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

Mechthild Thalhammer

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Contents and related work

Contents.

- Commutator-free quasi-Magnus (CFQM) exponential integrators for non-autonomous linear evolution equations
  Appropriate name thanks to Arieh Iserles
- Splitting methods for nonlinear autonomous evolution equations
  Possibility of local error control with negligible additional cost
- CFQM exponential integrators combined with splitting methods for non-autonomous nonlinear evolution equations

Focus in this talk.

- Joint work with SERGIO BLANES and FERNANDO CASAS.

Related work.

- With WINFRIED AUZINGER, KARSTEN HELD, OTHMAR KOCH.
- With ERIKA HAUSENBLAS.

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.* IMA J. Numer. Anal. (2017).
  - 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)

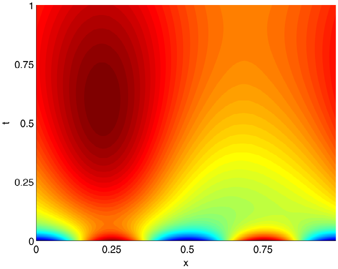
Test equation. Consider non-autonomous linear evolution equation

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

Impose periodic boundary conditions and regular initial condition.

Special choice. In particular, set

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



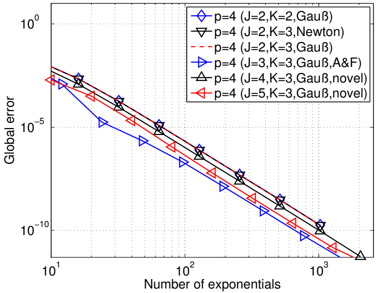
First illustration (Parabolic equation)

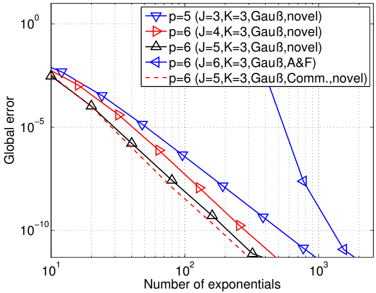
One must watch the convergence of a numerical code as carefully as a father watching his four year old play near a busy road. J. P. Boyd

Time integration. Apply commutator-free quasi-Magnus exponential integrators and related method of non-stiff orders $p = 4, 5, 6$. 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

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

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

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

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).
- possibly high 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

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

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

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

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

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

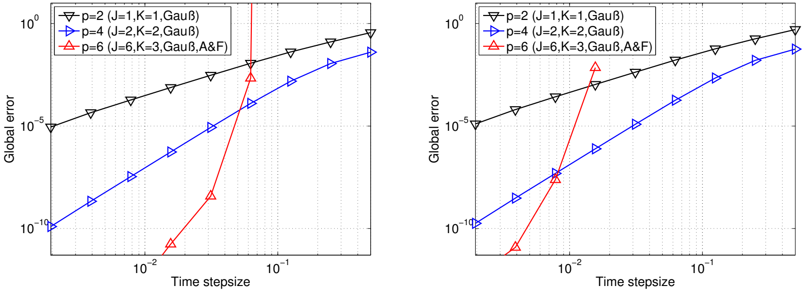
$$b_1 = a_{11} + a_{12} = \tfrac{1}{2} = a_{21} + a_{22} = b_2\,.$$

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

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

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

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

Basic assumptions on methods

Commutator-free quasi-Magnus exponential integrators. High-order commutator-free quasi-Magnus exponential 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 quasi-Magnus exponential 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 CFQM exponential 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* $n \in \{0, 1, \dots, N\}$ *and time increments* $0 < \tau_n \leq \tau_{\max}$

$$\big\| u_n - u(t_n) \big\|_X \leq C \left(\big\| u_0 - u(t_0) \big\|_X + \tau_{\max}^p \right).$$

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 $\partial_x^{p-1} u(t) \in L^2(\Omega, \mathbb{C})$ sufficient.

Main tools of proof

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

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

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

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

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 $\tau > 0$)

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

- 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.)

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

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

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

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

Design of novel schemes

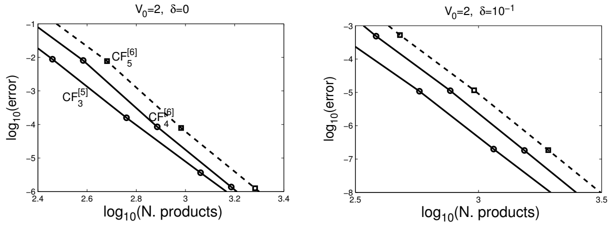
Additional practical constraints.

- 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))

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

- 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.

Remarks on operator splitting methods for nonlinear evolution equations

Possibility of local error control with negligible additional cost

Splitting methods

Situation. Consider autonomous linear evolution equation of form

$$\begin{cases} u'(t) = A\,u(t) + B\,u(t)\,, & t \in (0,T)\,, \\ u(0) = u_0\,. \end{cases}$$

Approach. Apply pth-order splitting method involving s compositions

$$u_{n+1} = \mathrm{e}^{b_s \tau_n B}\,\mathrm{e}^{a_s \tau_n A} \cdots \mathrm{e}^{b_1 \tau_n B}\,\mathrm{e}^{a_1 \tau_n A}\,u_n \;\approx\; u(t_{n+1}) = \mathrm{e}^{\tau_n (A+B)}\,u(t_n)\,.$$

Realisation straightforward

$$\begin{aligned} & u = u_n \\ & \text{for } j = 1:s \\ & \qquad u = \mathrm{e}^{a_j \tau_n A}\,u \\ & \qquad u = \mathrm{e}^{b_j \tau_n B}\,u \\ & \text{end} \\ & u_{n+1} = u \end{aligned}$$

Basic approach for local error estimation

Approach for local error estimation. For instance, consider splitting method by Blanes, Moan or splitting method by Yoshida (complex coefficients, melt two subsequent time steps), where

$$p = 4\,, \qquad s = 7\,.$$

Auxiliary third-order approximation obtained by suitable linear combination of intermediate values used for local error estimation

$$\begin{aligned}
&u = u_n\,, && u_{\text{Estimator}} = \alpha_0\, u\\
&\text{for } j = 1 : s &&\\
&\qquad u = \mathrm{e}^{a_j \tau_n A}\, u\,, && u_{\text{Estimator}} = u_{\text{Estimator}} + \alpha_{2j-1}\, u\\
&\qquad u = \mathrm{e}^{b_j \tau_n B}\, u\,, && u_{\text{Estimator}} = u_{\text{Estimator}} + \alpha_{2j}\, u\\
&\text{end} &&\\
&u_{n+1} = u\,, && \text{Local error estimator} = u - u_{\text{Estimator}}
\end{aligned}$$

Remark. Extension to nonlinear evolution equations straightforward.

Illustration (Semi-classical nonlinear Schrödinger equ.)

Situation. Consider nonlinear Schrödinger equation in semi-classical regime (decisive parameter $\varepsilon > 0$). Time integration by fourth-order splitting method with constant time stepsize $\Delta t = \varepsilon$ fails.

Blanes & Moan (novel, p = 4)
Solution at time t = 3, Tolerance tol = 0, Number of time steps N = 300
Semi–classical parameter eps = 0.01, M = 4096

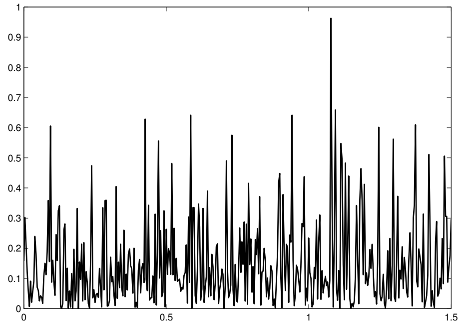


Illustration (Semi-classical nonlinear Schrödinger equ.)

Approach. Use novel approach for local error control. Obtain reliable result for initial time stepsize $\Delta t = \varepsilon$ and different tolerances.

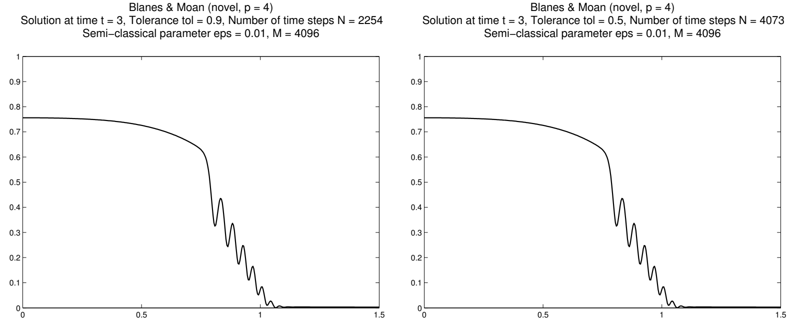
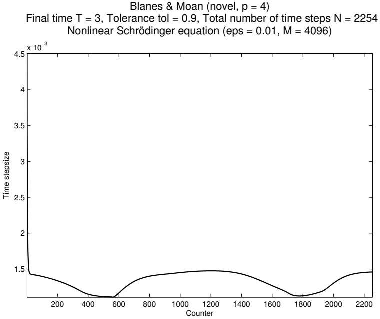


Illustration (Semi-classical nonlinear Schrödinger equ.)



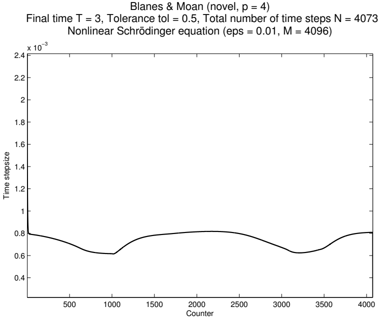


Illustration (Gray–Scott equations)

Yoshida (complex, novel, p = 4)
Solution at time t = 3000, Tolerance tol = 0.9, Number of time steps N = 2481
Second component, M = 10000

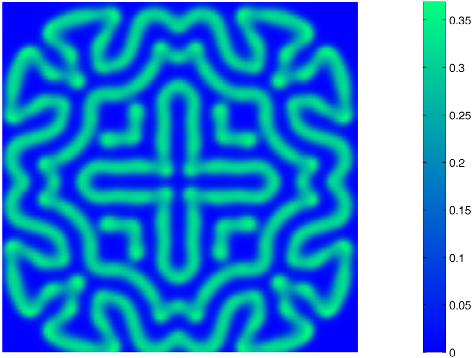


Illustration (Gray–Scott equations)

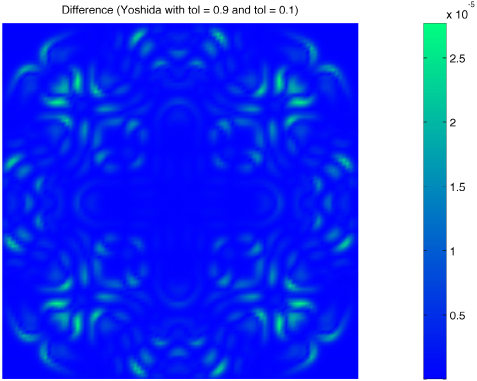
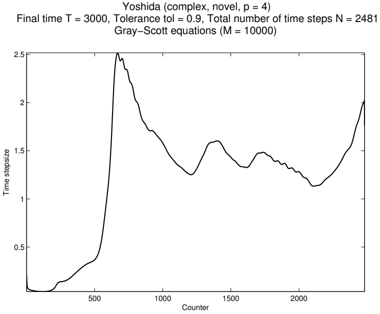
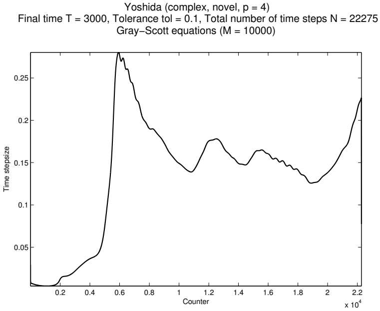


Illustration (Gray–Scott equations)





Remarks on extension to non-autonomous nonlinear evolution equations

Extension to nonlinear evolution equations

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

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

that is, solve sequence of related autonomous nonlinear equations

$$u'(t) = \mathscr{A}_{jn}\, u(t) + b_j\, B\big(u(t)\big), \qquad t \in (t_n, t_{n+1}),$$

$$\mathscr{A}_{jn} = \sum_{k=1}^{K} a_{jk}\, A(t_n + c_k \tau_n), \qquad b_j = \sum_{k=1}^{K} a_{jk}, \qquad j \in \{1, \dots, J\},$$

by means of splitting methods.

Areas of application

Situation. Consider nonlinear evolution equation of form

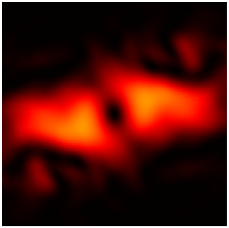
$$u'(t) = A(t)\,u(t) + B\big(u(t)\big)\,, \quad t \in (t_0, T)\,.$$

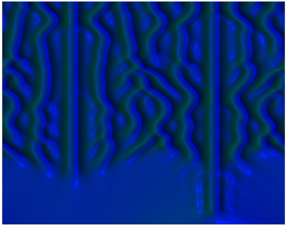
Areas of application.

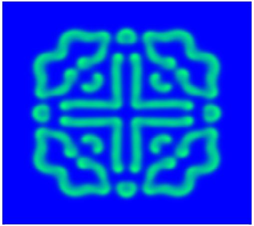
- Nonlinear Schrödinger equations
  Gross–Pitaevskii equations with opening trap
  Gross–Pitaevskii equations with rotation (moving frame)

- 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)







Movies

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.

- Study approach used for local error estimation of splitting methods.
- Study commutator-free integrators in combination with splitting methods for nonlinear equations.
  - Provide implementation for GPE (quantum turbulence).
  - Improve performance of implementation for deterministic Gray–Scott equations (GPU).

Thank you!