Favourable time integration methods for non-autonomous evolution equations

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International Conference on
Scientific Computation and Differential Equations (SciCADE)
Session on Numerical integration of non-autonomous
dynamical systems organised by Sergio Blanes

Bath, United Kingdom, September 2017

Contents and related work

Contents.

- Commutator-free quasi-Magnus (CFQM) exponential integrators for non-autonomous linear evolution equations

  Appropriate name thanks to Arieh Iserles

- 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.* Computer Physics Communications (2017).

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

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

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

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

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)

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

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

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

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

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

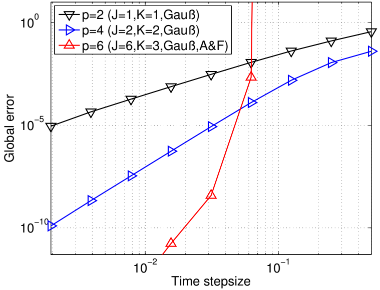
$$b_1 = a_{11} + a_{12} = \tfrac{1}{2} = a_{21} + a_{22} = b_2\,.$$

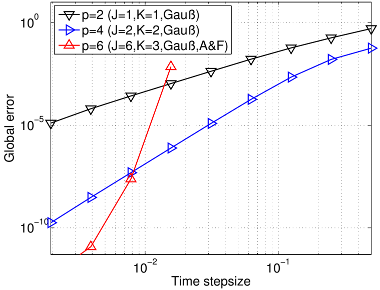
Order 6. Sixth-order method obtained from coefficients given in Alvermann, Fehske. Scheme suitable for evolution equations of Schrödinger type, but poor stability behaviour observed for evolution equations of parabolic type, since

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

Counter-example

Numerical experiment. Apply commutator-free quasi-Magnus exponential integrators of nonstiff orders $p = 2, 4, 6$ to parabolic test equation. 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

... omitted due to lack of time ...

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

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

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

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

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

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

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)

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

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* $0 < \tau_n \leq \tau_{\max}$

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

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.

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.)

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

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

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

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

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).

Dissipative quantum system

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

$$u'(t) = A(t)\,u(t) = -\mathrm{i}\,H(t)\,u(t)\,, \quad t \in (t_0, T)\,,$$
$$H(t) = f_1(t)\,\sigma_1 \otimes I + f_2(t)\,\sigma_2 \otimes R + \delta D \in \mathbb{C}^{d\times d}\,, \quad d = 2\,k\,,$$
$$I = \operatorname{diag}\big(1\big) \in \mathbb{R}^{k\times k}\,, \quad R = \operatorname{tridiag}\big(1,0,1\big) \in \mathbb{R}^{k\times k}\,, \quad D = -\mathrm{i}\operatorname{diag}\big(1^2, 2^2, \dots, d^2\big) \in \mathbb{C}^{d\times d}\,.$$

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 ($p = 4$)

Favourable fourth-order schemes. Design fourth-order time-symmetric commutator-free quasi-Magnus exponential integrators with real coefficients satisfying positivity condition

$$\forall\, j \in \{1, \dots, J\}: \quad x_{j1} > 0\,.$$

Use additional degrees of freedom due to inclusion of sixth-order quadrature nodes and further exponentials to verify certain conditions at order five and to minimise deviation of the remaining fifth-order conditions without increasing the overall computational cost

$$p = 4: \quad \mathrm{CF}_4^{[4]}\,, \quad \mathrm{CF}_5^{[4]}\,.$$

Compare novel schemes with optimised commutator-free quasi-Magnus exponential integrator proposed in ALVERMANN, FEHSKE (see eq. (43))

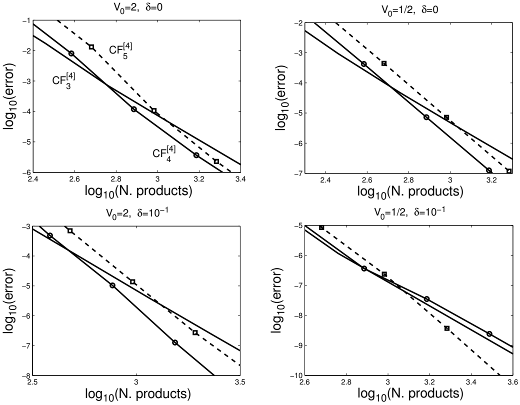
$$p = 4: \quad \mathrm{CF}_3^{[4]}\,.$$

Illustration ($p = 4$)

Numerical results. Time integration of Rosen–Zener model by fourth-order CFQM exponential integrators

$$p = 4: \quad \mathrm{CF}_3^{[4]} \text{ (A \& F)}, \quad \mathrm{CF}_4^{[4]}, \mathrm{CF}_5^{[4]} \text{ (novel)}.$$

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 favourable for higher accuracy.



Favourable novel scheme ($p = 6$, commutator)

Favourable novel scheme (commutator). Design unconventional scheme of order six involving single commutator

$$p = 6\,, \quad J = 5\,, \quad K = 3\,,$$

$$\mathrm{CF}_{5C}^{[6]}(\tau) = \prod_{j=4}^{5} \mathrm{e}^{\tau a_{j1} A_1(\tau) + \tau a_{j2} A_2(\tau) + \tau a_{j3} A_3(\tau)}\, \mathrm{e}^{D(\tau)} \prod_{j=1}^{2} \mathrm{e}^{\tau a_{j1} A_1(\tau) + \tau a_{j2} A_2(\tau) + \tau a_{j3} A_3(\tau)}\,,$$

$$D(\tau) = \tau^2 \big[C_1(\tau), C_2(\tau)\big]\,, \quad C_1 = e_1 \big(A_1 + A_3\big) + e_2 A_2\,, \quad C_2 = A_3 - A_1\,.$$

Contrary to classical interpolatory Magnus integrators, where arising commutators only of first order, additional computational cost low due to

$$D(\tau) \simeq \big[d_1\, \alpha_1(\tau) + d_2\, \alpha_3(\tau), \alpha_2(\tau)\big] = \mathscr{O}\big(\tau^3\big)\,, \quad \alpha_k(\tau) = \mathscr{O}\big(\tau^k\big)\,.$$

Compare novel scheme with optimised commutator-free quasi-Magnus exponential integrator proposed in ALVERMANN, FEHSKE (see Table 3, stability issues for $\delta > 0$)

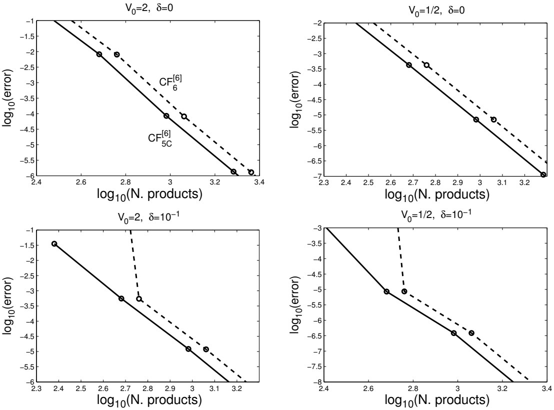
$$p = 6: \quad \mathrm{CF}_6^{[6]}\,.$$

Illustration ($p = 6$)

Numerical results. Time integration of Rosen–Zener model by sixth-order CFQM exponential integrators

$$p = 6: \quad \mathrm{CF}_{6}^{[6]}\ (\text{A \& F}), \quad \mathrm{CF}_{5C}^{[6]}\ (\text{novel}).$$

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 scheme favourable in all cases.



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

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

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

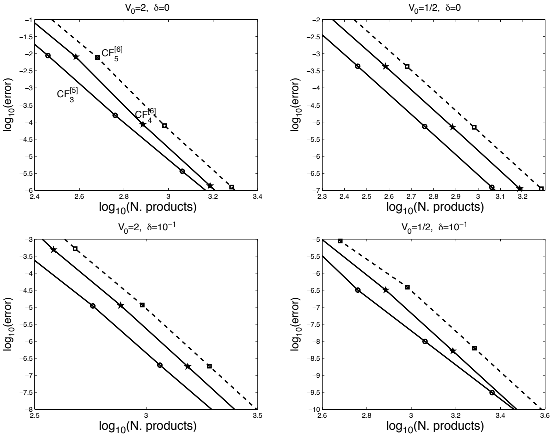
- Expect schemes to remain stable for $\delta > 0$.
- Expect scheme with $J = 3$ to be most efficient.

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

Numerical results. Time integration of Rosen–Zener model by fifth- and sixth-order CFQM exponential integrators

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

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 $\delta > 0$.



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

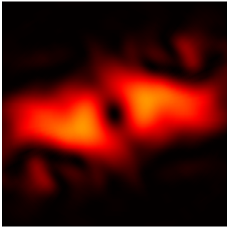
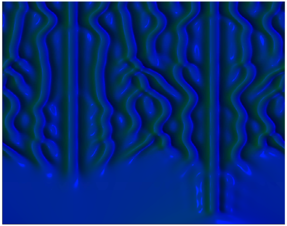
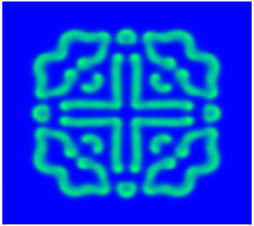
Situation. Consider nonlinear evolution equation of form

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

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

http://techmath.uibk.ac.at/mecht/MyHomepage/Research.html

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 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!