Convergence analysis of high-order commutator-free exponential integrators for non-autonomous linear evolution equations

Mechthild Thalhammer
Leopold–Franzens Universität Innsbruck, Austria

The 10th AIMS Conference on
Dynamical Systems, Differential Equations and Applications
Special Session 63 on Advanced High Order Geometric Numerical Integration Methods for Differential Equations
July 2014, Madrid, Spain

Theme

Exponential integrators. Efficient time integration of non-autonomous linear evolution equations by commutator-free exponential integrators

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = A(t)\, u(t)\,, \quad t \in (t_0, T)\,, \\ u(t_0) \text{ given}\,, \end{cases}$$

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

$$A_{nk} = A(t_n + c_k \tau_n)\,, \quad B_{nj} = \sum_{k=1}^{K} a_{jk}\, A_{nk}\,, \quad (j,k) \in \{1,\dots,J\} \times \{1,\dots,K\}\,,$$

$$\mathscr{S}(\tau_n, t_n) = \prod_{j=1}^{J} \mathrm{e}^{\tau_n B_{nj}} = \mathrm{e}^{\tau_n B_{nJ}} \cdots \mathrm{e}^{\tau_n B_{n1}}\,, \quad n \in \{0,1,\dots,N-1\}\,.$$

Applications.

- Linear evolution equations of Schrödinger type (time-dependent Hamilton operators)
- Linear evolution equations of parabolic type (dissipative systems)

Outline

Theme. Theoretical analysis of commutator-free exponential integrators for time integration of non-autonomous linear evolution equations.

Outline.

- Commutator-free exponential integrators
- Stability and error analysis
  - Evolution equations of Schrödinger type
  - Evolution equations of parabolic type
- Numerical illustrations

References

Main inspiration.

- Application of commutator-free 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.

- Previous work on construction of commutator-free exponential integrators.

S. Blanes and 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.

- Previous work on error analysis of fourth-order commutator-free exponential integrator for initial-boundary value problems of parabolic type.

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

Main reference.

Sergio Blanes, Fernando Casas, M. Th.
Convergence analysis of high-order commutator-free exponential integrators for non-autonomous linear evolution equations.
In preparation.

High-order commutator-free exponential integrators

Magnus expansion

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = A(t)\, u(t)\,, \quad t \in (t_0, T)\,, \quad u(t_0) \text{ given}\,,$$

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

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

Magnus integrators. Truncation of Magnus expansion and application of suitable quadrature formulae for approximations of integrals leads to 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)

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

Magnus integrators and related exponential methods

Higher-order Magnus integrators.

- Fourth-order 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

- larger computational costs for realisation of exponentials,
- loss of structure (decisive factor for evolution equations of parabolic type).

Alternative. Commutator-free exponential integrators provide useful alternative to integrators based on Magnus expansion.

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 exponential integrators

Time-stepping approach. Time integration of non-autonomous linear evolution equation on Banach space $(X, \|\cdot\|_X)$

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = A(t)\, u(t)\,, \quad t \in (t_0, T)\,, \quad u(t_0) \text{ given}\,.$$

Approximations at time grid points $t_0 < t_1 < \dots < t_N \leq T$ with increments $\tau_n = t_{n+1} - t_n$ given by recurrence

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

Commutator-free methods. Commutator-free exponential integrators rely on presumption that exponential of $A_{nk} = A(t_n + c_k \tau_n)$ and linear combinations computable in accurate and efficient manner.

General form. High-order commutator-free exponential integrators cast into general form with real nodes $c_k \in \mathbb{R}$ and real or complex coefficients $a_{jk} \in \mathbb{K}$ for $(j,k) \in \{1, \dots, J\} \times \{1, \dots, K\}$

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

Basic assumptions

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

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

Nodes and coefficients.

- Relate nodes to quadrature nodes and suppose

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

- 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 require

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

to ensure well-definededness of commutator-free methods within analytical framework of sectorial operators and analytic semigroups.

Examples (Nonstiff orders $p = 2, 3, 4$)

Order 2. Commutator-free method based on single Gaussian node involves single exponential at each time step

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

Method coincides with exponential midpoint rule (Magnus integrator).

Order 3. Commutator-free method based on two Gaussian nodes requires evaluation of two exponentials at each time step

$$p = 3\,, \quad J = 2 = K\,, \quad c_k = \tfrac{1}{2} \mp \tfrac{\sqrt{3}}{6}\,, \quad \beta = \tfrac{1}{4} - \tfrac{\sqrt{3}}{4}\,,$$
$$a_{11} = \tfrac{\sqrt{3}}{3}\,, \quad a_{12} = 0\,, \quad a_{21} = \big(1 - \tfrac{\sqrt{3}}{3}\big)\beta\,, \quad a_{22} = \big(1 - \tfrac{\sqrt{3}}{3}\big)(1-\beta)\,, \quad b_1 = \tfrac{\sqrt{3}}{3}\,, \quad b_2 = 1 - \tfrac{\sqrt{3}}{3}\,,$$
$$\mathscr{S}(\tau_n, t_n) = \mathrm{e}^{\tau_n (a_{21} A_{n1} + a_{22} A_{n2})}\, \mathrm{e}^{\tau_n (a_{11} A_{n1} + a_{12} A_{n2})}\,.$$

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

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

Method suitable for evolution equations of parabolic type, since

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

Example (Nonstiff order $p = 6$)

Order 6. Example of (non-optimised) commutator-free method obtained from coefficients given in ALVERMANN, FEHSKE combined with sixth-order quadrature approximation based on three Gaussian nodes and corresponding weights

$$c_1 = \tfrac{1}{2}\Big(1-\sqrt{\tfrac{3}{5}}\Big), \quad c_2 = \tfrac{1}{2}, \quad c_3 = \tfrac{1}{2}\Big(1+\sqrt{\tfrac{3}{5}}\Big), \quad w_1 = \tfrac{5}{18} = w_3, \quad w_2 = \tfrac{4}{9},$$

$$f = \begin{pmatrix} 0.160000000000000 & 0.151015389377465 & 0.133046168132396 \\ -0.227381647426963 & -0.087654259755115 & 0.069919836812657 \\ 0.567381647426963 & 0.210351545122098 & -0.202966004945053 \end{pmatrix},$$

$$F = \begin{pmatrix} f_{11} & -f_{12} & f_{13} \\ f_{21} & -f_{22} & f_{23} \\ f_{31} & -f_{32} & f_{33} \\ f_{31} & f_{32} & f_{33} \\ f_{21} & f_{22} & f_{23} \\ f_{11} & f_{12} & f_{13} \end{pmatrix}, \quad G = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 6 & 0 \\ -\frac{5}{2} & 0 & 30 \end{pmatrix}, \quad Q = \begin{pmatrix} w_1 & w_2 & w_3 \\ w_1(c_1-\frac{1}{2}) & w_2(c_2-\frac{1}{2}) & w_3(c_3-\frac{1}{2}) \\ w_1(c_1-\frac{1}{2})^2 & w_2(c_2-\frac{1}{2})^2 & w_3(c_3-\frac{1}{2})^2 \end{pmatrix},$$

$$a = FGQ = \begin{pmatrix} 0.215838996975768 & -0.076717964591551 & 0.020878967615784 \\ -0.080897796320853 & -0.178747217537158 & 0.032263366431047 \\ 0.180628460055830 & 0.477687404350931 & -0.090934216979798 \\ -0.090934216979798 & 0.477687404350931 & 0.180628460055830 \\ 0.032263366431047 & -0.178747217537158 & -0.080897796320853 \\ 0.020878967615784 & -0.076717964591551 & 0.215838996975768 \end{pmatrix},$$

$$\mathscr{S}(\tau_n, t_n) = \prod_{j=1}^{6} \mathrm{e}^{\tau_n (a_{j1} A_{n1} + a_{j2} A_{n2} + a_{j3} A_{n3})}.$$

Method suitable for evolution equations of Schrödinger type. Poor stability behaviour for evolution equations of parabolic type, since

$$b_j = \sum_{k=1}^{K} a_{jk} = f_{j1}, \quad j \in \{1,\dots,J\}.$$

Analytical framework

Evolution equations of Schrödinger type

Evolution equations of parabolic type

Model problem

Model problem. For purpose of illustration study academic initial-boundary value problem for $U : \overline{\Omega} \times [t_0, T] \to \mathbb{K}$

$$\begin{cases} \partial_t U(x,t) = \big(\alpha(x,t)\,\partial_{xx} + \beta(x,t)\,\partial_x + \gamma(x,t)\,I\big)\,U(x,t)\,, & (x,t) \in \Omega \times (t_0,T)\,, \\ U(x,t_0) \text{ given}\,. \end{cases}$$

Abstract formulation. In regard to introduction and error analysis of commutator-free exponential integrators rewrite model problem as abstract initial value problem for $u : [t_0, T] \to X$

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\,u(t) = A(t)\,u(t)\,, & t \in (t_0,T)\,, \\ u(t_0) \text{ given}\,. \end{cases}$$

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.

Basic assumption. Assume that domain of defining linear operator $A(t) : D \subset X \to X$ time-independent, dense and continuously embedded.

Evolution equation of Schrödinger type

Schrödinger equation. Consider time-dependent linear Schrödinger equation for $U : \overline{\Omega} \times [t_0, T] \to \mathbb{C}$

$$\partial_t U(x,t) = \big(\alpha(x,t)\,\partial_{xx} + \beta(x,t)\,\partial_x + \gamma(x,t)\,I\big)\,U(x,t)\,, \quad (x,t) \in \Omega \times (t_0, T)\,.$$

Impose periodic boundary conditions and regular initial condition.

Analytical framework. Employ abstract formulation

$$\frac{\mathrm{d}}{\mathrm{d}t}\,u(t) = A(t)\,u(t)\,, \quad t \in (t_0, T)\,.$$

Utilise basic assumption that defining linear operator $A(t) : D \subset X \to X$ generates unitary group $(\mathrm{e}^{\sigma A(t)})_{\sigma \in \mathbb{R}}$ on underlying Hilbert space X.

Stability. Note that basic assumption satisfied, whenever $\mathrm{i}\,A(t)$ defines selfadjoint operator on Hilbert space (Stone's Theorem). As basic property of selfadjointness preserved by linear combinations involving real coefficients, unitarity of discrete evolution operator follows

$$\Big\| \prod_{n=N_0}^{N_1} \mathscr{S}(\tau_n, t_n) \Big\|_{X \leftarrow X} = 1\,, \quad a_{jk} \in \mathbb{R}\,, \quad (j,k) \in \{1,\dots,J\} \times \{1,\dots,K\}\,.$$

Evolution equation of Schrödinger type

Schrödinger equation. Consider time-dependent linear Schrödinger equation

$$\partial_t U(x,t) = \big(\alpha(x,t)\,\partial_{xx} + \beta(x,t)\,\partial_x + \gamma(x,t)\,I\big)\,U(x,t)\,, \quad (x,t) \in \Omega \times (t_0,T)\,.$$

Special case. Relevant applications justify study of simplest case, where defining operator comprises Laplacian and regular real-valued time-space-dependent multiplication operator

$$\alpha = \mathrm{i}\,, \quad \beta = 0\,, \quad \gamma(x,t) = \mathrm{i}\,V(x,t) \in \mathrm{i}\,\mathbb{R}\,, \qquad \frac{\mathrm{d}}{\mathrm{d}t}\,u(t) = A(t)\,u(t) = \mathrm{i}\,\big(\partial_{xx} + V(t)\big)\,u(t)\,, \quad t \in (t_0,T)\,.$$

Straightforward argument proves preservation of L^2-norm which implies unitarity of evolution operator on Hilbert space $X = L^2(\Omega)$ and in particular ensures well-definededness of evolution operator on X

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\|u(t)\|_{L^2} = 2\,\Re\big(A(t)u(t)\big|u(t)\big)_{L^2} = 2\,\Re\Big(\mathrm{i}\,\underbrace{\big(\partial_{xx}u(t)\big|u(t)\big)_{L^2}}_{\in\mathbb{R}} + \mathrm{i}\,\underbrace{\big(V(t)u(t)\big|u(t)\big)_{L^2}}_{\in\mathbb{R}}\Big) = 0\,,$$

$$\|u(t)\|_{L^2} = \|u(t_0)\|_{L^2}\,, \quad u(t) = \mathrm{e}^{\Omega(t-t_0,t_0)}\,u(t_0) \in L^2(\Omega)\,, \quad u(t_0) \in L^2(\Omega)\,, \quad t \in (t_0,T)\,.$$

Remarks.

- Note that spatial derivative $v = \partial_x u$ satisfies evolution equation $\frac{\mathrm{d}}{\mathrm{d}t}\,v(t) = A(t)\,v(t) + \partial_x V(t)u(t)$. Variation-of-constants formula implies $v(t) \in X$ if $v(0) \in X$ and $\partial_x V$ regular.
- Involved task to justify $\mathrm{e}^{\Omega(t-t_0,t_0)} : X \to X$ for parabolic equations!

Evolution equation of parabolic type

Parabolic equation. Consider linear diffusion-advection-reaction equation for $U : \overline{\Omega} \times [t_0, T] \to \mathbb{R}$

$$\partial_t U(x,t) = \big(\alpha(x,t)\,\partial_{xx} + \beta(x,t)\,\partial_x + \gamma(x,t)\,I\big)\,U(x,t)\,, \quad (x,t) \in \Omega \times (t_0, T)\,.$$

Impose certain boundary conditions and regular initial condition.

Analytical framework. Employ abstract formulation

$$\frac{\mathrm{d}}{\mathrm{d}t}\,u(t) = A(t)\,u(t)\,, \quad t \in (t_0, T)\,.$$

Utilise basic assumption that defining linear operator $A(t) : D \subset X \to X$ sectorial and generates analytic semigroup $(\mathrm{e}^{\sigma A(t)})_{\sigma \in [0,\infty)}$ on underlying Banach space X.

Stability. As basic property of sectoriality is preserved by suitable linear combinations, boundedness of discrete evolution operator follows (details given below)

$$\Big\| \prod_{n=N_0}^{N_1} \mathscr{S}(\tau_n, t_n) \Big\|_{X \leftarrow X} \leq C\,, \quad \Re\, b_j \geq 0\,, \quad b_j = \sum_{k=1}^{K} a_{jk}\,, \quad j \in \{1, \dots, J\}\,.$$

Evolution equation of parabolic type

Hypothesis

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

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

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

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

Defining operator satisfies $A \in \mathscr{C}^\vartheta\big([t_0, T], L(D, X)\big)$ for some $0 < \vartheta \leq 1$, i.e., there exists $C_3 > 0$ such that

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

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

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

Evolution equation of parabolic type

Well-definedness. Employ analytical framework of sectorial operators and analytic semigroups. Basic assumption on coefficients

$$\Re\, b_j \geq 0\,, \quad b_j = \sum_{k=1}^{K} a_{jk}\,, \quad 1 \leq j \leq J\,,$$

ensures that high-order commutator-free methods remain well-defined on underlying Banach space. Indeed, sum of sectorial operator $b_j\, A(t_n) : D \to X$ and bounded remainder (Hölder continuity assumption) defines sectorial operator

$$B_{nj} = \sum_{k=1}^{K} a_{jk}\, A(t_n + c_k \tau_n) = b_j\, A(t_n) + \sum_{k=1}^{K} a_{jk} \big(A(t_n + c_k \tau_n) - A(t_n) \big) : D \to X\,.$$

Theorem (Stability)

Under basic hypotheses on operator family, sequence of time stepsizes, and coefficients, discrete evolution operator associated with high-order commutator-free method satisfies bound

$$\Big\| \prod_{n=N_0}^{N_1} \mathscr{S}(\tau_n, t_n) \Big\|_{X \leftarrow X} \leq C\,, \quad \mathscr{S}(\tau_n, t_n) = \prod_{j=1}^{J} \mathrm{e}^{\tau_n B_{nj}}\,,$$

with constant $C > 0$ independent of stepsize sequence.

Convergence result
Numerical illustrations

Convergence result

Convergence result. Employ fundamental hypotheses on operator family defining non-autonomous linear evolution equations of Schrödinger or parabolic type. Assume that coefficients of commutator-free methods fulfill basic assumptions and conditions for nonstiff order p. Recall assumption on ratios of subsequent time stepsizes.

Theorem

Provided that operator family and exact solution sufficiently regular such that remainder arising in local error expansion bounded in underlying Banach space, convergence estimate holds with constant $C > 0$ *independent of* n *and time increments* $0 < \tau_n \leq \tau_{\max}$

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

Crucial point. Specify regularity and compatibility requirements on initial state.

Special case. Details included below for special case $A(t) = \mathrm{i}\,\Delta + \mathrm{i}\,V(t)$ with regular potential and exponential midpoint rule ($p = 2$). Straightforward approach based on step-wise Taylor series expansions yields restrictive regularity requirement $\partial_x^6 u(0) \in X$, whereas favourable approach based on variable-of-constants formula leads to condition $\partial_x u(0) \in X$.

Illustration (Evolution equation of Schrödinger type)

Schrödinger equation. Consider time-dependent linear Schrödinger equation for $U:\overline{\Omega}\times[t_0,T]\to\mathbb{C}$

$$\partial_t U(x,t) = \big(\alpha(x,t)\,\partial_{xx} + \beta(x,t)\,\partial_x + \gamma(x,t)\,I\big)\,U(x,t)\,, \quad (x,t)\in\Omega\times(t_0,T)\,.$$

Impose periodic boundary conditions and regular initial condition.

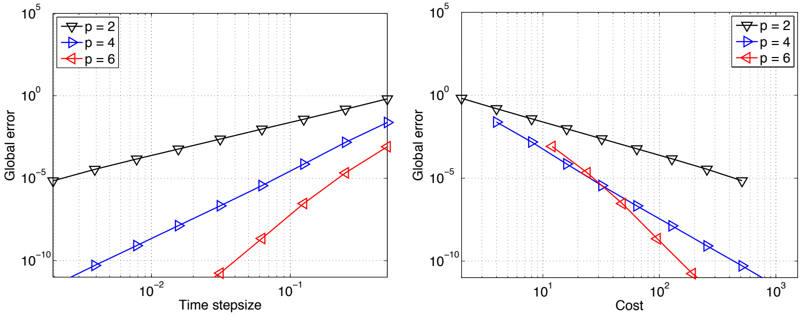
Special choice. For numerical example set

$$\Omega=(0,2\pi)\,,\quad t_0=0\,,$$
$$\alpha(x,t)=\mathrm{i}\,\mathrm{e}^{-\cos x}\,(\sin t)^2\,,\quad \beta(x,t)=0\,,\quad \gamma(x,t)=\mathrm{i}\,\mathrm{e}^{\sin x}\,\big(1+\mathrm{e}^{-t}\big)\,,$$
$$U(x,0)=\sin(2x)\,.$$

Space and time discretisation. Spatial discretisation by standard symmetric finite differences ($M=100$). Time integration by commutator-free methods of nonstiff orders $p=2,4,6$ with time increments $2^{-1},\dots,2^{-9}$. Numerical approximation for finest time stepsize serves as reference solution.

Illustration (Evolution equation of Schrödinger type)

Illustration. Numerical example for initial-boundary value problem of Schrödinger type confirms convergence result for commutator-free methods of nonstiff orders $p = 2, 4, 6$.



Global errors at time $T = 1$ versus chosen time stepsizes or cost (number of matrix exponentials $J \times N$).

Illustration (Evolution equation of parabolic type)

Diffusion-advection-reaction equation. Consider linear diffusion-advection-reaction equation for $U : \overline{\Omega} \times [t_0, T] \to \mathbb{R}$

$$\partial_t U(x,t) = \big(\alpha(x,t)\,\partial_{xx} + \beta(x,t)\,\partial_x + \gamma(x,t)\,I\big)\,U(x,t)\,, \quad (x,t) \in \Omega \times (t_0, T)\,.$$

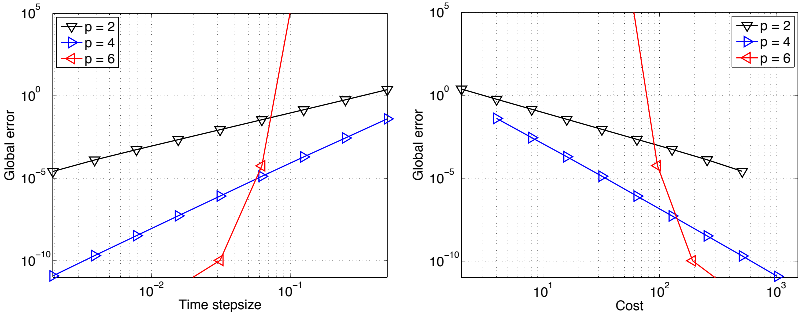
Impose periodic boundary conditions and regular initial condition.

Special choice. For numerical example set

$$\Omega = (0, 2\pi)\,, \qquad t_0 = 0\,,$$
$$\alpha(x,t) = \mathrm{e}^{-\cos x}\,(\sin t)^2\,, \quad \beta(x,t) = \partial_x \alpha(x,t)\,, \quad \gamma(x,t) = \mathrm{e}^{\sin x}\,\big(1 + \mathrm{e}^{-t}\big)\,,$$
$$U(x,0) = \sin(2x)\,.$$

Illustration (Evolution equation of parabolic type)

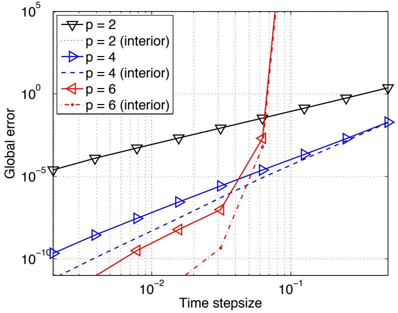
Illustration. Numerical example for initial-boundary value problem of parabolic type confirms convergence result for commutator-free methods of nonstiff orders $p = 2, 4, 6$ (periodic boundary conditions, full order of convergence). Note that sixth-order commutator-free method involving negative coefficients shows poor stability behaviour.

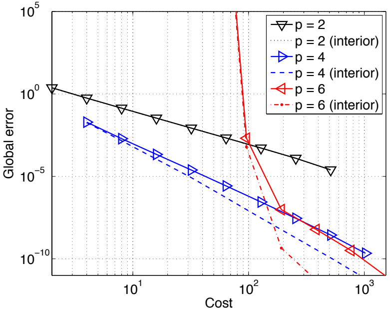


Global errors at $T = 1$ versus chosen time stepsizes or cost.

Illustration (Evolution equation of parabolic type)

Additional illustration. Numerical example for initial-boundary value problem of parabolic type illustrates expected (rather mild) order reductions for commutator-free methods of nonstiff orders $p = 4, 6$ (homogeneous Dirichlet boundary conditions, higher convergence rates obtained in interior of spatial domain).

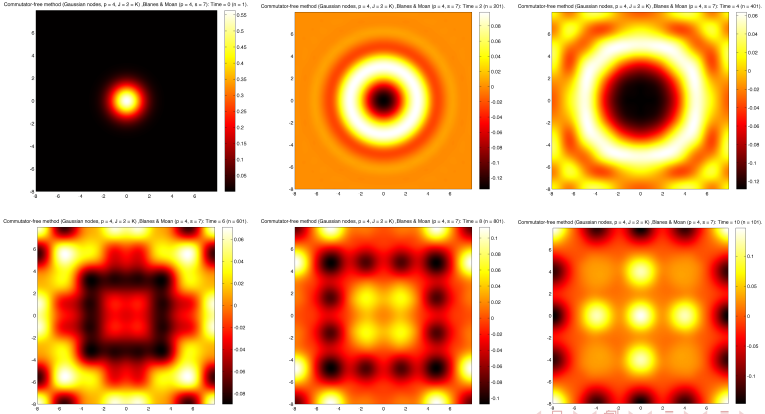




Global errors at $T = 1$, measured on entire spatial domain and in interior, respectively, versus chosen time stepsizes or cost.

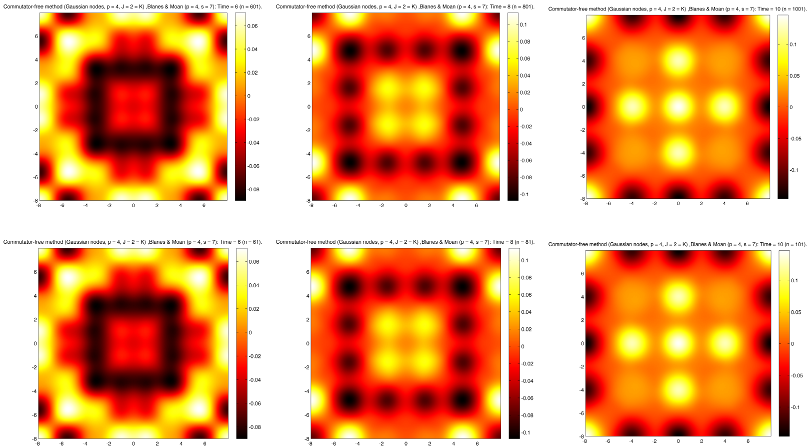
Further illustration

Schrödinger equation with time-dependent Hamiltonian. Inspired by paraxial model for light propagation in inhomogeneous media (refractive index), see G. THALHAMMER. Time integration of linear Schrödinger equation with time-dependent Hamiltonian (non-smooth time-space dependent potential, 2D) by commutator-free methods combined with time-splitting Fourier spectral methods.



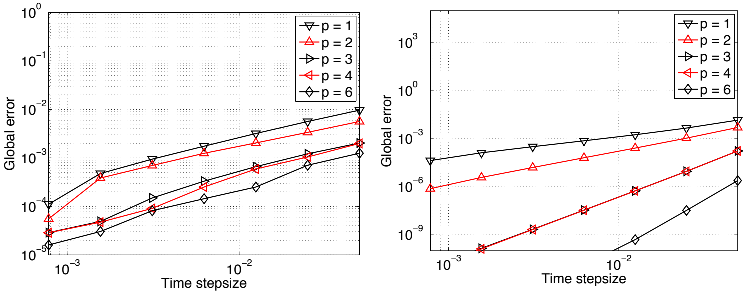
Further illustration

Comparison of obtained results for $N = 1000$ ($\tau = \frac{1}{100}$, first row) and reduced number of time steps $N = 100$ ($\tau = \frac{1}{10}$, second row).



Further illustration

Schrödinger equation with time-dependent Hamiltonian. Time integration of linear Schrödinger equation in 2D with time-dependent Hamiltonian (time-space dependent potential) by commutator-free methods combined with time-splitting Fourier spectral methods. Global errors for non-smooth (order reductions) versus smooth potential (full order of convergence).



Local error analysis

Local error analysis

Aim. Deduce local error expansion suitable for evolution equations involving unbounded operators

$$\delta_{n+1} = \mathscr{S}(\tau_n, t_n)\, u(t_n) - u(t_{n+1}) = \prod_{j=1}^{J} \mathrm{e}^{\tau_n B_{nj}}\, u(t_n) - u(t_{n+1}) \,.$$

Main tool. Representation of exact solution value obtained by suitable linearisation and application of variation-of-constants formula.

- Favourable approach utilised e.g. in LUNARDI (1995) for construction of evolution operator associated with non-autonomous evolution equation of parabolic type (involved task to justify $\mathrm{e}^{\Omega(t-t_0,t_0)} : X \to X$).
- Approach turns out to be favourable in connection with evolution equations of Schrödinger type. Allows to simplify considerations given in HOCHBRUCK, LUBICH (2003) for exponential midpoint rule ($A(t) = \mathrm{i}\,\Delta + \mathrm{i}\,V(t)$, see below).

Further tools. Taylor series expansions for differences of form $A(t) - A(s)$ appropriate. Differentiation of terms of form $\mathrm{e}^{(t-\tau)A(t)}\, A'(\sigma)\, \mathrm{e}^{\tau A(t)}$ yields iterated commutators.

Special case

Aim. Study local error behaviour of exponential midpoint rule for approximation of solution to non-autonomous linear evolution equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = A(t)\, u(t)\,, \quad t \in (t_0, T)\,, \quad u(t_0) \text{ given}\,.$$

Focus on simplest case, where defining operator comprises Laplacian and real-valued multiplication operator

$$A(t) = \mathrm{i}\,\partial_{xx} + \mathrm{i}\, V(t) : D \to X\,.$$

Recall that associated evolution operator unitary on Hilbert space $X = L^2(\Omega)$

$$u(t) = \mathrm{e}^{\Omega(t-t_0, t_0)}\, u(0)\,, \quad \|u(t)\|_{L^2} = \|u(t_0)\|_{L^2}\,, \quad u(t_0) \in X\,, \quad t \in (t_0, T)\,.$$

Consider first time step and employ simplifiying assumptions $t_0 = 0$ and $u_0 = u(0)$

$$u_1 = \mathrm{e}^{\tau A\left(\frac{\tau}{2}\right)}\, u(0) \approx u(\tau)\,.$$

Aim at derivation of local error expansion reflecting nonstiff order of convergence, avoiding restrictive regularity requirements

$$u_1 - u(\tau) = \mathrm{e}^{\tau A\left(\frac{\tau}{2}\right)}\, u(0) - u(\tau) = \mathscr{O}\left(\tau^3\right).$$

Approaches

Approaches.

- **Infinite series.** Expansions based on infinite series useful for construction of novel schemes, but not suitable for local error analysis of commutator-free methods applied to evolution equations involving unbounded operators, since arguments persist at formal level.

- **Step-wise Taylor series expansions.** Straightforward step-wise expansions of exact solution and evolution operator yield well-defined local error representations, but imply unnatural restrictions.
  In present situation expansion of exact solution

$$u(\tau) = u(0) + \tau A(0) u(0) + \tfrac{1}{2}\, \tau^2 \big(A'(0) + A(0) A(0)\big) u(0)$$
$$+ \tfrac{1}{2} \int_0^1 (1-\zeta)^2\, \tau^3 \big(A''(\zeta\tau) + 2A'(\zeta\tau) A(\zeta\tau) + A(\zeta\tau) A'(\zeta\tau) + A(\zeta\tau) A(\zeta\tau) A(\zeta\tau)\big) u(\zeta\tau)\, \mathrm{d}\zeta$$

  well-defined, provided that $A^3 u \in X$, i.e. $\partial_x^6 u(0) \in X$.

- **Linearisation and variation-of-constants-formula.** Employ favourable approach based on suitable linearisation

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = A(t_{\text{frozen}})\, u(t) + \big(A(t) - A(t_{\text{frozen}})\big)\, u(t)$$

  and application of variation-of-constants formula, see A. Lunardi.
  In present situation regularity requirement $[A, A']u = [A, V']u \in X$, i.e. $\partial_x u(0) \in X$ results.
  Challenge to extend approach to high-order commutator-free methods.

Local error expansion (Exponential midpoint rule)

Initial local error representation. Favourable approach based on suitable linearisation of evolution equation and application of variation-of-constants formula yields

$$\frac{\mathrm{d}}{\mathrm{d}t}\, u(t) = A(t)\, u(t) = A\big(\tfrac{\tau}{2}\big)\, u(t) + \big(A(t) - A\big(\tfrac{\tau}{2}\big)\big)\, u(t)\,,$$

$$u(\tau) = \mathrm{e}^{\tau A\left(\frac{\tau}{2}\right)}\, u(0) + I_0\,, \quad I_0 = \int_0^\tau \mathrm{e}^{(\tau-\sigma) A\left(\frac{\tau}{2}\right)} \big(A(\sigma) - A\big(\tfrac{\tau}{2}\big)\big)\, u(\sigma)\, \mathrm{d}\sigma\,, \quad u_1 = \mathrm{e}^{\tau A\left(\frac{\tau}{2}\right)}\, u(0)\,,$$

$$u(\tau) - u_1 = I_0 = \int_0^\tau \mathrm{e}^{(\tau-\sigma) A\left(\frac{\tau}{2}\right)} \big(A\big(\tfrac{\tau}{2}\big) - A(\sigma)\big)\, u(\sigma)\, \mathrm{d}\sigma\,.$$

Remark. For special case $A(t) = \mathrm{i}\,(\partial_{xx} + V(t))$ evident that representation well-defined in underlying space

$$u(\tau) - u_1 = \int_0^\tau \underbrace{\mathrm{e}^{(\tau-\sigma) A\left(\frac{\tau}{2}\right)}}_{X \leftarrow X} \underbrace{\mathrm{i}\big(V\big(\tfrac{\tau}{2}\big) - V(\sigma)\big)\, u(\sigma)}_{\in X}\, \mathrm{d}\sigma \in X \quad \text{if} \quad u(0) \in X\,.$$

First expansion step. Employ auxiliary expansion to obtain first local error expansion

$$A\big(\tfrac{\tau}{2}\big) - A(\sigma) = \big(\tfrac{\tau}{2} - \sigma\big)\, A'(\sigma) + \int_0^1 (1-\zeta)\, \big(\tfrac{\tau}{2} - \sigma\big)^2 A''\big(\sigma + \zeta\big(\tfrac{\tau}{2} - \sigma\big)\big)\, \mathrm{d}\zeta\,,$$

$$u(\tau) - u_1 = I_1 + R_1\,, \quad I_1 = \int_0^\tau \big(\tfrac{\tau}{2} - \sigma\big)\, \mathrm{e}^{(\tau-\sigma) A\left(\frac{\tau}{2}\right)} A'(\sigma)\, u(\sigma)\, \mathrm{d}\sigma\,,$$

$$R_1 = \int_0^\tau \int_0^1 (1-\zeta)\, \big(\tfrac{\tau}{2} - \sigma\big)^2 \mathrm{e}^{(\tau-\sigma) A\left(\frac{\tau}{2}\right)} A''\big(\sigma + \zeta\big(\tfrac{\tau}{2} - \sigma\big)\big)\, u(\sigma)\, \mathrm{d}\zeta\, \mathrm{d}\sigma = \mathscr{O}\big(\tau^3, \mathrm{e}^{\tau A} A'' u\big)\,.$$

Local error expansion (Exponential midpoint rule)

Second expansion step. Further application of variation-of-constants formula yields

$$u(\sigma) = \mathrm{e}^{\sigma A\left(\frac{\tau}{2}\right)} u(0) + \int_0^\sigma \mathrm{e}^{(\sigma-\zeta) A\left(\frac{\tau}{2}\right)} \left(A(\zeta) - A\left(\tfrac{\tau}{2}\right)\right) u(\zeta)\, \mathrm{d}\zeta\,,$$

$$u(\tau) - u_1 = I_2 + R_1 + R_2\,, \quad I_2 = \int_0^\tau \left(\tfrac{\tau}{2} - \sigma\right) \mathrm{e}^{(\tau-\sigma) A\left(\frac{\tau}{2}\right)} A'(\sigma)\, \mathrm{e}^{\sigma A\left(\frac{\tau}{2}\right)} u(0)\, \mathrm{d}\sigma\,,$$

$$R_2 = \int_0^\tau \int_0^\sigma \left(\tfrac{\tau}{2} - \sigma\right) \mathrm{e}^{(\tau-\sigma) A\left(\frac{\tau}{2}\right)} A'(\sigma)\, \mathrm{e}^{(\sigma-\zeta) A\left(\frac{\tau}{2}\right)} \left(A(\zeta) - A\left(\tfrac{\tau}{2}\right)\right) u(\zeta)\, \mathrm{d}\zeta\, \mathrm{d}\sigma = \mathscr{O}\left(\tau^3, \mathrm{e}^{\tau A} A' \mathrm{e}^{\tau A} (A_1 - A_2) u\right).$$

Third expansion step. Rewrite dominant contribution and employ symmetry

$$f(\sigma) = \mathrm{e}^{(\tau-\sigma) A\left(\frac{\tau}{2}\right)} A'(\sigma)\, \mathrm{e}^{\sigma A\left(\frac{\tau}{2}\right)} u(0) = f(0) + \int_0^1 \sigma f'(\zeta\sigma)\, \mathrm{d}\zeta\,,$$

$$f'(\sigma) = \mathrm{e}^{(\tau-\sigma) A\left(\frac{\tau}{2}\right)} \left[A'(\sigma), A\left(\tfrac{\tau}{2}\right)\right] \mathrm{e}^{\sigma A\left(\frac{\tau}{2}\right)} u(0) + \mathrm{e}^{(\tau-\sigma) A\left(\frac{\tau}{2}\right)} A''(\sigma)\, \mathrm{e}^{\sigma A\left(\frac{\tau}{2}\right)} u(0)\,,$$

$$I_2 = \int_0^\tau \left(\tfrac{\tau}{2} - \sigma\right) f(\sigma)\, \mathrm{d}\sigma = \underbrace{\int_0^\tau \left(\tfrac{\tau}{2} - \sigma\right) f(0)\, \mathrm{d}\sigma}_{=0} + R_3\,,$$

$$R_3 = \int_0^\tau \int_0^1 \sigma \left(\tfrac{\tau}{2} - \sigma\right) f'(\zeta\sigma)\, \mathrm{d}\zeta\, \mathrm{d}\sigma = \mathscr{O}\left(\tau^3, \mathrm{e}^{\tau A} [A', A]\, \mathrm{e}^{\tau A} u, \mathrm{e}^{\tau A} A'' \mathrm{e}^{\tau A} u\right).$$

Local error expansion (Exponential midpoint rule)

Local error expansion. Altogether, this leads to local error expansion

$$u_1 - u(\tau) = \mathscr{O}\big(\tau^3, \mathrm{e}^{\tau A} A'' u, \mathrm{e}^{\tau A} A' \mathrm{e}^{\tau A} (A_1 - A_2) u, \mathrm{e}^{\tau A} [A', A]\, \mathrm{e}^{\tau A} u, \mathrm{e}^{\tau A} A'' \mathrm{e}^{\tau A} u\big).$$

Special case. For special case $A(t) = \mathrm{i}\,(\partial_{xx} + V(t))$ desired dependence $u_1 - u(\tau) = \mathscr{O}\big(\tau^3\big)$ obtained, provided that conditions satisfied

$$\mathrm{e}^{\tau A} V'' u \in X\,, \quad \mathrm{e}^{\tau A} V' \mathrm{e}^{\tau A} (V_1 - V_2) u \in X\,, \quad \mathrm{e}^{\tau A} [V', A]\, \mathrm{e}^{\tau A} u \in X, \quad \mathrm{e}^{\tau A} V'' \mathrm{e}^{\tau A} u \in X\,.$$

Reduces to regularity requirement

$$[V', A]\, u(0) = [\partial_{xx}, V']\, u(0) = 2\,\partial_x V' \partial_x u(0) + \partial_{xx} V' u(0) \in X\,.$$

Conclusion. Straightforward approach based on step-wise Taylor series expansions yields restrictive regularity requirement

$$\partial_x^6 u(0) \in X\,,$$

whereas favourable approach based on variable-of-constants formula leads to

$$\partial_x u(0) \in X\,.$$

Conclusions and future work

Summary.

- High-order commutator-free exponential 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 exponential integrators provides better understanding when order reductions and thus significant loss of accuracy for higher-order methods have to be expected.

Open questions.

- Construction of higher-order commutator-free exponential integrators suitable for time integration of parabolic initial-boundary value problems.

Thank you!