

Convergence analysis of commutator-free quasi-Magnus exponential integrators for non-autonomous linear Schrödinger equations

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Collaborators

My collaborators.

SERGIO BLANES, FERNANDO CASAS, CESÁREO GONZÁLEZ

Our former work on design and error analysis of commutator-free quasi-Magnus exponential integrators applied to parabolic equations.

S. BLANES, F. CASAS, M. TH.

Convergence analysis of high-order commutator-free quasi-Magnus exponential integrators for nonautonomous linear evolution equations of parabolic type.
IMA J. Numer. Anal. 38/2 (2018) 743–778.

S. BLANES, F. CASAS, M. TH.

High-order commutator-free quasi-Magnus exponential integrators for non-autonomous linear evolution equations.
Comp. Phys. Commun. 220 (2017) 243–262.

Related work on construction of local error estimators for Magnus-type integrators.

W. AUZINGER, H. HOFSTÄTTER, O. KOCH, M. QUELL, M. TH.

A posteriori error estimation for Magnus-type integrators.
Submitted (2018).

Setting

CFQM exponential integrators

Class of evolution equations

Class of evolution equations. Consider **non-autonomous linear evolution equations** of form

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

Applications. Relevant applications include (large) systems of ordinary differential equations and **partial differential equations**.

- Linear evolution equations of **Schrödinger type** involving time-dependent Hamilton operators (**focus in this talk**)

$$A(t) = -iH(t).$$

- Linear evolution equations of **parabolic type** (former work).

Illustrations

Illustrations.

- Linear Schrödinger equations with space-time-dependent potential.
See also work by ARIEH ISERLES, KAROLINA KROPIELNICKA, PRANAV SINGH and talk by SERGIO BLANES.
- Time-dependent Gross–Pitaevskii equations with rotation term (transformation to rotating frame, additional nonlinearity).
See also work by WEIZHU BAO and co-authors.

[HTTP://TECHMATH.UIBK.AC.AT/MECHT/MyHOMEPAGE/RESEARCH.HTML](http://TECHMATH.UIBK.AC.AT/MECHT/MyHOMEPAGE/RESEARCH.HTML)

Class of time integrators

Class of time integrators. Study **commutator-free quasi-Magnus (CFQM) exponential integrators** for efficient time integration.

- Consider time grid points and associated time stepsizes

$$t_0 < \dots < t_n < \dots < t_N = T, \quad \tau_n = t_{n+1} - t_n, \quad n \in \{0, 1, \dots, N-1\}.$$

- Choose quadrature nodes and adjust (real) method coefficients to attain certain order of consistency

$$c_k \in [0, 1], \quad a_{jk} \in \mathbb{R}, \quad (j, k) \in \{1, \dots, J\} \times \{1, \dots, K\}.$$

- Determine **numerical solution values by recurrence** of form

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

$$\mathcal{S}(\tau_n, t_n) = e^{\tau_n B_{nJ}(\tau_n)} \dots e^{\tau_n B_{n1}(\tau_n)},$$

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

Which time integration methods perform best?

Which time integration methods perform best? Apparently not possible to provide **generally valid answer**, since performance of time integration methods substantially depends on problems under consideration and realisations of exponentials.

- Numerical examples that confirm favourable behaviour of CFQM integrators are found in literature. For **comparisons with Magnus integrators and Runge–Kutta methods** in context of parabolic and Schrödinger equations, see BLANES, CASAS, TH. (2017).
- See talks by SERGIO BLANES and PRANAV SINGH.

Intrinsic benefit. Intrinsic benefit of CFQM exponential integrators is that **structural properties** of defining operator family are well-preserved.

- Good stability behaviour (no stepsize restriction).
- Preservation of geometric properties.

Main objective

Main objective (in this talk). Study CFQM exponential integrators in context of **linear Schrödinger equations**. Provide **rigorous theoretical convergence analysis** (**stability**, **local error**). Note that difficulty in derivation of local error representation lies in suitable expansion of product of exponentials defining numerical solution.¹

Convergence analysis.

- For general case, adapt approach detailed in former work on parabolic equations.
- For relevant special case $H(t) = \Delta + V(t)$, deduce error representation that captures correctly low regularity requirements on initial state. Contrast convergence result for CFQM exponential integrators to convergence result for Magnus integrators.

¹ *Be aware of presence of unbounded operators. Care about remainders. Do not use representations involving infinite series such as BCH-formula.*

Convergence result (General case)

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Theorem

Assume that the considered non-autonomous linear evolution equation is defined by a family of self-adjoint space-time-dependent operators

$$\begin{cases} u'(t) = A(t) u(t) = i H(t) u(t), & H(t) : D \rightarrow X = L_2(\Omega, \mathbb{R}), \quad t \in (t_0, T), \\ u(t_0) \text{ given.} \end{cases}$$

Suppose that the coefficients of the applied CFQM exponential integrator are real and fulfill the nonstiff p -th order conditions. Provided that compositions of the form $A^{(\ell)}(s) u^{(m)}(t)$ with $\ell \in \{0, 1, \dots, p\}$ and $m \in \{0, 1, \dots, p-1\}$ remain bounded for $s, t \in [0, T]$, the global error estimate

$$\|u_n - u(t_n)\|_X \leq C \left(\|u_0 - u(t_0)\|_X + \tau^p \right), \quad n \in \{0, 1, \dots, N\},$$

is valid with a constant $C > 0$ that does not depend on the number of time steps n and the (maximal) time stepsize $\tau > 0$.

Implication. For family of second-order differential operators involving regular coefficients, assumption $A(t) u^{(p-1)}(t) \sim (A(t))^p u(t) \sim \partial_{x_1}^{2p} u(t)$ bounded in $L_2(\Omega, \mathbb{R})$, uniformly for $t \in [0, T]$, corresponds to regularity requirement $u(t_0) \in H^{2p}(\Omega, \mathbb{R})$.

Convergence result (General case)

Proof (Initial step in local error expansion). On first sub-subinterval, employ linearisation and represent exact solution value by variation-of-constants formula

$$u'(t) = A(t) u(t) = \frac{1}{b_1} B_{n1} u(t) + \left(A(t) - \frac{1}{b_1} B_{n1} \right) u(t), \quad t \in (t_n, t_n + b_1 \tau_n),$$

$$u(t_n + b_1 \tau_n) = e^{\tau_n B_{n1}} u(t_n) + b_1 \int_0^{\tau_n} e^{(\tau_n - \sigma) B_{n1}} R_{n1}(t_n + b_1 \sigma) d\sigma.$$

Observe that remainder satisfies relation

$$R_{n1}(t) = \left(A(t) - \frac{1}{b_1} B_{n1} \right) u(t) \sim \left(A(t) - A(s) \right) u(t) \sim (t - s) A'(s) u(t),$$


$$u(t_n + b_1 \tau_n) - e^{\tau_n B_{n1}} u(t_n) = \mathcal{O}(\tau_n^2, \|A' u\|_X).$$

Proceed inductively to attain solution representation on subinterval

$$\underbrace{u(t_n + \tau_n) = u(t_n + (b_1 + \dots + b_j) \tau_n)}_{\text{exact solution value}} = \underbrace{e^{\tau_n B_{nJ}(\tau_n)} \dots e^{\tau_n B_{n1}(\tau_n)} u(t_n)}_{\text{numerical solution value}} + \underbrace{\text{remainder}}_{\mathcal{O}(\tau_n^2, \|A' u\|_X)}.$$

For $p = 1$, this implies stated result under regularity requirement

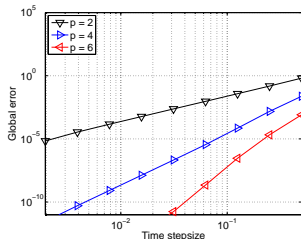
$$A^{(p)}(s) u^{(p-1)}(t) \in X, \quad s, t \in [t_0, T].$$

For $p \geq 2$, use similar approach for further expansion of remainder (involved calculations). 

Convergence result (General case)

Illustration. Numerical examples for *characteristical test equation* confirm theoretical convergence result.

- Unconditional stability of CFQM exponential integrators.
- Full order of convergence for regular data.



Open questions (Special case)

Optimality of regularity requirements?

Optimality of regularity requirements?

- Numerical verification that regularity requirements on exact solution (initial state) are optimal is difficult, since space discretisation error and errors in computation of exponentials in general dominate time discretisation error.
- Hope: In relevant special case $H(t) = \Delta + V(t)$, use of operator splitting methods and their realisation by Fourier spectral method permits to reduce space discretisation error and provides possibility to verify regularity requirements numerically.

Open questions (Special case)

Special case. Study convergence behaviour of CFQM exponential integrators for special case

$$H(t) = \Delta + V(t).$$

Open questions.

- What are the optimal regularity requirements on the exact solution (initial state)?
Rigorous derivation provided for special schemes. Conjecture stated for method class.
- Does our former proof capture these regularity requirements?
Suitable adaptation needed, since local error analysis becomes more delicate. In particular, observe that Laplacian cancels in difference $A(t) - A(s) \sim V(t) - V(s)$.
- Do numerical examples verify the optimal regularity requirements?
First tests give a hint, but numerical study needs to be refined.

Objective

Objective. Conjecture that for non-autonomous linear evolution equations that involve **Hamilton operators of special structure**

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

significantly lower regularity requirements are sufficient to attain full order of convergence

general case: $u(t_0) \in H^{2p}(\Omega, \mathbb{R})$, special case: $u(t_0) \in H^{p-1}(\Omega, \mathbb{R})$.

Explain this observation by rigorous error analysis.

In this talk.

- Present (briefly) basic approach.
- Contrast obtained result for CFQM exponential integrators to result for other integration methods.

Convergence analysis (Special case)

Basic assumption

Basic assumption. Consider non-autonomous linear evolution equation involving **Hamilton operator of special structure** on **first subinterval**

$$\begin{cases} u'(t) = A(t) u(t), & A(t) = i(\Delta + V(t)), \quad t \in (t_0, t_0 + \tau), \\ u(t_0) \text{ given.} \end{cases}$$

Assume that initial state and real-valued space-time-dependent potential satisfy certain regularity requirements. Employ short notation

$$\begin{aligned} \|u(t_0)\|_{H^\ell} &= \|u(t_0)\|_{H^\ell(\Omega, \mathbb{R})}, \\ \|V^{(\ell)}\|_{W_\infty^m} &= \sup_{t \in [t_0, t_0 + \tau]} \|V^{(\ell)}(t)\|_{W_\infty^m(\Omega, \mathbb{R})}. \end{aligned}$$

Implication

Implication. Use unitarity of evolution operator (integration-by-parts, potential real-valued)

$$\frac{d}{dt} \|u(t)\|_{L_2}^2 = 2 \Re \left(u(t) \middle| u'(t) \right)_{L_2} = 2 \Re \left(i \|\nabla u(t)\|_{L_2}^2 - i \left(V(t) \middle| |u(t)|^2 \right)_{L_2} \right) = 0,$$
$$\|u(t)\|_{L_2} = \|u(t_0)\|_{L_2}, \quad t \in [t_0, t_0 + \tau],$$

and representation by variation-of-constants formula to justify that **exact solution inherits regularity of initial state**, e.g.

$$\chi(t) = \partial_x u(t), \quad \chi'(t) = i(\Delta + V(t))\chi(t) + i\partial_x V(t)u(t),$$
$$\|u(t)\|_{H^1} \leq \left(1 + \tau \|V\|_{W_\infty^1}\right) \|u(t_0)\|_{H^1}.$$

Integrators

CFQM exponential integrators. Study lower- and higher-order CFQM exponential integrators (first time step).

- Apply **second-order exponential midpoint rule** based on single Gaussian quadrature node and single exponential

$$p = 2, \quad J = 1 = K, \quad \mathcal{S}(\tau) u(t_0) = e^{\tau A(t_0 + \frac{1}{2}\tau)} u(t_0) \approx u(t_0 + \tau).$$

- Apply **fourth-order CFQM exponential integrator** based on two Gaussian quadrature nodes and two exponentials

$$p = 4, \quad J = 2 = K, \quad \alpha = \frac{\sqrt{3}}{6}, \quad c_1 = \frac{1}{2} - \alpha, \quad c_2 = \frac{1}{2} + \alpha,$$

$$a_{11} = \frac{1}{4} + \alpha = a_{22}, \quad a_{12} = \frac{1}{4} - \alpha = a_{21},$$

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

$$B_j(\tau) = a_{j1} A(t_0 + c_1\tau) + a_{j2} A(t_0 + c_2\tau), \quad j \in \{1, 2\},$$

$$\mathcal{S}(\tau) u(t_0) = e^{\tau B_2(\tau)} e^{\tau B_1(\tau)} u(t_0) \approx u(t_0 + \tau).$$

Note that symmetry suggests linearisation about midpoint $A_* = A(t_0 + \frac{\tau}{2})$.

Stability

Stability. Assume that **method coefficients** are **real**

$$a_{jk} \in \mathbb{R}, \quad (j, k) \in \{1, \dots, J\} \times \{1, \dots, K\}.$$

As operators defining CFQM exponential integrators rewrite as follows

$$B_j(\tau) = \sum_{k=1}^K a_{jk} A(t_0 + c_k \tau),$$

$$A(t) = i(\Delta + V(t)), \quad b_j = \sum_{k=1}^K a_{jk},$$

$$B_j(\tau) = i\left(b_j \Delta + \sum_{k=1}^K a_{jk} V(t_0 + c_k \tau)\right),$$

stability in $L_2(\Omega, \mathbb{R})$ is ensured by **unitarity** of arising evolution operators

$$\left\| e^{tB_j(\tau)} \dots e^{tB_1(\tau)} u(t_0) \right\|_{L_2} = \|u(t_0)\|_{L_2}, \quad t \in [0, \tau].$$

Approach

Approach.

- Deduce **local error expansion** that remains appropriate for **unbounded Hamilton operators**, reflects **correct order** with respect to time stepsize, and captures observed **regularity requirements** on exact solution

$$\mathcal{S}(\tau) u(t_0) - u(t_0 + \tau) = \mathcal{O}\left(\tau^{p+1}, \|V^{(\ell)}\|_{W_\infty^m}, \|u\|_{H^{p-1}}\right).$$

- Consider evolution equations satisfied by exact solution and by exponentials defining numerical solution.
- Employ linearisations about midpoint and representations by variation-of- constants formula.
- Observe that in expansions of integrands iterated commutators implying certain regularity requirements arise naturally.
- Together with stability bound, obtain **global error bound** of form

$$\|u_n - u(t_n)\|_{L_2} \leq C\left(\|V^{(\ell)}\|_{W_\infty^m}\right) t_n \tau^p \|u\|_{H^{p-1}}.$$

Conjecture

Theorem

Assume that the considered non-autonomous linear evolution equation is defined by a family of self-adjoint space-time-dependent operators

$$\begin{cases} u'(t) = A(t) u(t) = i H(t) u(t), & H(t) : D \rightarrow X = L_2(\Omega, \mathbb{R}), \quad t \in (t_0, T), \\ u(t_0) \text{ given,} \end{cases}$$

Then, any p -th order CFQM exponential integrator with real coefficients satisfies the global error estimate

$$\|u_n - u(t_n)\|_{L_2} \leq C \left(\|u_0 - u(t_0)\|_{L_2} + \tau^p \right), \quad n \in \{0, 1, \dots, N\},$$

with a constant that depends on $\|V^{(\ell)}\|_{W_\infty^m}$ and $\|u\|_{H^{p-1}}$ but is independent of the number of time steps n and the (maximal) time stepsize $\tau > 0$.

Proof. Rigorous derivation completed for $p = 4$ and $J = K = 2$. ◇

Comparison

Comparison with classical methods. Note that boundedness of higher time derivatives of solution corresponds to spatial regularity, since

$$u'(t) = A(t) u(t), \quad u''(t) = A'(t) u(t) + A(t) u'(t) \sim (A(t))^2 u(t), \\ u'''(t) \sim (A(t))^3 u(t), \quad \|u'''\|_{L_2} \sim \|u\|_{H^6}.$$

Convergence result for CFQM exponential integrators confirms superior behaviour compared to classical methods, e.g. of exponential midpoint rule versus implicit midpoint rule

$$\|u_n - u(t_n)\|_{L_2} \leq C t_n \tau^2 \|u'''\|_{L_2}.$$

Comparison

Comparison with Magnus integrators. Conjectured convergence result for CFQM exponential integrators compares with work on (interpolatory) **Magnus integrators** (in context of spatial semi-discretisation).

- CFQM exponential integrators: **Same regularity requirement on exact solution.** **Time stepsize restriction not needed.**

Theorem (HOCHBRUCK, LUBICH, 2003)

Consider $A(t) = i(U + V(t))$ with symmetric positive-definite matrix U and Hermitian matrix-valued function V . Assume that the time-derivatives of V are uniformly bounded and that the commutator bounds $(m \in \{0, 1, \dots, p\}, k \in \{1, \dots, (p-1)p-1\})$

$$\|V^{(m)}(t)\| \leq M_p, \quad \|[A(t_k), \dots, [A(t_1), V^{(m)}(t)] \dots] w\| \leq K \|D^k w\|, \quad D = U^{\frac{1}{2}},$$

hold. Under the **stepsize restriction** $\tau \|D\| \leq c$, the p -th order Magnus integrator satisfies the error bound

$$\|u_n - u(t_n)\| \leq C(p, c, M_p, K) t_n \tau^p \sup_{t \in [0, t_n]} \|D^{p-1} u(t)\|.$$

Conclusions

Conclusions. Convergence analysis provided for CFQM exponential integrators applied to non-autonomous linear Schrödinger equations.

Open questions. Proceed with study of special case $H(t) = \Delta + V(t)$.

- Extend rigorous derivation to other higher-order methods.
- Confirm optimality of regularity requirements by numerical examples.

Thank you!