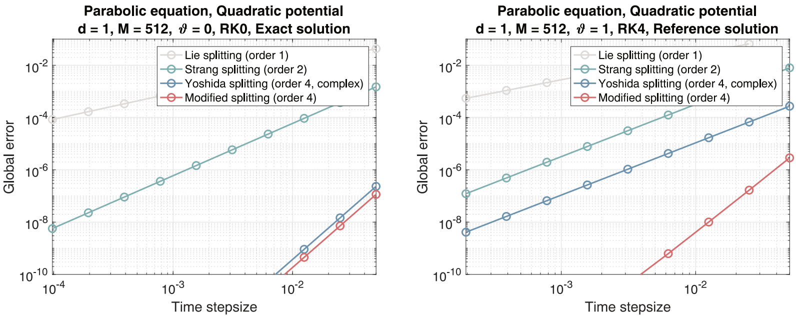




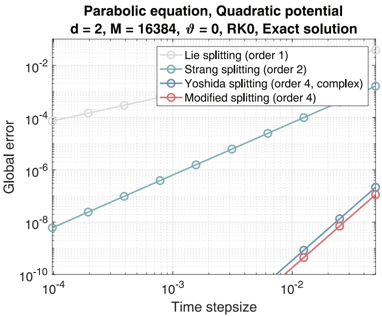
Numerical experiments

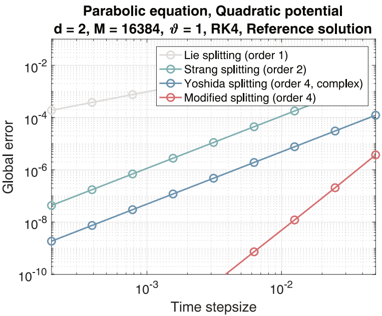
- Time integration of the parabolic problem involving a quadratic potential by standard splitting methods and the novel modified operator splitting method.
- Global errors versus time stepsizes in space dimensions $d \in \{1,2,3\}$.
- Nonlinear $(\vartheta = 1)$ versus simplified linear $(\vartheta = 0)$ case.
- In order to resolve the nonlinear subproblem, a fourth-order explicit Runge–Kutta method is applied (RK4).
- Depending on the stiffness of the equation, stability is ensured for sufficiently small time stepsizes.
- For a naive implementation of the Yoshida splitting method with complex coefficients, an order reduction is observed.

Numerical experiments

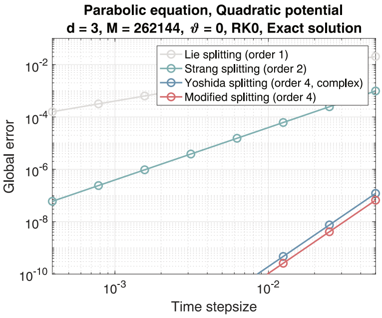


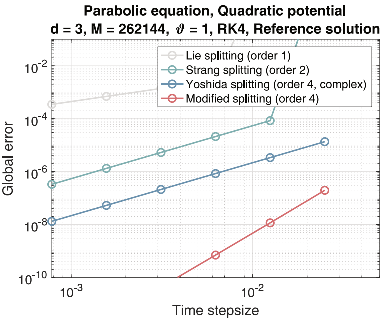
Numerical experiments





Numerical experiments



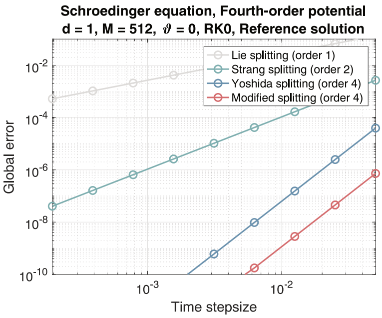


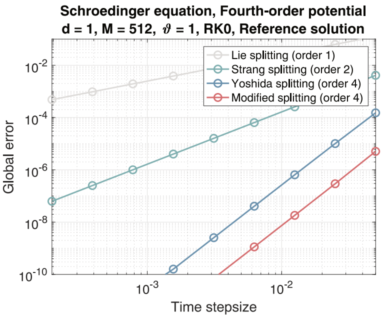
Further numerical experiments

Numerical experiments

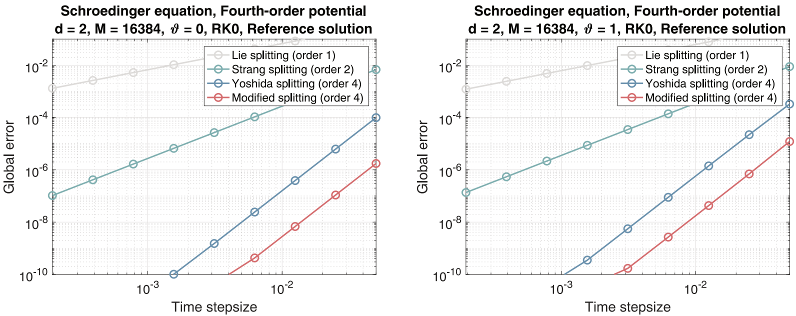
Corresponding results for the time-dependent Gross–Pitaevskii equation involving a fourth-order polynomial potential.

Numerical experiments

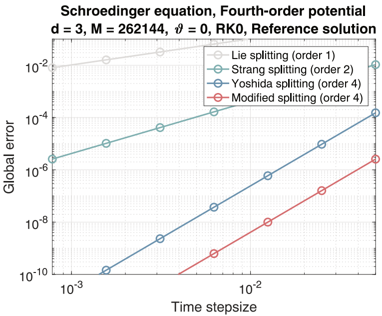


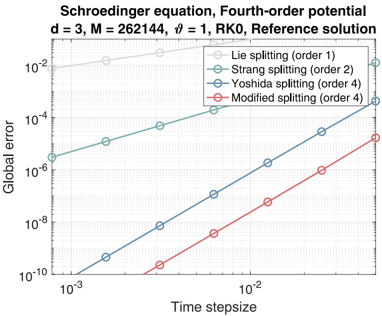


Numerical experiments



Numerical experiments

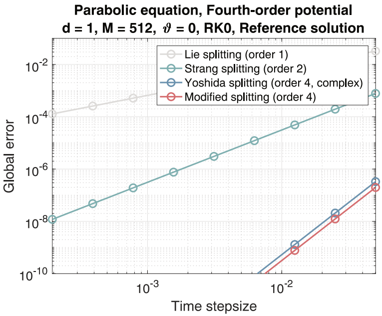


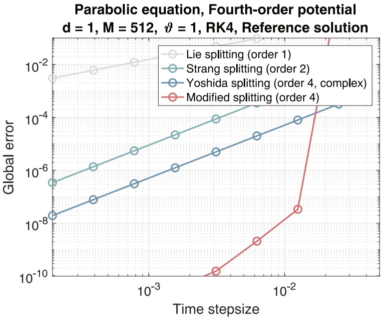


Numerical experiments

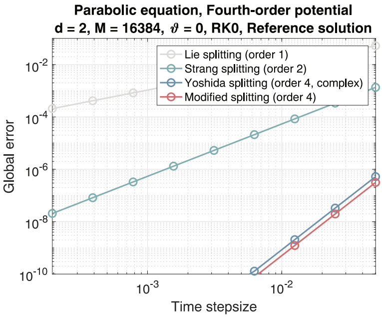
Corresponding results for the parabolic problem involving a fourth-order polynomial potential.

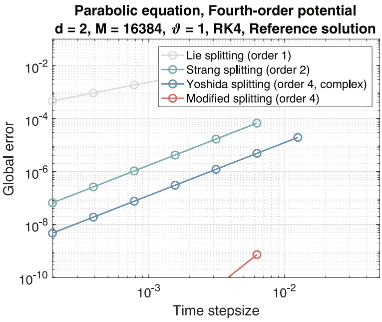
Numerical experiments



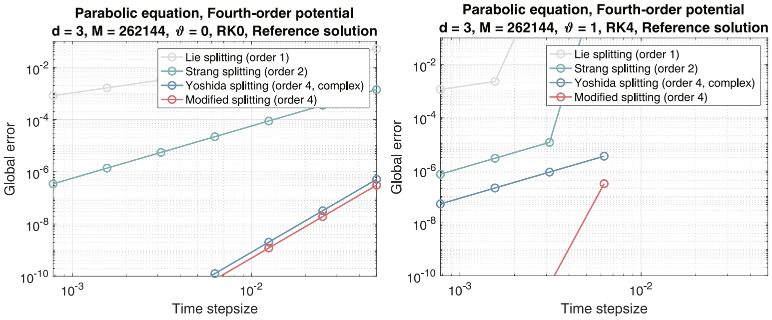


Numerical experiments





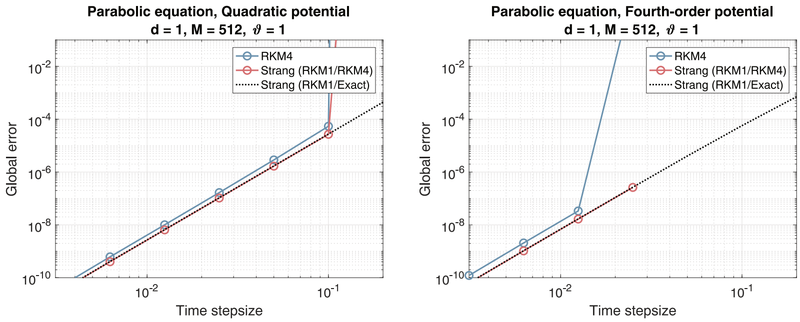
Numerical experiments



Numerical experiments

- Time integration of the one-dimensional parabolic equation involving a quadratic potential (left) or a fourth-order potential (right), respectively, by the modified operator splitting method.
- Global errors versus time stepsizes.
- The original approach is based on the application of an explicit fourth-order Runge–Kutta method for the numerical solution of the nonlinear subproblem involving the double commutator $\mathcal{E}_{\tau, \frac{2}{3} F_2 - \frac{1}{72}\tau^2 G_2}$.
- Alternative approaches are based on the Strang splitting method $\mathcal{E}_{\frac{1}{2}\tau, \frac{2}{3} F_2} \circ \mathcal{E}_{\tau, -\frac{1}{72}\tau^2 G_2} \circ \mathcal{E}_{\frac{1}{2}\tau, \frac{2}{3} F_2}$. Here, a reduced number of (inverse) fast Fourier transforms is required and an improved accuracy is observed. Furthermore, the knowledge of the exact solution to the component $\mathcal{E}_{\frac{1}{2}\tau, \frac{2}{3} F_2}$ enhances the stability behaviour of the resulting time integration method for larger time increments.

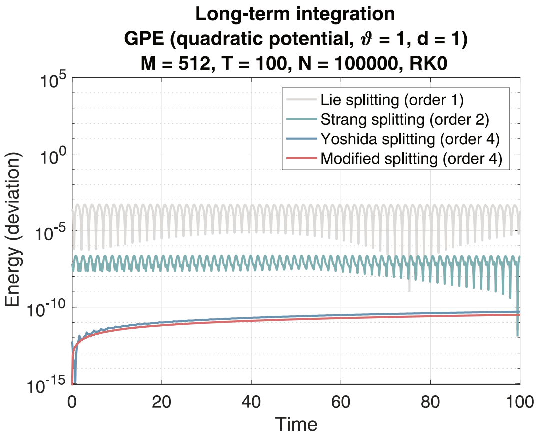
Numerical experiments



Numerical experiments

- Long-term integration of the one-dimensional Gross–Pitaevskii equation by standard and modified operator splitting methods.
- Computation of numerical approximations to the values of the energy at time grid points $t_n = n\tau$ for $\tau = 10^{-3}$ and $n \in \{0, 1, \dots, 10^5\}$ as well as corresponding deviations with respect to the minimal values.
- The obtained results confirm the favourable geometric properties of the modified operator splitting method.

Numerical experiments



Conclusions and future work

Conclusions and future work

Summary.

- Introduction of a general framework for the extension of Chin's fourth-order modified potential operator splitting method to nonlinear evolution equations.
- Specification of the resulting fourth-order modified operator splitting method for the time-dependent Gross–Pitaevskii equation and its parabolic counterpart.

Conclusions and future work

Future work.

- Rigorous analysis (stability, error) of modified operator splitting methods applied to the time-dependent Gross–Pitaevskii equation and its parabolic analogue.
- Extensions of modified operator splitting methods to complex Ginzburg–Landau equations and higher-order reaction-diffusion equations with pattern formation describing quasicrystals.
- Design of high-order modified operator splitting methods for nonlinear evolution equations that are optimal with regard to a preselected criterium such as efficiency.

Thank you very much!