Time integration methods for non-autonomous evolution equations

Mechthild Thalhammer

Karlsruhe PDE Seminar, February 2017

Scope

Numerical methods for differential equations.

- Study numerical methods for different classes of partial differential equations arising in applications.
- Provide convergence analysis of space and time discretisations. Identify benefits or possible limitations. Improve existing methods or design novel methods.

Focus in this talk.

- Joint work with SERGIO BLANES, FERNANDO CASAS (Valencia, Castellón, Spain).

Related work.

- With WINFRIED AUZINGER, KARSTEN HELD, OTHMAR KOCH (Wien).
- With ERIKA HAUSENBLAS (Leoben).

First remarks on commutator-free quasi-Magnus exponential integrators for linear evolution equations

Areas of application

Situation. Consider non-autonomous linear evolution equation

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

Areas of application.

- Linear evolution equations of Schrödinger type
  Linear Schrödinger equations involving space-time-dependent potential
  Quantum systems
  Models for oxide solar cells (with W. AUZINGER, K. HELD, O. KOCH)
- Linear evolution equations of parabolic type
  Variational equations related to diffusion-advection-reaction equations
  Dissipative quantum systems
  Rosen–Zener models with dissipation

Remark. Abstract formulation helps to recognise common structure of complex processes.

Commutator-free quasi-Magnus exponential integrators

Issue. Exact solution of non-autonomous linear evolution equation not available (used only theoretically as ideal case)

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

Remark. In autonomous case, solution (formally) given by exponential

$$w'(t) = A_0\, w(t)\,, \qquad w(t_0 + \tau) = \mathrm{e}^{\tau A_0}\, w(t_0)\,.$$

Approach. In non-autonomous case, compute numerical approximation (time stepsize $\tau > 0$, second-order scheme)

$$\mathscr{S}(\tau)\, u(t_0) \approx u(t_0 + \tau)\,, \qquad \mathscr{S}(\tau) = \mathrm{e}^{\tau A(t_0 + \frac{\tau}{2})}\,.$$

Desirable to use higher-order approximations (favourable in efficiency).
Study class of commutator-free quasi-Magnus exponential integrators

$$\mathscr{S}(\tau) = \mathrm{e}^{\tau B_J(\tau)} \cdots \mathrm{e}^{\tau B_1(\tau)}\,, \qquad B_j(\tau) = \sum_{k=1}^{K} a_{jk}\, A(t_n + c_k \tau)\,.$$

Secret of success. *Smart* choice of arising coefficients.

References

Our background.

Previous work on design of higher-order commutator-free quasi-Magnus exponential 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 stability and error analysis of fourth-order scheme for parabolic equations. Explanation of order reductions due to imposed homogeneous Dirichlet 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.

References

Our main inspiration.

Application of commutator-free quasi-Magnus exponential 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.

Complete the big picture ...

Main objectives.

- Stability and error analysis of commutator-free quasi-Magnus exponential 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 quasi-Magnus exponential 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 quasi-Magnus exponential integrators and related methods for non-autonomous linear evolution equations.* Submitted.

First illustration (Parabolic equation)

Practice in numerical methods is the only way of learning it.

H. Jeffreys, B. Jeffreys

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.

First illustration (Parabolic equation)

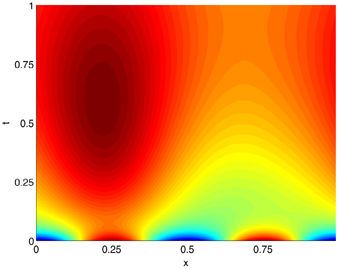
Test equation. Consider non-autonomous linear evolution equation

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

Impose periodic boundary conditions and regular initial condition.

Special choice. In particular, set

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



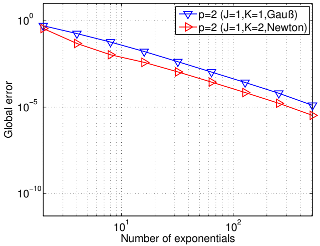
First illustration (Parabolic equation)

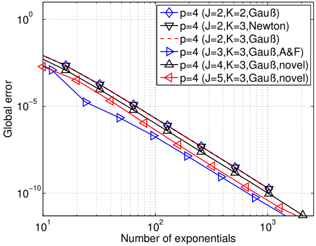
One must watch the convergence of a numerical code as carefully as a father watching his four year old play near a busy road. J. P. Boyd

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

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

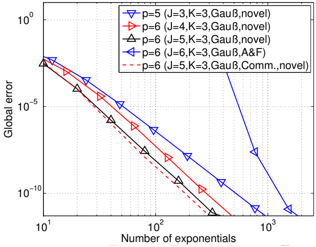
First illustration (Parabolic equation)





Observations.

- Commutator-free integrators retain nonstiff orders of convergence.
- Poor stability of high-order schemes found in literature (e.g. 6th-order scheme by ALVERMANN, FEHSKE).



Further remarks

Magnus versus commutator-free quasi-Magnus exponential integrators
Approach to resolve stability issues

Magnus expansion

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

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

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

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

Magnus integrators

Magnus integrators. Truncation of Magnus 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 Magnus integrator, see Blanes, Casas, Ros (2000)

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

Issue. Presence of iterated commutators.

Magnus-type integrators

Disadvantages. Presence of iterated commutators causes

- loss of structure (issues of well-definedness and stability for PDEs involving differential operators).
- large computational cost (for realisation of action of arising matrix-exponentials on vectors by Krylov-type methods, e.g.).

Alternative. Commutator-free quasi-Magnus exponential 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 quasi-Magnus exponential integrators

Situation. Consider non-autonomous linear evolution equation

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

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

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

General format. Cast high-order commutator-free quasi-Magnus exponential integrators into general form

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

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

Commutator-free quasi-Magnus exponential integrators

General format. Recall general format

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

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

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

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

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

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

Order 4. Fourth-order method based on two Gaussian quadrature nodes requires evaluation of two exponentials at each time step

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

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

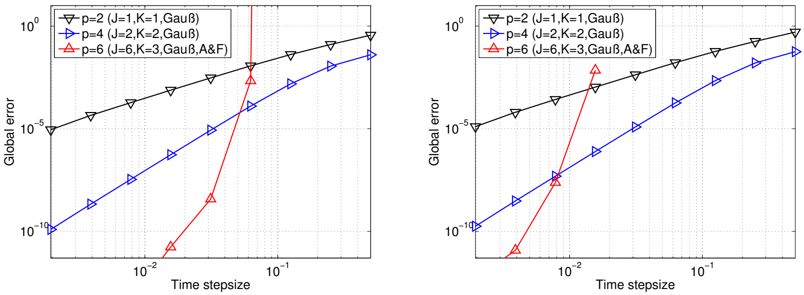
$$b_1 = a_{11} + a_{12} = \tfrac{1}{2} = a_{21} + a_{22} = b_2\,.$$

Order 6. Sixth-order method 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 quasi-Magnus exponential integrators of nonstiff orders $p = 2, 4, 6$ to parabolic test equation (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.



First conclusions

First conclusions.

- Order barrier at order four, i.e. commutator-free quasi-Magnus exponential integrators of order five or higher necessarily involve negative coefficients which cause integration backward in time (ill-posed problem).
- Close connexion to class of time-splitting methods gives reasons for the study of *unconventional* commutator-free quasi-Magnus exponential integrators involving complex coefficients under additional positivity condition.

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

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

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

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

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

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

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

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

Basic assumptions on methods

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

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

Employ standard assumption that ratios of subsequent time stepsizes remain bounded

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

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)

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

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

$$\Re\, b_j > 0\,, \qquad j \in \{1, \dots, J\}\,.$$

Convergence result

Situation.

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

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

- Use that coefficients of considered high-order commutator-free Magnus integrator fulfill basic assumptions (positivity condition for parabolic case) and order conditions.

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

$$\big\| u_n - u(t_n) \big\|_X \leq C \Big(\big\| u_0 - u(t_0) \big\|_X + \tau_{\max}^p \Big), \quad 0 < \tau_n \leq \tau_{\max}, \quad n \in \{0, 1, \dots, N\}.$$

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

- Test equation: For $X = \mathscr{C}(\Omega, \mathbb{R})$ obtain regularity requirement $u(t) \in \mathscr{C}^{2p}(\Omega, \mathbb{R})$.
- Schrödinger equation with $A(t) = \mathrm{i}\,\Delta + \mathrm{i}\,V(t)$: For $X = L^2(\Omega, \mathbb{C})$ weaker assumption $\partial_x^p u(t) \in L^2(\Omega, \mathbb{C})$ sufficient.

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 suitable representation 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.

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 $\tau > 0$)

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

- 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.)

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

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

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

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

Design of novel schemes

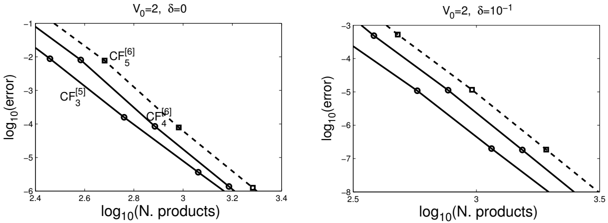
Additional practical constraints.

- In certain cases, require time-symmetry to further reduce number of order conditions (for $p=6$ obtain $q=7$ conditions (1), (3), (1,2), (2,3), (1,1,3), (1,2,2), (1,1,1,2))

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

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

Favourable novel schemes. Illustrate favourable behaviour of resulting novel schemes for dissipative quantum system (Rosen–Zener model). Display results for schemes of order $p=5,6$ with complex coefficients satisfying positivity condition



Observations. Schemes remain stable for $\delta > 0$. Scheme with $J=3$ favourable in efficiency.

A step aside ...

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

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

Illustration (Smooth versus non-smooth potential)

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 (slight improvement in accuracy and efficiency for higher-order schemes).

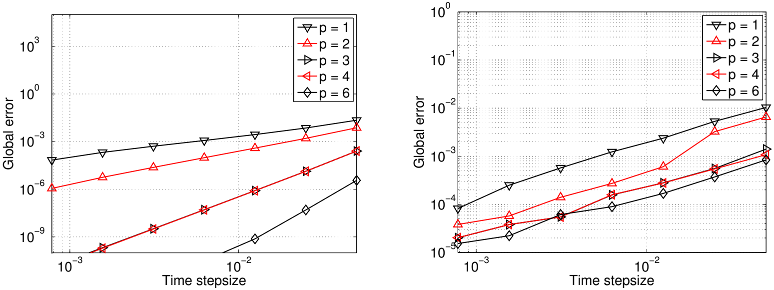
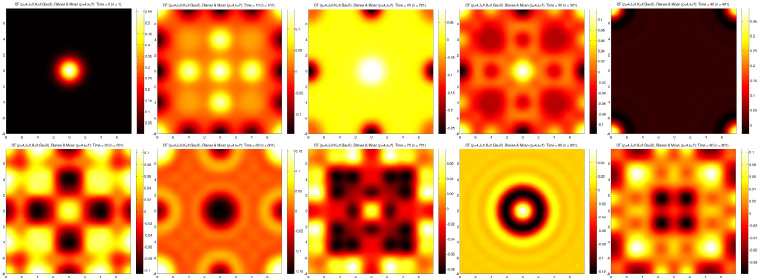


Illustration (Non-smooth potential)

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.



Serious aspect. Evolution equations with pattern formation reveal qualitity of numerical approximations, since differences in solution readily identified.

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

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

Former work. Results on operator splitting methods in different contexts are provided by former work (with W. Auzinger & H. Hofstätter & O. Koch, Ph. Chartier & F. Méhats, B. Kaltenbacher).

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

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

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

Areas of application

Situation. Consider nonlinear evolution equation of form

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

Areas of application.

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

Illustrations (BEC, Pattern formation)

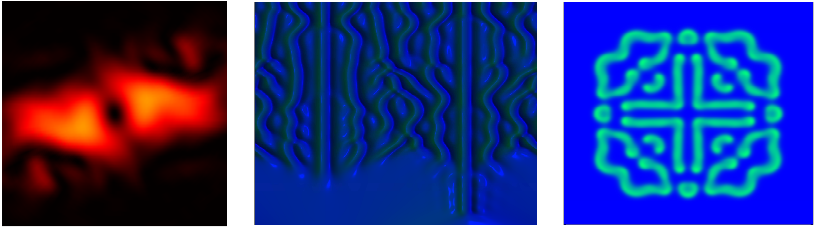


Illustration (Gray–Scott equations)

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

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

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

MOVIES

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!

Conclusions and future work

Conclusions and future work

Summary.

- Commutator-free quasi-Magnus exponential integrators form favourable class of time discretisation methods for linear evolution equations of Schrödinger type and of parabolic type. Theoretical analysis contributes to deeper understanding (reveals approach to resolve stability issues, explains order reductions causing signifcant loss of accuracy).

Current and future work.

- Design time-adaptive schemes (optimisation of solar cells).
- Study commutator-free integrators in combination with splitting for nonlinear equations.
  - Provide implementation for GPE (quantum turbulence).
  - Improve performance of implementation for deterministic Gray–Scott equations. Introduce time integrators for stochastic counterpart (multiplicative noise).

Thank you!