Commutator-free Magnus integrators combined with operator splitting methods and their areas of application

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Recent Contributions of Women to PDEs
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First remarks on commutator-free Magnus integrators for linear evolution equations

Commutator-free Magnus integrators

Approach. Analysis and design of commutator-free Magnus integrators for time integration of non-autonomous linear evolution equations

$$\begin{cases} u'(t) = A(t)\, u(t)\,, \quad t \in (t_0, T)\,, \\ u(t_0) \text{ given}\,, \end{cases}$$

$$t_0 < t_1 < \cdots < t_n < t_{n+1} < \cdots < t_N = T\,, \quad \tau_n = t_{n+1} - t_n\,,$$

$$u_{n+1} = \mathscr{S}(\tau_n, t_n)\, u_n \approx u(t_{n+1}) = \mathscr{E}(\tau_n, t_n)\, u(t_n)\,,$$

$$\mathscr{S}(\tau_n, t_n) = \mathrm{e}^{\tau_n B_{nJ}(\tau_n)} \cdots \mathrm{e}^{\tau_n B_{n1}(\tau_n)}\,,$$

$$B_{nj}(\tau_n) = \sum_{k=1}^{K} a_{jk}\, A(t_n + c_k \tau_n)\,.$$

Example. Second-order (commutator-free) Magnus integrator (first step)

$$\mathrm{e}^{\tau A(t_0 + \frac{\tau}{2})}\, u_0 \approx u(t_0 + \tau)\,.$$

Areas of application

Situation. Consider non-autonomous linear evolution equation

$$u'(t) = A(t)\,u(t)\,, \quad t \in (t_0, T)\,.$$

Areas of application.

- **Quantum systems**

  Models for oxide solar cells (with W. Auzinger, K. Held, O. Koch)

  Linear evolution equations of Schrödinger type

  Linear Schrödinger equations involving time-dependent potential

- **Dissipative quantum systems**

  Rosen–Zener models with dissipation

  Linear evolution equations of parabolic type

  Variational equations related to diffusion-advection-reaction equations

First illustration (Parabolic equation)

Test equation. Consider nonlinear diffusion-advection-reaction equation

$$\partial_t U(x,t) = f_2\big(U(x,t)\big)\,\partial_{xx} U(x,t) + f_1\big(U(x,t)\big)\,\partial_x U(x,t) + f_0\big(U(x,t)\big) + g(x,t)\,.$$

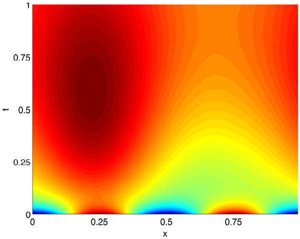
Associated variational equation has form of non-autonomous linear evolution equation

$$\partial_t u(x,t) = \alpha_2(x,t)\,\partial_{xx} u(x,t) + \alpha_1(x,t)\,\partial_x u(x,t) + \alpha_0(x,t)\,u(x,t)\,.$$

Impose periodic boundary conditions and regular initial condition.

Special choice. In particular, set

$$(x,t) \in \Omega \times [0,T]\,, \quad \Omega = [0,1]\,, \quad T = 1\,,$$
$$U(x,t) = \mathrm{e}^{-t} \sin(2\pi x)\,, \quad u(x,0) = \big(\sin(2\pi x)\big)^2\,,$$
$$f_2(w) = \tfrac{1}{10}\big(\cos(w) + \tfrac{11}{10}\big)\,, \quad f_1(w) = \tfrac{1}{10}\,w\,, \quad f_0(w) = w\big(w - \tfrac{1}{2}\big)\,,$$
$$\alpha_2(x,t) = f_2\big(U(x,t)\big)\,, \quad \alpha_1(x,t) = f_1\big(U(x,t)\big)\,,$$
$$\alpha_0(x,t) = f_2'\big(U(x,t)\big)\,\partial_{xx} U(x,t) + f_1'\big(U(x,t)\big)\,\partial_x U(x,t) + f_0'\big(U(x,t)\big)\,.$$



First illustration (Parabolic equation)

Test equation. Consider non-autonomous linear evolution equation of parabolic type

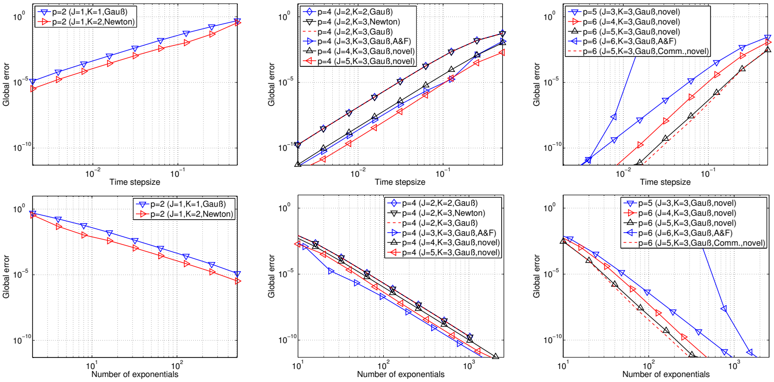
$$\partial_t u(x,t) = \alpha_2(x,t)\,\partial_{xx} u(x,t) + \alpha_1(x,t)\,\partial_x u(x,t) + \alpha_0(x,t)\,u(x,t)\,.$$

Impose periodic boundary conditions and regular initial condition.

Time integration. Apply commutator-free Magnus integrators and related method of non-stiff orders $p = 2, 4, 5, 6$. Choose spatial grid width sufficiently small such that temporal error dominates.

- ◊ Display global errors versus time stepsizes (accuracy).
- ◊ Display global errors versus number of exponentials (efficiency).
  More appropriate indicator for efficiency used for Rosen–Zener model. Improved performance of novel schemes.

First illustration (Parabolic equation)



Observations.

- Commutator-free Magnus integrators retain nonstiff orders of convergence.
- Poor stability behaviour of optimised sixth-order scheme by ALVERMANN, FEHSKE.

Objectives

Main objectives.

- Stability and error analysis of commutator-free Magnus integrators and related methods for different classes of evolution equations
  - Evolution equations of parabolic type
    SERGIO BLANES, FERNANDO CASAS, M. TH.
    Convergence analysis of high-order commutator-free Magnus integrators for non-autonomous linear evolution equations of parabolic type.
    Submitted.
  - Evolution equations of Schrödinger type
    Time-dependent Hamiltonian ($A(t) = \mathrm{i}\,\Delta + \mathrm{i}\,V(t)$, e.g.)
- Design of efficient schemes

  SERGIO BLANES, FERNANDO CASAS, M. TH.
  High-order commutator-free Magnus integrators and related methods for non-autonomous linear evolution equations.
  In preparation.

References

Main inspiration.

Application of commutator-free Magnus integrators in quantum dynamics.

A. ALVERMANN, H. FEHSKE.
High-order commutator-free exponential time-propagation of driven quantum systems.
Journal of Computational Physics 230 (2011) 5930–5956.

A. ALVERMANN, H. FEHSKE, P. B. LITTLEWOOD.
Numerical time propagation of quantum systems in radiation fields.
New Journal of Physics 14 (2012) 105008.

Previous work on design of higher-order commutator-free Magnus integrators.

S. BLANES, P. C. MOAN.
Fourth- and sixth-order commutator-free Magnus integrators for linear and non-linear dynamical systems.
Applied Numerical Mathematics 56 (2006) 1519–1537.

S. BLANES, F. CASAS, J. A. OTEO, J. ROS.
The Magnus expansion and some of its applications.
Phys. Rep. 470 (2009) 151–238.

Previous work on error analysis of fourth-order scheme for parabolic equations.
Explanation of order reductions due to imposed boundary conditions.

M. TH.
A fourth-order commutator-free exponential integrator for nonautonomous differential equations.
SIAM Journal on Numerical Analysis 44/2 (2006) 851–864.

Remarks on extension to nonlinear evolution equations

Extension by operator splitting

Approach. Apply commutator-free Magnus integrators in combination with operator splitting methods to nonlinear evolution equations of form

$$\begin{cases} u'(t) = A(t)\,u(t) + B\big(u(t)\big)\,, \quad t \in (t_0, T)\,, \\ u(t_0) \text{ given}\,, \end{cases}$$

i.e., employ suitable compositions of solutions to associated subproblems

$$v'(t) = A(t)\,v(t)\,, \quad w'(t) = B\big(w(t)\big)\,.$$

Example. Second-order splitting method (Strang, special case of autonomous linear equation, first step)

$$\begin{cases} u'(t) = A\,u(t) + B\,u(t)\,, \quad t \in (t_0, T)\,, \\ u(t_0) \text{ given}\,, \end{cases}$$

$$\mathrm{e}^{\frac{1}{2}\tau A}\,\mathrm{e}^{\tau B}\,\mathrm{e}^{\frac{1}{2}\tau A} u_0 \approx u(t_0+\tau) = \mathrm{e}^{\tau(A+B)}\,u_0\,.$$

Areas of application

Situation. Consider nonlinear evolution equation of form

$$u'(t) = A(t)\,u(t) + B\big(u(t)\big)\,, \qquad t \in (t_0, T)\,.$$

Areas of application.

- Nonlinear Schrödinger equations
  - Gross–Pitaevskii equations with opening trap
  - Gross–Pitaevskii equations with rotation (moving frame, see illustration)
- Diffusion-advection-reaction systems with multiplicative noise
  - Formation of patterns in deterministic case, see illustrations
  - Gray–Scott equations with multiplicative noise (with E. Hausenblas)

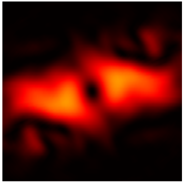
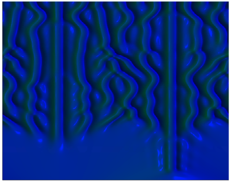
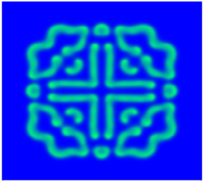




Illustration (Gray–Scott equations)

Solution behaviour (deterministic case). Consider diffusion-reaction system with additional space-time-dependent term (multiplicative form). Observe great variety of patterns (over long times).

MOVIE_GRAYSCOTT   MOVIE_GRAYSCOTT_TIMEDEPENDENCIES

Solution behaviour (stochastic case). Consider additional space-time-dependent noise term (multiplicative form). Display single path.

MOVIE_GRAYSCOTT_PURENOISE   MOVIE_GRAYSCOTT_WITHNOISE

Aim. Study effect of noise on patterns (stability, diversity).

Questions.

- ◇ Numerical analysis of space and time discretisation over short times (stability, accuracy, convergence rate in dependence of noise term).
- ◇ Use of local error control powerful in deterministic case (reliability, efficiency). Any hope for use of automatic time stepsize control in stochastic case?
- ◇ Efficient realisation essential for computation of numerous paths over long times. Challenging task!

High-order versus low-order methods

Main objectives.

- ◇ Provide stability and error analysis of considered time integration methods for different classes of evolution equations (specify regularity and compatibility requirements for general format of methods, explain order reductions).
- ◇ Design efficient schemes.

Guide line.

- ◇ Higher-order methods expected to be beneficial in efficiency for equations of Schrödinger type (no stability and regularity issues expected).
- ◇ Poor stability behaviour expected for equations of parabolic type (circumvented by study of complex coefficients under additional positivity condition).

  Significant order reductions expected for equations of parabolic type when Dirichlet or Neuman boundary conditions are imposed.
- ◇ Efficiency of high-order methods limited by exactness of measurements in physical experiments or by low regularity of data (e.g. for SPDEs). Low-order methods expected to be adequate in such situations.

Remark. Focus on results for commutator-free Magnus integrators. Results on operator splitting methods are provided by former work.

High-order commutator-free Magnus integrators

Magnus expansion

Magnus expansion (Magnus, 1954). Formal representation of solution to non-autonomous linear evolution equation based on Magnus expansion

$$u'(t) = A(t)\,u(t)\,, \quad t \in (t_0, T)\,, \quad u(t_0) \text{ given}\,,$$

$$u(t_n + \tau_n) = \mathrm{e}^{\Omega(\tau_n, t_n)}\,u(t_n)\,, \quad t_0 \le t_n < t_n + \tau_n \le T\,,$$

$$\Omega(\tau_n, t_n) = \int_{t_n}^{t_n+\tau_n} A(\sigma)\,\mathrm{d}\sigma + \tfrac{1}{2}\int_{t_n}^{t_n+\tau_n}\int_{t_n}^{\sigma_1} \big[A(\sigma_1), A(\sigma_2)\big]\,\mathrm{d}\sigma_2 \mathrm{d}\sigma_1$$
$$+ \tfrac{1}{6}\int_{t_n}^{t_n+\tau_n}\int_{t_n}^{\sigma_1}\int_{t_n}^{\sigma_2} \Big(\big[A(\sigma_1), \big[A(\sigma_2), A(\sigma_3)\big]\big] + \big[A(\sigma_3), \big[A(\sigma_2), A(\sigma_1)\big]\big]\Big)\,\mathrm{d}\sigma_3 \mathrm{d}\sigma_2 \mathrm{d}\sigma_1 + \dots$$

Magnus integrators. Truncation of expansion and application of quadrature formulae for approximation of multiple integrals leads to class of interpolatory Magnus integrators.

- Second-order Magnus integrator (exponential midpoint rule)

$$\tau_n\,A\big(t_n + \tfrac{\tau_n}{2}\big) \;\approx\; \Omega(\tau_n, t_n)\,.$$

- Fourth-order interpolatory Magnus integrator, see Blanes, Casas, Ros (2000)

$$\tfrac{1}{6}\Big(A(t_n) + 4\,A\big(t_n + \tfrac{\tau_n}{2}\big) + A(t_n + \tau_n)\Big) - \tfrac{1}{12}\,\tau_n^2\big[A(t_n), A(t_n + \tau_n)\big] \;\approx\; \Omega(\tau_n, t_n)\,.$$

Magnus-type integrators

Higher-order interpolatory Magnus integrators.

◇ Fourth-order interpolatory Magnus integrator, see BLANES, CASAS, ROS (2000)

$$\tfrac{1}{6}\big(A(t_n) + 4\,A(t_n + \tfrac{1}{2}\,\tau_n) + A(t_n + \tau_n)\big) - \tfrac{1}{12}\,\tau_n^2\big[A(t_n), A(t_n + \tau_n)\big] \approx \Omega(\tau_n, t_n)\,.$$

Disadvantages. Presence of commutators causes

- large computational cost (for realisation of action of arising matrix-exponentials on vectors by Krylov-type methods, e.g.),
- loss of structure (issues of well-definededness and stability for evolution equations).

Alternative. Commutator-free Magnus integrators provide useful alternative to interpolatory Magnus integrators.

A. ALVERMANN, H. FEHSKE, P. B. LITTLEWOOD.
Numerical time propagation of quantum systems in radiation fields.
New Journal of Physics 14 (2012) 105008.

... We explain the use of commutator-free exponential time propagators for the numerical solution of the associated Schrödinger or master equations with a time-dependent Hamilton operator. These time propagators are based on the Magnus series but avoid the computation of commutators, which makes them suitable for the efficient propagation of systems with a large number of degrees of freedom. ...

Commutator-free Magnus integrators

Situation. Consider non-autonomous linear evolution equation

$$u'(t) = A(t)\,u(t)\,, \quad t \in (t_0, T)\,, \quad u(t_0) \text{ given}\,.$$

Use time-stepping approach, i.e., determine approximations at certain time grid points $t_0 < t_1 < \cdots < t_N \leq T$ by recurrence

$$u_{n+1} = \mathscr{S}(\tau_n, t_n)\,u_n \approx u(t_{n+1}) = \mathscr{E}(\tau_n, t_n)\,u(t_n)\,, \quad \tau_n = t_{n+1} - t_n\,, \quad n \in \{0, 1, \dots, N-1\}\,.$$

Commutator-free Magnus integrators. High-order commutator-free Magnus integrators cast into general form

$$\mathscr{S}(\tau_n, t_n) = \prod_{j=1}^{J} \mathrm{e}^{\tau_n B_{nj}} = \mathrm{e}^{\tau_n B_{nJ}} \cdots \mathrm{e}^{\tau_n B_{n1}}\,, \quad B_{nj} = \sum_{k=1}^{K} a_{jk}\,A_{nk}\,, \quad A_{nk} = A(t_n + c_k \tau_n)\,.$$

Realisation. Action of arising matrix-exponentials on vectors commonly computed by Krylov-type methods. Computational effort determined by cost for matrix-vector products.

Remark. Commutator-free Magnus integrators generalise time-splitting methods defined by coefficients $(\alpha_\ell, \beta_\ell)_{\ell=1}^{s}$ (freeze time by adding differential equation $\frac{\mathrm{d}}{\mathrm{d}t}\,t = 1$)

$$u_{n+1} = \mathrm{e}^{\tau_n \alpha_s A_{ns}} \cdots \mathrm{e}^{\tau_n \alpha_1 A_{n1}}\,u_n\,, \quad c_k = \sum_{\ell=1}^{k} \beta_\ell\,,$$

with the merit of a significantly reduced number of exponentials, which enhances efficiency.

Examples (Nonstiff orders $p = 2, 4, 6$)

Order 2 (Exponential midpoint rule). Commutator-free Magnus integrator based on single Gaussian quadrature node involves single exponential at each time step

$$p = 2, \quad J = 1 = K, \quad c_1 = \tfrac{1}{2}, \quad a_{11} = 1, \quad A_{n1} = A\big(t_n + \tfrac{\tau_n}{2}\big),$$
$$\mathscr{S}(\tau_n, t_n) = \mathrm{e}^{\tau_n A(t_n + \frac{1}{2}\tau_n)}.$$

Order 4. Commutator-free Magnus integrator based on two Gaussian quadrature nodes requires evaluation of two exponentials at each time step

$$p = 4, \quad J = 2 = K, \quad c_k = \tfrac{1}{2} \mp \tfrac{\sqrt{3}}{6}, \quad a_{1k} = \tfrac{1}{4} \pm \tfrac{\sqrt{3}}{6}, \quad a_{21} = a_{12}, \quad a_{22} = a_{11},$$
$$\mathscr{S}(\tau_n, t_n) = \mathrm{e}^{\tau_n (a_{21} A_{n1} + a_{22} A_{n2})} \, \mathrm{e}^{\tau_n (a_{11} A_{n1} + a_{12} A_{n2})}.$$

Scheme suitable for evolution equations of Schrödinger and parabolic type, since

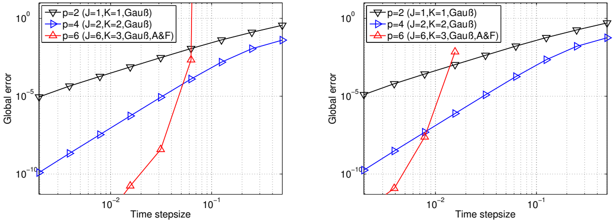
$$b_1 = a_{11} + a_{12} = \tfrac{1}{2} = a_{21} + a_{22} = b_2.$$

Order 6. Sixth-order commutator-free Magnus integrator obtained from coefficients given in Alvermann, Fehske. Scheme suitable for evolution equations of Schrödinger type, but poor stability behaviour observed for evolution equations of parabolic type, since

$$\exists\, j \in \{1, \dots, J\}: \quad b_j = \sum_{k=1}^{K} a_{jk} < 0.$$

Counter-example

Numerical experiment. Apply commutator-free Magnus integrators of nonstiff orders $p = 2, 4, 6$ to test equation of parabolic type (see before). Display global errors versus time stepsizes for $M = 50$ (left) and $M = 100$ (right) space grid points. Sixth-order scheme shows poor stability behaviour.



Explanation. Sixth-order scheme involves negative coefficients which cause integration backward in time (ill-posed problem).

Conclusions. Order barrier at order four conjectured. Connexion to class of time-splitting methods gives reasons for the study of *unconventional* commutator-free Magnus integrators involving complex coefficients under additional positivity condition.

Basic assumptions

Commutator-free Magnus integrators. High-order commutator-free Magnus integrators cast into general form

$$\mathscr{S}(\tau_n, t_n) = \prod_{j=1}^{J} \mathrm{e}^{\tau_n B_{nj}}\,, \quad B_{nj} = \sum_{k=1}^{K} a_{jk}\, A_{nk}\,, \quad A_{nk} = A(t_n + c_k \tau_n)\,.$$

Employ standard assumption that ratios of subsequent time stepsizes remain bounded from below and above

$$\varrho_{\min} \le \frac{\tau_{n+1}}{\tau_n} \le \varrho_{\max}\,, \quad n \in \{0, 1, \dots, N-2\}\,.$$

Nodes and coefficients. Relate nodes to quadrature nodes and suppose

$$0 \le c_1 < \cdots < c_K \le 1\,.$$

Assume basic consistency condition to be satisfied (direct consequence of elementary requirement $\mathscr{S}(\tau_n, t_n) = \mathrm{e}^{\tau_n A}$ for time-independent operator A)

$$\sum_{j=1}^{J} \sum_{k=1}^{K} a_{jk} = 1\,.$$

In connection with evolution equations of parabolic type employ positivity condition, which ensures well-definededness of commutator-free Magnus integrators within analytical framework of sectorial operators and analytic semigroups

$$\Re\, b_j > 0\,, \quad b_j = \sum_{k=1}^{K} a_{jk}\,, \quad j \in \{1, \dots, J\}\,.$$

Design of novel schemes

Numerical comparisons for dissipative quantum system

Derivation of order conditions

Approach.

- ◇ Focus on design of efficient schemes of non-stiff orders $p = 4, 5$ involving $K = 3$ Gaussian quadrature nodes. By time-symmetry of schemes achieve $p = 6$.
- ◇ Employ advantageous reformulation (suffices to study first time step, indicate dependence on time stepsize $\tau > 0$)

$$\prod_{j=1}^{J} \mathrm{e}^{\tau(a_{j1} A_1(\tau) + a_{j2} A_2(\tau) + a_{j3} A_3(\tau))} = \prod_{j=1}^{J} \mathrm{e}^{x_{j1}\alpha_1(\tau) + x_{j2}\alpha_2(\tau) + x_{j3}\alpha_3(\tau)} + \mathcal{O}(\tau^{p+1}), \quad \alpha_k(\tau) = \mathcal{O}(\tau^k).$$

- ◇ Determine set of independent order conditions (obtain $q = 10$ conditions for $p = 5$, use Lyndon multi-index $(1,2)$ and corresponding word $\alpha_1 \alpha_2$ etc.)

$$(1):\ y_J = \sum_{\ell=1}^{J} x_{\ell 1} = 1, \quad (2):\ z_J = \sum_{\ell=1}^{J} x_{\ell 2} = 0, \quad (3):\ \sum_{j=1}^{J} x_{j3} = \tfrac{1}{12},$$

$$(1,2):\ \sum_{j=1}^{J} x_{j2}\,(x_{j1} + 2\,y_{j-1}) = -\tfrac{1}{6}, \quad (1,3):\ \sum_{j=1}^{J} x_{j3}\,(x_{j1} + 2\,y_{j-1}) = \tfrac{1}{12}, \quad (2,3):\ \sum_{j=1}^{J} x_{j3}\,(x_{j2} + 2\,z_{j-1}) = \tfrac{1}{120},$$

$$(1,1,2):\ \sum_{j=1}^{J} x_{j2}\,(x_{j1}^2 + 3\,y_{j-1}^2 + 3\,x_{j1}\,y_{j-1}) = -\tfrac{1}{4}, \quad (1,1,3):\ \sum_{j=1}^{J} x_{j3}\,(x_{j1}^2 + 3\,y_{j-1}^2 + 3\,x_{j1}\,y_{j-1}) = \tfrac{1}{10},$$

$$(1,2,2):\ \sum_{j=1}^{J} x_{j1}\,(x_{j2}^2 - 3\,x_{j2}\,z_j + 3\,z_j^2) = \tfrac{1}{40}, \quad (1,1,1,2):\ \sum_{j=1}^{J} x_{j2}\,(x_{j1}^3 + 4\,y_{j-1}^3 + 6\,x_{j1}\,y_{j-1}^2 + 4\,x_{j1}^2\,y_{j-1}) = \tfrac{3}{10}.$$

Derivation of order conditions

Additional practical constraints.

- In certain cases, impose requirement of time-symmetry to further reduce number of order conditions (obtain $q = 7$ conditions for $p = 6$)

$$\Psi_J^{[r]}(-\tau) = \big(\Psi_J^{[r]}(\tau)\big)^{-1}, \quad x_{J+1-j,k} = (-1)^{k+1} x_{jk},$$
$$(1), (3), (1,2), (2,3), (1,1,3), (1,2,2), (1,1,1,2).$$

- In certain cases, express solutions to order conditions in terms of few coefficients and minimise amount by which higher-order conditions (e.g. related to $(1,1,1,1,1,2)$ at order seven) are not satisfied.

Numerical comparisons. Illustrate favourable behaviour of resulting novel schemes for dissipative quantum system.

Remark. For reason of time, focus on schemes of orders $p = 5, 6$ with complex coefficients and omit results for $p = 4$.

Dissipative quantum system

Rosen–Zener model with dissipation. For Rosen–Zener model with dissipation, associated Schrödinger equation in normalised form reads

$$u'(t) = A(t)\,u(t) = -\mathrm{i}\,H(t)\,u(t)\,, \quad t \in (t_0, T)\,,$$

$$H(t) = f_1(t)\,\sigma_1 \otimes I + f_2(t)\,\sigma_2 \otimes R + \delta D \in \mathbb{C}^{d\times d}\,, \quad d = 2\,k\,,$$

$$I = \mathrm{diag}\big(1\big) \in \mathbb{R}^{k\times k}\,, \quad R = \mathrm{tridiag}\big(1,0,1\big) \in \mathbb{R}^{k\times k}\,, \quad D = -\mathrm{i}\,\mathrm{diag}\big(1^2, 2^2, \dots, d^2\big) \in \mathbb{C}^{d\times d}\,.$$

Notation and special choice. Recall definitions of Pauli matrices and Kronecker product

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma_1 \otimes I = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \quad \sigma_2 \otimes R = \begin{pmatrix} 0 & -\mathrm{i}R \\ \mathrm{i}R & 0 \end{pmatrix}.$$

Special choice of arising functions and parameters

$$d = 10\,, \quad T_0 = 1\,, \quad t_0 = -4\,T_0\,, \quad T = 4\,T_0\,, \quad V_0 = \tfrac{1}{2}\,, \quad \omega = 5\,, \quad \delta = 10^{-1}\,,$$

$$f_1(t) = V_0\,\cos(\omega t)\,\big(\cosh\big(\tfrac{t}{T}\big)\big)^{-1}\,, \quad f_2(t) = -\,V_0\,\sin(\omega t)\big(\cosh\big(\tfrac{t}{T}\big)\big)^{-1}\,.$$

Remark.

- Ordinary differential equation of simple form that shows characteristics of parabolic equations if $\delta > 0$ and $d \gg 1$.
- Straightforward realisation of matrix-exponentials by low-order Taylor series expansions.

Favourable novel schemes ($p = 5, 6$, complex)

Favourable novel schemes (complex coefficients). Design commutator-free Magnus integrators with complex coefficients satisfying positivity condition

$$p = 5: \quad \mathrm{CF}_3^{[5]}, \qquad p = 6: \quad \mathrm{CF}_4^{[6]}, \quad \mathrm{CF}_5^{[6]}.$$

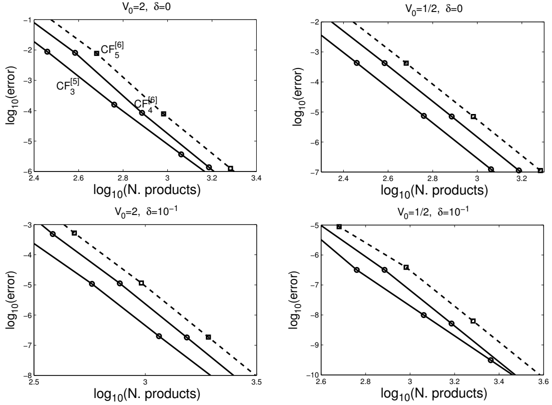
- ◇ Expect schemes to remain stable for $\delta > 0$.
- ◇ Expect scheme with $J = 3$ to be most efficient.

Illustration ($p = 5, 6$)

Numerical results. Time integration of Rosen–Zener model by fifth- and sixth-order commutator-free Magnus integrators

$$p = 5: \quad CF_3^{[5]}, \qquad p = 6: \quad CF_4^{[6]}, \quad CF_5^{[6]}.$$

Implementation by Taylor series approximation of order $M = 6$. Display global errors in fundamental matrix solution at final time versus number of matrix-vector products. Novel schemes remain stable for $\delta > 0$.



Convergence result

Analytical framework

Analytical framework. Suitable functional analytical framework for evolution equations of Schrödinger or parabolic type based on

- selfadjoint operators and unitary evolution operators on Hilbert spaces or
- sectorial operators and analytic semigroups on Banach spaces.

Hypotheses (Parabolic case). Domain of $A(t) : D \subset X \to X$ time-independent, dense and continuously embedded. Linear operator $A(t) : D \subset X \to X$ sectorial, uniformly in $t \in [t_0, T]$, i.e., there exist $a \in \mathbb{R}$, $0 < \phi < \frac{\pi}{2}$, $C_1 > 0$ such that

$$\left\|(\lambda I - A(t))^{-1}\right\|_{X \leftarrow X} \le \frac{C_1}{|\lambda - a|}\,, \quad t \in [t_0, T]\,, \quad \lambda \notin S_\phi(a) = \{a\} \cup \big\{\mu \in \mathbb{C} : |\arg(a-\mu)| \le \phi\big\}\,.$$

Graph norm of $A(t)$ and norm in D equivalent for $t \in [t_0, T]$, i.e., there exists $C_2 > 0$ such that

$$C_2^{-1}\,\|x\|_D \le \|x\|_X + \big\|A(t)\,x\big\|_X \le C_2\,\|x\|_D\,, \quad t \in [t_0, T]\,, \quad x \in D\,.$$

Defining operator family is Hölder-continuous for some exponent $\vartheta \in (0,1]$, i.e., there exists $C_3 > 0$ such that

$$\big\|A(t) - A(s)\big\|_{X \leftarrow D} \le C_3\,|t-s|^\vartheta\,, \quad s,t \in [t_0, T]\,.$$

Consequence. Sectorial operator $A(t)$ generates analytic semigroup $(\mathrm{e}^{\sigma A(t)})_{\sigma \in [0,\infty)}$ on X. By integral formula of Cauchy representation follows

$$\mathrm{e}^{\sigma A(t)} = \frac{1}{2\pi\mathrm{i}} \int_\Gamma \mathrm{e}^\lambda \big(\lambda I - \sigma A(t)\big)^{-1}\,\mathrm{d}\lambda\,, \quad \sigma > 0\,, \qquad \mathrm{e}^{\sigma A(t)} = I\,, \quad \sigma = 0\,.$$

Convergence result

Situation.

- Employ standard hypotheses on operator family defining non-autonomous linear evolution equation of Schrödinger or parabolic type.

  See Blanes, Casas, Th. (parabolic case) and draft (Schrödinger case included).

- Assume that coefficients of considered high-order commutator-free Magnus integrator fulfill basic assumptions and nonstiff order conditions.

- Recall assumption on ratios of subsequent time stepsizes.

Theorem

Provided that operator family and exact solution are sufficiently regular, following estimate holds in underlying Banach space with constant $C > 0$ independent of n and time increments

$$\|u_n - u(t_n)\|_X \leq C\left(\|u_0 - u(0)\|_X + \tau_{\max}^p\right), \quad 0 < \tau_n \leq \tau_{\max}, \quad n \in \{0, 1, \dots, N\}.$$

Crucial point. Specify regularity and compatibility requirements on exact solution.

- For test equation and $X = \mathscr{C}(\Omega, \mathbb{R})$, obtain regularity requirement $u(t) \in \mathscr{C}^{2p}(\Omega, \mathbb{R})$ for $t \in [t_0, T]$.
- For Schrödinger equation with $A(t) = \mathrm{i}\,\Delta + \mathrm{i}\,V(t)$ and $X = L^2(\Omega, \mathbb{C})$, weaker assumption $\partial_x^p u(t) \in L^2(\Omega, \mathbb{C})$ sufficient. Error analysis of classical fourth-order scheme completed, but rigorous proof for high-order schemes remains open.

Main tools of proof

Stability. Relate stability function of commutator-free Magnus integrator to analytic semigroup (suitable choice of frozen time t)

$$\Delta_{n_0}^{n} = \prod_{i=n_0}^{n} \mathscr{S}_i(\tau_i, t_i) - \mathrm{e}^{(t_{n+1}-t_{n_0})\,A(t)}\,, \quad \|\mathrm{e}^{sA(t)}\|_{X\leftarrow X} + s\,\|\mathrm{e}^{sA(t)}\|_{D\leftarrow X} \le C\,.$$

Employ telescopic identity, bounds for analytic semigroup, Hölder-continuity of defining operator family, and Gronwall-type inequality to deduce desired stability bound

$$\Big\| \prod_{i=n_0}^{n} \mathscr{S}_i(\tau_i, t_i) \Big\|_{X\leftarrow X} \le C\,.$$

Local error. Repeated application of variation-of-constants formula yields relation which is starting point for further expansions

$$u(t_{n+1}) - \mathscr{S}(\tau_n, t_n)\,u(t_n) = \sum_{j=1}^{J} \sum_{k=1}^{K} a_{jk} \Big(\prod_{i=j+1}^{J} \mathrm{e}^{\tau_n B_{ni}(\tau_n)} \Big) \int_0^{\tau_n} \mathrm{e}^{(\tau_n-\sigma) B_{nj}(\tau_n)}\, g_{njk}(\sigma)\,\mathrm{d}\sigma\,,$$

$$g_{njk}(\sigma) = \big(A(t_n + d_{j-1}\tau_n + b_j\sigma) - A(t_n + c_k\tau_n)\big)\,u(t_n + d_{j-1}\tau_n + b_j\sigma)\,.$$

Resulting local error representation involved for high-order schemes.

Further illustrations

Illustration (Smooth versus non-smooth potential)

Illustration. Time integration of linear Schrödinger equation with space-time-dependent Hamiltonian by commutator-free Magnus integrators of orders $p = 1,2,3,4,6$ combined with time-splitting methods of same orders and Fourier-spectral method ($M = 100 \times 100$). Study non-smooth versus smooth space-time-dependent potential

$$V(x,t) = \sin(\omega t)\left(\gamma_1^4 x_1^2 + \gamma_2^4 x_2^2\right), \qquad V(x,t) = \begin{cases} c_1 & \text{if } x_1^2 + x_2^2 + t^2 < r^2\,, \\ c_2 & \text{else}\,. \end{cases}$$

Observations. Display global errors at time $T = 1$ versus time stepsizes. For smooth potential, in accordance with theoretical result, retain full orders of convergence (superconvergence for $p = 3$). For non-smooth potential, observe severe order reductions (only slight improvement in accuracy and efficiency for higher-order schemes).

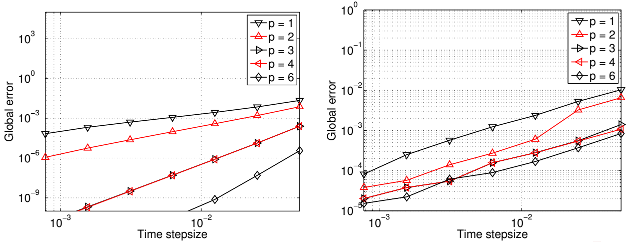
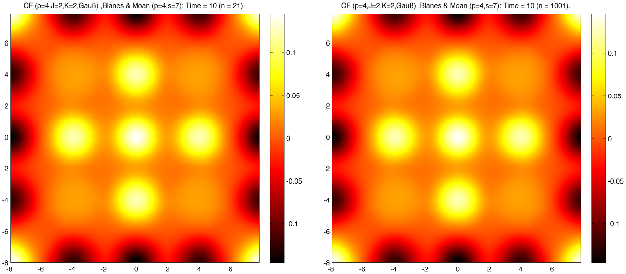


Illustration (Non-smooth potential)

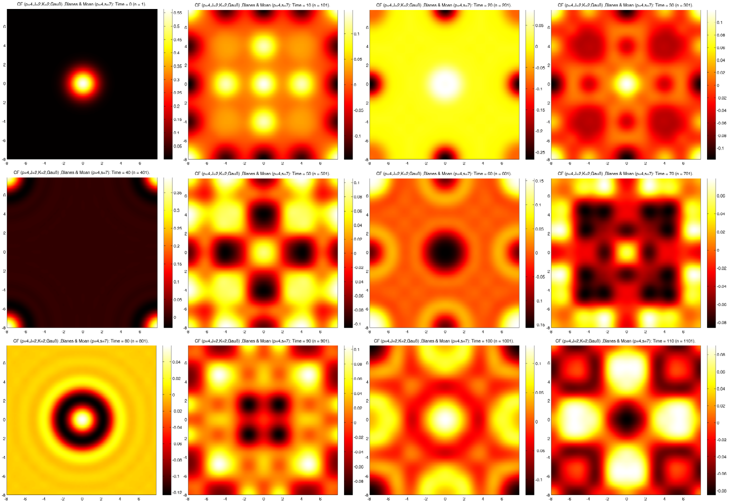
Model (non-smooth potential). Inspired by paraxial model for light propagation in inhomogeneous media (refractive index), see G. Thalhammer.

- Impose (unphysical) periodic boundary conditions to observe formation of beautiful patterns over longer times, see movie and next slide.
- Solution profile remains stable for coarse time stepsizes.



Solution profile at $T = 10$, computed by coarse time stepsize $\tau = \frac{1}{2}$ (left) and refined time stepsize $\tau = \frac{1}{100}$ (right).

Illustration (Non-smooth potential)



Conclusions and future work

Conclusions and future work

Summary.

- High-order commutator-free Magnus integrators form favourable class of time integration methods for non-autonomous linear evolution equations of Schrödinger and parabolic type.
- Theoretical analysis of high-order commutator-free Magnus integrators provides better understanding when order reductions and thus significant loss of accuracy for higher-order methods have to be expected.

Future work.

- Design of time-adaptive schemes for local error control (optimisation of solar cells).
- Study of commutator-free Magnus integrators in combination with operator splitting methods for nonlinear problems of form

$$u'(t) = A(t)\,u(t) + B\big(u(t)\big)\,.$$

  Relevant applications include Gross–Pitaevskii equations (quantum turbulence).
- Improve performance of implementation for deterministic Gray–Scott equations. Introduce time integrators for stochastic counterpart (multiplicative noise).

Thank you!