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

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

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)

$$A(t) = -\,\mathrm{i}\,H(t)\,.$$

- 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

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

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

- 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

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

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

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

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)

Convergence result (General case)

Theorem

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

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

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

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

is valid with a constant $C > 0$ that does not dependent 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

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

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

Observe that remainder satisfies relation

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

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

Proceed inductively to attain solution representation on subinterval

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

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

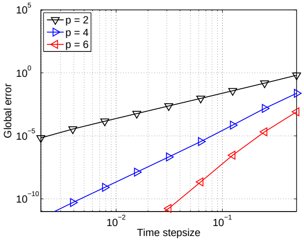
$$A^{(p)}(s)\,u^{(p-1)}(t) \in X\,, \quad s, t \in [t_0, T]\,.$$

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

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

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

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

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

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

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

$$\big\| u(t_0) \big\|_{H^\ell} = \big\| u(t_0) \big\|_{H^\ell(\Omega,\mathbb{R})}\,,$$
$$\big\| V^{(\ell)} \big\|_{W^m_\infty} = \sup_{t \in [t_0, t_0+\tau]} \big\| V^{(\ell)}(t) \big\|_{W^m_\infty(\Omega,\mathbb{R})}\,.$$

Implication

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

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\|u(t)\|_{L_2}^2 = 2\,\Re\left(u(t)\middle|u'(t)\right)_{L_2} = 2\,\Re\left(\mathrm{i}\,\|\nabla u(t)\|_{L_2}^2 - \mathrm{i}\left(V(t)\middle|\,|u(t)|^2\right)_{L_2}\right) = 0\,,$$

$$\|u(t)\|_{L_2} = \|u(t_0)\|_{L_2}\,, \quad t \in [t_0, t_0+\tau]\,,$$

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

$$\chi(t) = \partial_x u(t)\,, \quad \chi'(t) = \mathrm{i}\left(\Delta + V(t)\right)\chi(t) + \mathrm{i}\,\partial_x V(t)\,u(t)\,,$$

$$\|u(t)\|_{H^1} \leq \left(1 + \tau\,\|V\|_{W^1_\infty}\right)\|u(t_0)\|_{H^1}\,.$$

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

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

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

$$p = 4\,, \quad J = 2 = K\,, \quad \alpha = \frac{\sqrt{3}}{6}\,, \quad c_1 = \tfrac{1}{2} - \alpha\,, \quad c_2 = \tfrac{1}{2} + \alpha\,,$$
$$a_{11} = \tfrac{1}{4} + \alpha = a_{22}\,, \quad a_{12} = \tfrac{1}{4} - \alpha = a_{21}\,,$$
$$b_1 = a_{11} + a_{12} = b_2 = a_{21} + a_{22} = \tfrac{1}{2}\,,$$
$$B_j(\tau) = a_{j1}\, A(t_0 + c_1 \tau) + a_{j2}\, A(t_0 + c_2 \tau)\,, \quad j \in \{1,2\}\,,$$
$$\mathscr{S}(\tau)\, u(t_0) = \mathrm{e}^{\tau B_2(\tau)}\, \mathrm{e}^{\tau B_1(\tau)}\, u(t_0) \approx u(t_0 + \tau)\,.$$

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

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

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

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

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

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

$$\Big\| \mathrm{e}^{tB_J(\tau)} \cdots \mathrm{e}^{tB_1(\tau)}\, u(t_0) \Big\|_{L_2} = \big\| u(t_0) \big\|_{L_2}, \quad t \in [0,\tau].$$

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

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

  - 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

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

Conjecture

Theorem

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

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

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

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

with a constant that depends on $\| V^{(\ell)} \|_{W^m_\infty}$ 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

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

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

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

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 $A(t) = \mathrm{i}\,(U + V(t))$ 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 ($m \in \{0,1,\dots,p\}, k \in \{1,\dots,(p-1)p-1\}$)

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

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

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

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!

Proof
Local error expansion

Linearisations

Linearisations. Consider evolution equations for numerical and exact solutions, and employ linearisations about midpoint of first subinterval.

- Employ abbreviations

$$A(t) = \mathrm{i}\,\big(\Delta + V(t)\big)\,, \quad A_* = A\big(t_0 + \tfrac{\tau}{2}\big)\,, \quad V_* = V\big(t_0 + \tfrac{\tau}{2}\big)\,,$$
$$R(t) = A(t) - A_* = \mathrm{i}\,\big(V(t) - V_*\big) = \mathscr{O}\Big(\tau, \|V'\|_{L_\infty}\Big)\,.$$

- Observe that numerical solution is composed by exponentials and that associated evolution equations rewrite as follows

$$\mathscr{S}(\tau)\,u(t_0) = \mathrm{e}^{\tau B_2(\tau)}\,\mathrm{e}^{\tau B_1(\tau)}\,u(t_0)\,,$$
$$w_j(t) = \mathrm{e}^{tB_j(\tau)}\,, \quad B_j(\tau) = a_{j1}\,A(t_0 + c_1\tau) + a_{j2}\,A(t_0 + c_2\tau)\,, \quad b_j = a_{j1} + a_{j2} = \tfrac{1}{2}\,,$$
$$S_j(\tau) = \tfrac{1}{b_j}\,\big(B_j(\tau) - b_j\,A_*\big) = 2\,\big(a_{j1}\,R(t_0 + c_1\tau) + a_{j2}\,R(t_0 + c_2\tau)\big) = \mathscr{O}\Big(\tau, \|V'\|_{L_\infty}\Big)\,,$$
$$w_j'(t) = B_j(\tau)\,w_j(t) = b_j\,A_*\,w_j(t) + b_j\,S_j(\tau)\,w_j(t) = \tfrac{1}{2}\,A_*\,w_j(t) + \tfrac{1}{2}\,S_j(\tau)\,w_j(t)\,, \quad t \in (0,\tau)\,.$$

- Rewrite evolution equation in analogous manner

$$u'(t) = A(t)\,u(t) = A_*\,u(t) + R(t)\,u(t)\,, \quad t \in (t_0, t_0 + \tau)\,,$$
$$u(t_0 + \tau) = \mathscr{E}(\tau)\,u(t_0) = \mathscr{E}\big(\tfrac{\tau}{2}\big)\,\mathscr{E}\big(\tfrac{\tau}{2}\big)\,u(t_0)\,.$$

Auxiliary evolution equation

Auxiliary evolution equation. Above relations suggest consideration of linear evolution equation of form (neglect values of arising constants)

$$y'(t) = Z_* \, y(t) + z(t) \, y(t) \,, \quad t \in (s, s+\tau) \,,$$

Numerical solution: $\quad Z_* = \alpha \, A_* \,, \quad z(t) = \alpha \, S_j(\tau) = \mathcal{O}\Big(\tau, \|V'\|_{L_\infty}\Big) \,,$

Exact solution $\quad Z_* = \alpha \, A_* \,, \quad z(t) = \alpha \, R(t) = \mathcal{O}\Big(\tau, \|V'\|_{L_\infty}\Big) \,.$

Main tool

Main tool. Consider linear evolution equation of form

$$y'(t) = Z_* \, y(t) + z(t) \, y(t) \,, \quad t \in (s, s+\tau) \,.$$

Employ representations of solution values by variation-of-constants formula

$$y(s+t) = \mathrm{e}^{tZ_*} \, y(s) + \int_0^t \mathrm{e}^{(t-\sigma_1)Z_*} \, z(s+\sigma_1) \, y(s+\sigma_1) \, \mathrm{d}\sigma_1 \,, \quad t \in (0, \tau) \,,$$

$$y(s+\sigma_1) = \mathrm{e}^{\sigma_1 Z_*} \, y(s) + \int_0^{\sigma_1} \mathrm{e}^{(\sigma_1-\sigma_2)Z_*} \, z(s+\sigma_2) \, y(s+\sigma_2) \, \mathrm{d}\sigma_2 \,.$$

In view of further expansion for higher-order scheme, rewrite resulting identity as

$$y(s+t) = \mathrm{e}^{tZ_*} \Big(I + \int_0^t \underbrace{\mathrm{e}^{-\sigma_1 Z_*} \, z(s+\sigma_1) \, \mathrm{e}^{\sigma_1 Z_*}}_{= Z(s,\sigma_1)} \, \mathrm{d}\sigma_1 \Big) \, y(s)$$

$$+ \, \mathrm{e}^{tZ_*} \int_0^t \int_0^{\sigma_1} \underbrace{\mathrm{e}^{-\sigma_1 Z_*} \, z(s+\sigma_1) \, \mathrm{e}^{\sigma_1 Z_*}}_{= Z(s,\sigma_1)} \, \underbrace{\mathrm{e}^{-\sigma_2 Z_*} \, z(s+\sigma_2)}_{= Z(s,\sigma_2) \, \mathrm{e}^{-\sigma_2 Z_*}} \, y(s+\sigma_2) \, \mathrm{d}\sigma_2 \, \mathrm{d}\sigma_1 \,.$$

Representations

Representations. Use as well alternative representation obtained by linear tranformation $(\sigma_1, \sigma_2) \leftrightarrow (t-\sigma_1, t-\sigma_2)$

$$y(s+t) = \mathrm{e}^{tZ_*}\Big(I + \int_0^t \underbrace{\mathrm{e}^{-\sigma_1 Z_*}\, z(s+\sigma_1)\, \mathrm{e}^{\sigma_1 Z_*}}_{=Z(s,\sigma_1)}\, \mathrm{d}\sigma_1\Big)\, y(s)$$

$$+\, \mathrm{e}^{tZ_*} \int_0^t \int_0^{\sigma_1} \underbrace{\mathrm{e}^{-\sigma_1 Z_*}\, z(s+\sigma_1)\, \mathrm{e}^{\sigma_1 Z_*}}_{=Z(s,\sigma_1)}\ \underbrace{\mathrm{e}^{-\sigma_2 Z_*}\, z(s+\sigma_2)}_{=Z(s,\sigma_2)\,\mathrm{e}^{-\sigma_2 Z_*}}\ y(s+\sigma_2)\, \mathrm{d}\sigma_2\, \mathrm{d}\sigma_1$$

$$= \Big(I + \int_0^t \underbrace{\mathrm{e}^{\sigma_1 Z_*}\, z(s+t-\sigma_1)\, \mathrm{e}^{-\sigma_1 Z_*}}_{=Z(s+t,-\sigma_1)}\, \mathrm{d}\sigma_1\Big)\, \mathrm{e}^{tZ_*}\, y(s)$$

$$+ \int_0^t \int_{t-\sigma_1}^t \underbrace{\mathrm{e}^{\sigma_1 Z_*}\, z(s+t-\sigma_1)\, \mathrm{e}^{-\sigma_1 Z_*}}_{=Z(s+t,-\sigma_1)}\ \underbrace{\mathrm{e}^{\sigma_2 Z_*}\, z(s+t-\sigma_2)}_{=Z(s+t,-\sigma_2)\,\mathrm{e}^{tZ_*}\,\mathrm{e}^{(\sigma_2-t)Z_*}}\ y(s+t-\sigma_2)\, \mathrm{d}\sigma_2\, \mathrm{d}\sigma_1 \,.$$

Remark. Recall former relation and unitarity of evolution operator

$$z(s+\sigma) = \mathcal{O}\big(\tau, \|V'\|_{L_\infty}\big), \quad Z(s,\sigma) = \mathrm{e}^{-\sigma Z_*}\, z(s+\sigma)\, \mathrm{e}^{\sigma Z_*} = \mathcal{O}\big(\tau, \|V'\|_{L_\infty}\big), \quad \sigma \in [0,\tau] \,.$$

First expansion ($p = 2$)

First expansion. In context of 2nd-order method, employ expansion

$$y(s+t) = e^{tZ_*}\Big(I + \int_0^t \underbrace{e^{-\sigma_1 Z_*}\, z(s+\sigma_1)\, e^{\sigma_1 Z_*}}_{= Z(s,\sigma_1)}\, d\sigma_1\Big)\, y(s)$$

$$\underbrace{+\, e^{tZ_*} \int_0^t \int_0^{\sigma_1} \underbrace{e^{-\sigma_1 Z_*}\, z(s+\sigma_1)\, e^{\sigma_1 Z_*}}_{= Z(s,\sigma_1)}\; \underbrace{e^{-\sigma_2 Z_*}\, z(s+\sigma_2)}_{= Z(s,\sigma_2)\, e^{-\sigma_2 Z_*}}\; y(s+\sigma_2)\, d\sigma_2\, d\sigma_1}_{= \mathcal{O}\left(\tau^4, \|V'\|_{L_\infty}, \|y\|_{L_2}\right)}.$$

First expansion ($p = 4$)

First expansion. In context of 4th-order method, perform additional expansion step and employ equivalent representations

$$
\begin{aligned}
&y(s+t)\\
&= \mathrm{e}^{tZ_*}\left(I + \int_0^t \underbrace{\mathrm{e}^{-\sigma_1 Z_*}\, z(s+\sigma_1)\, \mathrm{e}^{\sigma_1 Z_*}}_{=\,Z(s,\sigma_1)}\, \mathrm{d}\sigma_1 + \int_0^t \int_0^{\sigma_1} Z(s,\sigma_1)\, Z(s,\sigma_2)\, \mathrm{d}\sigma_2\, \mathrm{d}\sigma_1\right) y(s)\\
&\quad + \underbrace{\mathrm{e}^{tZ_*} \int_0^t \int_0^{\sigma_1} \int_0^{\sigma_2} Z(s,\sigma_1)\, Z(s,\sigma_2)\, Z(s,\sigma_3)\, \mathrm{e}^{-\sigma_3 Z_*}\, y(s+\sigma_3)\, \mathrm{d}\sigma_3\, \mathrm{d}\sigma_2\, \mathrm{d}\sigma_1}_{=\,\mathscr{O}\left(\tau^6, \|V'\|_{L_\infty}, \|y\|_{L_2}\right)}\\
&= \left(I + \int_0^t Z(s+t,-\sigma_1)\, \mathrm{d}\sigma_1 + \int_0^t \int_{t-\sigma_1}^t Z(s+t,-\sigma_1)\, Z(s+t,-\sigma_2)\, \mathrm{d}\sigma_2\, \mathrm{d}\sigma_1\right) \mathrm{e}^{tZ_*}\, y(s)\\
&\quad + \underbrace{\int_0^t \int_{t-\sigma_1}^t \int_{t-\sigma_2}^t Z(s+t,-\sigma_1)\, Z(s+t,-\sigma_2)\, Z(s+t,-\sigma_3)\, \mathrm{e}^{tZ_*}\, \mathrm{e}^{(\sigma_3-t)Z_*}\, y(s+t-\sigma_3)\, \mathrm{d}\sigma_3\, \mathrm{d}\sigma_2\, \mathrm{d}\sigma_1}_{=\,\mathscr{O}\left(\tau^6, \|V'\|_{L_\infty}, \|y\|_{L_2}\right)}\,.
\end{aligned}
$$

Taylor series expansion

Taylor series expansion. Note that iterated commutators arise naturally

$$f(\sigma) = \mathrm{e}^{-\sigma Z_*} F \, \mathrm{e}^{\sigma Z_*} \,,$$

$$f'(\sigma) = \mathrm{e}^{-\sigma Z_*} \big(- Z_* F + F Z_* \big) \mathrm{e}^{\sigma Z_*} = \mathrm{e}^{-\sigma Z_*} \big[F, Z_* \big] \, \mathrm{e}^{\sigma Z_*} = \mathrm{e}^{-\sigma Z_*} \, \mathrm{ad}_{Z_*}(F) \, \mathrm{e}^{\sigma Z_*} \,,$$

$$f''(\sigma) = \mathrm{e}^{-\sigma Z_*} \big[[F, Z_*], Z_* \big] \, \mathrm{e}^{\sigma Z_*} = \mathrm{e}^{-\sigma Z_*} \, \mathrm{ad}^2_{Z_*}(F) \, \mathrm{e}^{\sigma Z_*} \,,$$

$$f'''(\sigma) = \mathrm{e}^{-\sigma Z_*} \, \mathrm{ad}^3_{Z_*}(F) \, \mathrm{e}^{\sigma Z_*} \,.$$

Stepwise Taylor series expansion yields relations

$$\begin{aligned}
f(\sigma) - f(\sigma_0) &= f\big(\theta\sigma + (1-\theta)\,\sigma_0\big)\Big|_{\theta=0}^{1} \\
&= (\sigma - \sigma_0) \int_0^1 f'\big(\theta\sigma + (1-\theta)\,\sigma_0\big)\,\mathrm{d}\theta\,, \\
&= (\sigma - \sigma_0)\, f'(\sigma_0) \\
&\quad + (\sigma - \sigma_0)^2 \int_0^1 (1-\theta)\, f''\big(\theta\sigma + (1-\theta)\,\sigma_0\big)\,\mathrm{d}\theta\,, \\
&= (\sigma - \sigma_0)\, f'(\sigma_0) + \tfrac{1}{2}\,(\sigma - \sigma_0)^2\, f''(\sigma_0) \\
&\quad + \tfrac{1}{2}\,(\sigma - \sigma_0)^3 \int_0^1 (1-\theta)^2\, f'''\big(\theta\sigma + (1-\theta)\,\sigma_0\big)\,\mathrm{d}\theta\,.
\end{aligned}$$

Commutators

Commutators. Recall that in present situation

$$Z_* \sim A_* \sim \Delta + V\big(t_0 + \tfrac{\tau}{2}\big)\,, \quad F \sim z(t) \sim \begin{cases} R(t)\,, \\ S_j(\tau)\,, \end{cases}$$

$$F \sim V(t) - V(s)\,, \quad s,t \in [t_0, t_0+\tau]\,, \quad F w = \mathcal{O}\Big(\|V\|_{L_\infty}, \|w\|_{L_2}\Big) = \mathcal{O}\Big(\tau, \|V'\|_{L_\infty}, \|w\|_{L_2}\Big)\,.$$

Determine iterated commutators

$$\begin{aligned} & W \sim V(t) - V(s)\,, \\ & [W, \partial_{xx}]\, w \sim \partial_x W\, \partial_x w + \partial_{xx} W\, w\,, \\ & \big\|[W, A_*]\, w\big\|_{L_2} = \mathcal{O}\Big(\|V\|_{W^2_\infty}, \|w\|_{H^1}\Big) = \mathcal{O}\Big(\tau, \|V'\|_{W^2_\infty}, \|w\|_{H^1}\Big)\,, \\ & \big\|[[W, A_*], A_*]\, w\big\|_{L_2} = \mathcal{O}\Big(\|V\|_{W^4_\infty}, \|w\|_{H^2}\Big) = \mathcal{O}\Big(\tau, \|V'\|_{W^4_\infty}, \|w\|_{H^2}\Big)\,, \\ & \Big\|\mathrm{ad}^k_{A_*}(W)\, w\Big\|_{L_2} = \mathcal{O}\Big(\|V\|_{W^{2k}_\infty}, \|w\|_{H^k}\Big) = \mathcal{O}\Big(\tau, \|V'\|_{W^{2k}_\infty}, \|w\|_{H^k}\Big)\,. \end{aligned}$$

Second expansion

Taylor series expansion. Obtain relations

$$
\begin{aligned}
\mathrm{e}^{-\sigma Z_*} F \,\mathrm{e}^{\sigma Z_*} w &= \mathrm{e}^{-\sigma_0 Z_*} F \,\mathrm{e}^{\sigma_0 Z_*} w \\
&\quad \underbrace{+ (\sigma - \sigma_0) \int_0^1 \mathrm{e}^{-(\theta\sigma + (1-\theta)\sigma_0) Z_*} [F, Z_*] \,\mathrm{e}^{(\theta\sigma + (1-\theta)\sigma_0) Z_*} w \,\mathrm{d}\theta}_{= \mathcal{O}\left(\tau, \|V\|_{W^2_\infty}, \|w\|_{H^1}\right) = \mathcal{O}\left(\tau^2, \|V'\|_{W^2_\infty}, \|w\|_{H^1}\right)},
\end{aligned}
$$

$$
\begin{aligned}
\mathrm{e}^{-\sigma Z_*} F \,\mathrm{e}^{\sigma Z_*} w &= \mathrm{e}^{-\sigma_0 Z_*} \Big(F + (\sigma - \sigma_0) [F, Z_*] + \tfrac{1}{2} (\sigma - \sigma_0)^2 \big[[F, Z_*], Z_*\big]\Big) \mathrm{e}^{\sigma_0 Z_*} w \\
&\quad \underbrace{+ \tfrac{1}{2} (\sigma - \sigma_0)^3 \int_0^1 (1-\theta)^2 \,\mathrm{e}^{-(\theta\sigma + (1-\theta)\sigma_0) Z_*} \mathrm{ad}^3_{Z_*}(F) \,\mathrm{e}^{(\theta\sigma + (1-\theta)\sigma_0) Z_*} w \,\mathrm{d}\theta}_{= \mathcal{O}\left(\tau^3, \|V\|_{W^6_\infty}, \|w\|_{H^3}\right) = \mathcal{O}\left(\tau^4, \|V'\|_{W^6_\infty}, \|w\|_{H^3}\right)}.
\end{aligned}
$$

Exponential midpoint rule

Summary

Summary ($p = 2$). Linearisation about midpoint of first subinterval, iterated application of variation-of-constants formula, and Taylor series expansion of integrand yields

$$
\begin{aligned}
y(s+t) &= \mathrm{e}^{tZ_*}\,y(s) \\
&\quad + \mathrm{e}^{(t-\sigma_0)Z_*}\int_0^t z(s+\sigma_1)\,\mathrm{d}\sigma_1\,\mathrm{e}^{\sigma_0 Z_*}\,y(s) \\
&\quad + \underbrace{\int_0^t\int_0^1 (\sigma_1-\sigma_0)\,\mathrm{e}^{(t-\theta\sigma_1-(1-\theta)\sigma_0)Z_*}\big[z(s+\sigma_1),Z_*\big]\,\mathrm{e}^{(\theta\sigma_1+(1-\theta)\sigma_0)Z_*}\,y(s)\,\mathrm{d}\theta\,\mathrm{d}\sigma_1}_{=\mathcal{O}\left(\tau^3,\,\|V'\|_{W^2_\infty},\,\|y\|_{H^1}\right)} \\
&\quad + \underbrace{\mathrm{e}^{tZ_*}\int_0^t\int_0^{\sigma_1} Z(s,\sigma_1)\,Z(s,\sigma_2)\,\mathrm{e}^{-\sigma_2 Z_*}\,y(s+\sigma_2)\,\mathrm{d}\sigma_2\,\mathrm{d}\sigma_1}_{=\mathcal{O}\left(\tau^4,\,\|V'\|_{L_\infty},\,\|y\|_{L_2}\right)} \\
&= \mathrm{e}^{tZ_*}\,y(s) \\
&\quad + \mathrm{e}^{(t-\sigma_0)Z_*}\int_0^t z(s+\sigma_1)\,\mathrm{d}\sigma_1\,\mathrm{e}^{\sigma_0 Z_*}\,y(s) \\
&\quad + \mathcal{O}\left(\tau^3,\,\|V'\|_{W^2_\infty},\,\|y\|_{H^1}\right).
\end{aligned}
$$

Local error expansion (Exponential midpoint rule)

Specification. Specification of above relation to exponential midpoint rule leads to relation $\left(y = u,\, s = t_0,\, t = \tau,\, Z_* = A_* = A\big(t_0 + \frac{\tau}{2}\big),\, z = R,\, \sigma_0 = 0\right)$

$$u(t_0+\tau) = \mathrm{e}^{\tau A_*}\, u(t_0) + \mathrm{e}^{\tau A_*} \int_0^\tau R(t_0+\sigma_1)\,\mathrm{d}\sigma_1\, u(t_0) + \mathscr{O}\Big(\tau^3, \|V'\|_{W^2_\infty}, \|u\|_{H^1}\Big).$$

Evidently this implies local error expansion

$$\begin{aligned} u(t_0+\tau) - \mathscr{S}(\tau)\, u(t_0) &= u(t_0+\tau) - \mathrm{e}^{\tau A_*}\, u(t_0) \\ &= \mathrm{e}^{\tau A_*} \int_0^\tau \underbrace{R(t_0+\sigma_1)}_{= \mathrm{i}\left(V(t) - V\left(t_0 + \frac{\tau}{2}\right)\right)} \mathrm{d}\sigma_1\, u(t_0) + \mathscr{O}\Big(\tau^3, \|V'\|_{W^2_\infty}, \|u\|_{H^1}\Big). \end{aligned}$$

In final step, use that $R\big(t_0 + \frac{\tau}{2}\big) = 0$, $R'(t) = \mathrm{i}\, V'(t)$, $R''(t) = \mathrm{i}\, V''(t)$ and hence by Taylor series expansion about midpoint

$$R(t_0+\sigma_1) = \big(\sigma_1 - \tfrac{\tau}{2}\big)\, \mathrm{i}\, V'\big(t_0 + \tfrac{\tau}{2}\big) + \big(\sigma_1 - \tfrac{\tau}{2}\big)^2 \int_0^1 (1-\theta)\, \mathrm{i}\, V''\big(t_0 + \theta\sigma_1 + (1-\theta)\, \tfrac{\tau}{2}\big)\,\mathrm{d}\theta\,,$$

$$\mathrm{e}^{\tau A_*} \int_0^\tau R(t_0+\sigma_1)\,\mathrm{d}\sigma_1\, u(t_0) = \mathrm{i}\,\mathrm{e}^{\tau A_*} \underbrace{\int_0^\tau \big(\sigma_1 - \tfrac{\tau}{2}\big)\,\mathrm{d}\sigma_1}_{=0}\, V'\big(t_0 + \tfrac{\tau}{2}\big)\, u(t_0) + \mathscr{O}\Big(\tau^3, \|V''\|_{L_\infty}, \|u\|_{H^1}\Big).$$

Local error expansion (Exponential midpoint rule)

Local error expansion. Altogether, attain local error expansion for exponential midpoint rule that reflects expected dependencies

$$u(t_0+\tau) - \mathrm{e}^{\tau A_*}\, u(t_0) = \mathscr{O}\Big(\tau^3, \|V'\|_{W_\infty^2}, \|V''\|_{L_\infty}, \|u\|_{H^1}\Big).$$

Theorem

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

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

Then, the exponential midpoint rule satisfies the global error estimate

$$\big\| u_n - u(t_n) \big\|_{L_2} \le C \Big(\big\| u_0 - u(t_0) \big\|_{L_2} + \tau^2 \Big), \quad n \in \{0, 1, \dots, N\},$$

with a constant $C > 0$ that depends on $\|V'\|_{W_\infty^2}$, $\|V''\|_{L_\infty}$ and $\|u\|_{H^1}$ but is independent of the number of time steps n and the (maximal) time stepsize $\tau > 0$.

Fourth-order method

Summary

Summary. In context of 4th-order method, employ expansion

$$y(s+t) = \mathrm{e}^{tZ_*}\big(I + \mathscr{J}_2(s,t,Z_*,z) + \mathscr{J}_4(s,t,Z_*,z)\big)\,y(s) + \mathscr{O}\Big(\tau^6, \|V'\|_{L_\infty}, \|y\|_{L_2}\Big),$$

$$\mathscr{J}_2(s,t,Z_*,z) = \int_0^t \mathrm{e}^{-\sigma_1 Z_*}\, z(s+\sigma_1)\, \mathrm{e}^{\sigma_1 Z_*}\, \mathrm{d}\sigma_1\,,$$

$$\mathscr{J}_4(s,t,Z_*,z) = \int_0^t \int_0^{\sigma_1} \mathrm{e}^{-\sigma_1 Z_*}\, z(s+\sigma_1)\, \mathrm{e}^{\sigma_1 Z_*}\, \mathrm{e}^{-\sigma_2 Z_*}\, z(s+\sigma_2)\, \mathrm{e}^{\sigma_2 Z_*}\, \mathrm{d}\sigma_2\, \mathrm{d}\sigma_1\,,$$

as well as alternative representation (for first integral, use transformation $\sigma \leftrightarrow -\sigma$)

$$y(s+t) = \big(I + \mathscr{K}_2(s,t,Z_*,z) + \mathscr{K}_4(s,t,Z_*,z)\big)\,\mathrm{e}^{tZ_*}\, y(s) + \mathscr{O}\Big(\tau^6, \|V'\|_{L_\infty}, \|y\|_{L_2}\Big),$$

$$\mathscr{K}_2(s,t,Z_*,z) = \int_0^t \mathrm{e}^{\sigma_1 Z_*}\, z(s+t-\sigma_1)\, \mathrm{e}^{-\sigma_1 Z_*}\, \mathrm{d}\sigma_1 = \int_{-t}^0 \mathrm{e}^{-\sigma_1 Z_*}\, z(s+t+\sigma_1)\, \mathrm{e}^{\sigma_1 Z_*}\, \mathrm{d}\sigma_1\,,$$

$$\mathscr{K}_4(s,t,Z_*,z) = \int_0^t \int_{t-\sigma_1}^t \mathrm{e}^{\sigma_1 Z_*}\, z(s+t-\sigma_1)\, \mathrm{e}^{-\sigma_1 Z_*}\, \mathrm{e}^{\sigma_2 Z_*}\, z(s+t-\sigma_2)\, \mathrm{e}^{-\sigma_2 Z_*}\, \mathrm{d}\sigma_2\, \mathrm{d}\sigma_1\,.$$

Note that for time-independent $z = S$

$$\mathscr{J}_2\big(\cdot, t, \tfrac{1}{2} Z_*, \tfrac{1}{2} S\big) = \mathscr{J}_2\big(\cdot, \tfrac{t}{2}, Z_*, S\big), \quad \mathscr{K}_2\big(\cdot, t, \tfrac{1}{2} Z_*, \tfrac{1}{2} S\big) = \mathscr{K}_2\big(\cdot, \tfrac{t}{2}, Z_*, S\big),$$

$$\mathscr{J}_4\big(\cdot, t, \tfrac{1}{2} Z_*, \tfrac{1}{2} S\big) = \mathscr{J}_4\big(\cdot, \tfrac{t}{2}, Z_*, S\big), \quad \mathscr{K}_4\big(\cdot, t, \tfrac{1}{2} Z_*, \tfrac{1}{2} S\big) = \mathscr{K}_4\big(\cdot, \tfrac{t}{2}, Z_*, S\big).$$

Application

Application. Recall abbreviations

$$A(t) = \mathrm{i}\,\big(\Delta + V(t)\big)\,, \quad A_* = A\big(t_0 + \tfrac{\tau}{2}\big)\,, \quad V_* = V\big(t_0 + \tfrac{\tau}{2}\big)\,,$$

$$R(t) = \mathrm{i}\,\big(V(t) - V_*\big) = \mathscr{O}\Big(\tau, \|V'\|_{L_\infty}\Big)\,,$$

$$S_j(\tau) = 2\,\big(a_{j1}\,R(t_0 + c_1\tau) + a_{j2}\,R(t_0 + c_2\tau)\big) = \mathscr{O}\Big(\tau, \|V'\|_{L_\infty}\Big)\,.$$

Recall relations for numerical and exact solutions

$$w_j'(t) = \tfrac{1}{2}\,A_*\,w_j(t) + \tfrac{1}{2}\,S_j(\tau)\,w_j(t)\,, \quad Z_* = \tfrac{1}{2}\,A_*\,, \quad z = \tfrac{1}{2}\,S_j(\tau)\,,$$

$$\mathscr{S}(\tau)\,u(t_0) = w_2(\tau)\,w_1(\tau)\,u(t_0)\,,$$

$$u'(t) = A_*\,u(t) + R(t)\,u(t)\,, \quad Z_* = A_*\,, \quad z = R\,,$$

$$u(t_0 + \tau) = \mathscr{E}\big(\tfrac{\tau}{2}\big)\,\mathscr{E}\big(\tfrac{\tau}{2}\big)\,u(t_0)\,.$$

Application

Application. Attain relation for numerical solution value

$$
\begin{aligned}
\mathscr{S}(\tau)\,u(t_0) &= \mathrm{e}^{\frac{\tau}{2}A_*}\Big(I + \mathscr{J}_2\big(\cdot,\tfrac{\tau}{2},A_*,S_2(\tau)\big) + \mathscr{J}_4\big(\cdot,\tfrac{\tau}{2},A_*,S_2(\tau)\big)\Big) \\
&\qquad \times \Big(I + \mathscr{K}_2\big(\cdot,\tfrac{\tau}{2},A_*,S_1(\tau)\big) + \mathscr{K}_4\big(\cdot,\tfrac{\tau}{2},A_*,S_1(\tau)\big)\Big)\,\mathrm{e}^{\frac{\tau}{2}A_*}\,u(t_0) \\
&\quad + \mathscr{O}\Big(\tau^6, \|V'\|_{L_\infty}, \|u\|_{L_2}\Big) \\
&= \mathrm{e}^{\frac{\tau}{2}A_*}\Big(I + \mathscr{J}_2\big(\cdot,\tfrac{\tau}{2},A_*,S_2(\tau)\big) + \mathscr{K}_2\big(\cdot,\tfrac{\tau}{2},A_*,S_1(\tau)\big) \\
&\qquad + \mathscr{J}_2\big(\cdot,\tfrac{\tau}{2},A_*,S_2(\tau)\big)\,\mathscr{K}_2\big(\cdot,\tfrac{\tau}{2},A_*,S_1(\tau)\big) \\
&\qquad + \mathscr{J}_4\big(\cdot,\tfrac{\tau}{2},A_*,S_2(\tau)\big) + \mathscr{K}_4\big(\cdot,\tfrac{\tau}{2},A_*,S_1(\tau)\big)\Big)\,\mathrm{e}^{\frac{\tau}{2}A_*}\,u(t_0) \\
&\quad + \mathscr{O}\Big(\tau^6, \|V'\|_{L_\infty}, \|u\|_{L_2}\Big).
\end{aligned}
$$

Application

Application. Attain relation for exact solution value

$$\begin{aligned} u(t_0+\tau) &= \mathrm{e}^{\frac{\tau}{2}A_*}\Big(I+\mathscr{J}_2\big(t_0+\tfrac{\tau}{2},\tfrac{\tau}{2},A_*,R\big)+\mathscr{J}_4\big(t_0+\tfrac{\tau}{2},\tfrac{\tau}{2},A_*,R\big)\Big) \\ &\qquad\times\Big(I+\mathscr{K}_2\big(t_0,\tfrac{\tau}{2},A_*,R\big)+\mathscr{K}_4\big(t_0,\tfrac{\tau}{2},A_*,R\big)\Big)\,\mathrm{e}^{\frac{\tau}{2}A_*}\,u(t_0) \\ &\quad+\mathscr{O}\Big(\tau^6,\|V'\|_{L_\infty},\|u\|_{L_2}\Big), \\ &= \mathrm{e}^{\frac{\tau}{2}A_*}\Big(I+\mathscr{J}_2\big(t_0+\tfrac{\tau}{2},\tfrac{\tau}{2},A_*,R\big)+\mathscr{K}_2\big(t_0,\tfrac{\tau}{2},A_*,R\big) \\ &\qquad+\mathscr{J}_2\big(t_0+\tfrac{\tau}{2},\tfrac{\tau}{2},A_*,R\big)\mathscr{K}_2\big(t_0,\tfrac{\tau}{2},A_*,R\big) \\ &\qquad+\mathscr{J}_4\big(t_0+\tfrac{\tau}{2},\tfrac{\tau}{2},A_*,R\big)+\mathscr{K}_4\big(t_0,\tfrac{\tau}{2},A_*,R\big)\Big)\,\mathrm{e}^{\frac{\tau}{2}A_*}\,u(t_0) \\ &\quad+\mathscr{O}\Big(\tau^6,\|V'\|_{L_\infty},\|u\|_{L_2}\Big). \end{aligned}$$

Local error (Integral representation)

Local error. Attain relation for local error

$$\begin{aligned}\mathscr{S}(\tau)\,u(t_0) - u(t_0+\tau) = \mathrm{e}^{\frac{\tau}{2}A_*}\Big(&\mathscr{J}_2\big(\cdot,\tfrac{\tau}{2},A_*,S_2(\tau)\big) - \mathscr{J}_2\big(t_0+\tfrac{\tau}{2},\tfrac{\tau}{2},A_*,R\big)\\
&+\mathscr{K}_2\big(\cdot,\tfrac{\tau}{2},A_*,S_1(\tau)\big) - \mathscr{K}_2\big(t_0,\tfrac{\tau}{2},A_*,R\big)\\
&+\mathscr{J}_2\big(\cdot,\tfrac{\tau}{2},A_*,S_2(\tau)\big)\,\mathscr{K}_2\big(\cdot,\tfrac{\tau}{2},A_*,S_1(\tau)\big)\\
&-\mathscr{J}_2\big(t_0+\tfrac{\tau}{2},\tfrac{\tau}{2},A_*,R\big)\,\mathscr{K}_2\big(t_0,\tfrac{\tau}{2},A_*,R\big)\\
&+\mathscr{J}_4\big(\cdot,\tfrac{\tau}{2},A_*,S_2(\tau)\big) - \mathscr{J}_4\big(t_0+\tfrac{\tau}{2},\tfrac{\tau}{2},A_*,R\big)\\
&+\mathscr{K}_4\big(\cdot,\tfrac{\tau}{2},A_*,S_1(\tau)\big) - \mathscr{K}_4\big(t_0,\tfrac{\tau}{2},A_*,R\big)\Big)\,\mathrm{e}^{\frac{\tau}{2}A_*}\,u(t_0)\\
+\mathscr{O}\Big(\tau^6,\|V'\|_{L_\infty},\|u\|_{L_2}\Big)&.\end{aligned}$$

Local error (Integral representation)

Local error. Rewrite local error expansion as follows

$$\mathscr{S}(\tau)\, u(t_0) - u(t_0+\tau) = \mathrm{e}^{\frac{\tau}{2} A_*} \big(D_{21}(\tau) + D_{22}(\tau) + D_{41}(\tau) + D_{42}(\tau) + D_{43}(\tau)\big)\, \mathrm{e}^{\frac{\tau}{2} A_*}\, u(t_0) + \mathscr{O}\Big(\tau^6, \|V'\|_{L_\infty}, \|u\|_{L_2}\Big),$$

and distinguish terms of different (a priori) orders

$$D_{21}(\tau) = \mathscr{J}_2\big(\cdot, \tfrac{\tau}{2}, A_*, S_2(\tau)\big) - \mathscr{J}_2\big(t_0 + \tfrac{\tau}{2}, \tfrac{\tau}{2}, A_*, R\big),$$
$$D_{22}(\tau) = \mathscr{K}_2\big(\cdot, \tfrac{\tau}{2}, A_*, S_1(\tau)\big) - \mathscr{K}_2\big(t_0, \tfrac{\tau}{2}, A_*, R\big),$$
$$D_{21}(\tau) = D_{22}(\tau) = \mathscr{O}\Big(\tau^2\Big),$$
$$D_{41}(\tau) = \mathscr{J}_4\big(\cdot, \tfrac{\tau}{2}, A_*, S_2(\tau)\big) - \mathscr{J}_4\big(t_0 + \tfrac{\tau}{2}, \tfrac{\tau}{2}, A_*, R\big),$$
$$D_{42}(\tau) = \mathscr{K}_4\big(\cdot, \tfrac{\tau}{2}, A_*, S_1(\tau)\big) - \mathscr{K}_4\big(t_0, \tfrac{\tau}{2}, A_*, R\big),$$
$$D_{43}(\tau) = \mathscr{J}_2\big(\cdot, \tfrac{\tau}{2}, A_*, S_2(\tau)\big)\mathscr{K}_2\big(\cdot, \tfrac{\tau}{2}, A_*, S_1(\tau)\big) - \mathscr{J}_2\big(t_0 + \tfrac{\tau}{2}, \tfrac{\tau}{2}, A_*, R\big)\mathscr{K}_2\big(t_0, \tfrac{\tau}{2}, A_*, R\big),$$
$$D_{41}(\tau) = D_{42}(\tau) = D_{43}(\tau) = \mathscr{O}\Big(\tau^4\Big).$$

Local error (Taylor series expansion)

Taylor series expansion. First, employ Taylor series expansion (certain simplification in computation of arising integrals for choice $\sigma_0 = 0$, seems that there is no reason for alternative choice)

$$\begin{aligned}\mathrm{e}^{-\sigma A_*} F \,\mathrm{e}^{\sigma A_*} w &= F\,w + \mathscr{O}\Big(\tau^2, \|V'\|_{W^2_\infty}, \|w\|_{H^1}\Big) \\ &= F\,w + \sigma\,[F, A_*]\,w + \tfrac{1}{2}\,\sigma^2\,\big[[F, A_*], A_*\big]\Big)\,w + \mathscr{O}\Big(\tau^4, \|V'\|_{W^6_\infty}, \|w\|_{H^3}\Big).\end{aligned}$$

Note also that

$$\Big\|\mathrm{e}^{-\sigma A_*}\big(V(t) - V(s)\big)\,\mathrm{e}^{\sigma A_*} w\Big\|_{H^1} = \mathscr{O}\Big(\tau, \|V'\|_{W^1_\infty}, \|w\|_{H^1}\Big)$$

implies for instance

$$\begin{aligned}\mathscr{I}_4\big(\cdot, \tfrac{\tau}{2}, A_*, S_2(\tau)\big)\,w &= \int_0^{\frac{\tau}{2}}\int_0^{\sigma_1} \mathrm{e}^{-\sigma_1 A_*} S_2(\tau)\,\mathrm{e}^{\sigma_1 A_*}\,\mathrm{e}^{-\sigma_2 A_*} S_2(\tau)\,\mathrm{e}^{\sigma_2 A_*}\,\mathrm{d}\sigma_2\,\mathrm{d}\sigma_1\,w \\ &= \int_0^{\frac{\tau}{2}}\int_0^{\sigma_1} S_2(\tau)\,\mathrm{e}^{-\sigma_2 A_*} S_2(\tau)\,\mathrm{e}^{\sigma_2 A_*}\,\mathrm{d}\sigma_2\,\mathrm{d}\sigma_1\,w + \mathscr{O}\Big(\tau^5, \|V'\|_{W^2_\infty}, \|w\|_{H^1}\Big) \\ &= \int_0^{\frac{\tau}{2}}\int_0^{\sigma_1} S_2(\tau)\,S_2(\tau)\,\mathrm{d}\sigma_2\,\mathrm{d}\sigma_1\,w + \mathscr{O}\Big(\tau^5, \|V'\|_{W^2_\infty}, \|w\|_{H^1}\Big).\end{aligned}$$

Local error (Taylor series expansion)

Obtain expansions

$$\mathscr{J}_2\big(\cdot,\tfrac{\tau}{2},A_*,S_2(\tau)\big)\,w = J_2\big(\cdot,\tfrac{\tau}{2},A_*,S_2(\tau)\big)\,w + \mathscr{O}\Big(\tau^5,\|V'\|_{W^6_\infty},\|w\|_{H^3}\Big),$$
$$\mathscr{J}_2\big(t_0+\tfrac{\tau}{2},\tfrac{\tau}{2},A_*,R\big)\,w = J_2\big(t_0+\tfrac{\tau}{2},\tfrac{\tau}{2},A_*,R\big)\,w + \mathscr{O}\Big(\tau^5,\|V'\|_{W^6_\infty},\|w\|_{H^3}\Big),$$
$$J_2\big(\cdot,\tfrac{\tau}{2},A_*,S_2(\tau)\big) = I^{(+)}_{21}(S_2) + \big[I^{(+)}_{22}(S_2),A_*\big] + \big[\big[I^{(+)}_{23}(S_2),A_*\big],A_*\big],$$
$$J_2\big(t_0+\tfrac{\tau}{2},\tfrac{\tau}{2},A_*,R\big) = I^{(+)}_{21}(R) + \big[I^{(+)}_{22}(R),A_*\big] + \big[\big[I^{(+)}_{23}(R),A_*\big],A_*\big],$$
$$\mathscr{J}_4\big(\cdot,\tfrac{\tau}{2},A_*,S_2(\tau)\big)\,w = I^{(+)}_{4}(S_2)\,w + \mathscr{O}\Big(\tau^5,\|V'\|_{W^2_\infty},\|w\|_{H^1}\Big),$$
$$\mathscr{J}_4\big(t_0+\tfrac{\tau}{2},\tfrac{\tau}{2},A_*,R\big)\,w = I^{(+)}_{4}(R)\,w + \mathscr{O}\Big(\tau^5,\|V'\|_{W^2_\infty},\|w\|_{H^1}\Big).$$

Local error (Taylor series expansion)

Obtain expansions

$$\mathscr{K}_2\big(\cdot, \tfrac{\tau}{2}, A_*, S_1(\tau)\big)\, w = K_2\big(\cdot, \tfrac{\tau}{2}, A_*, S_1(\tau)\big)\, w + \mathscr{O}\Big(\tau^5, \|V'\|_{W^6_\infty}, \|w\|_{H^3}\Big),$$

$$\mathscr{K}_2\big(t_0, \tfrac{\tau}{2}, A_*, R\big)\, w = K_2\big(t_0, \tfrac{\tau}{2}, A_*, R\big)\, w + \mathscr{O}\Big(\tau^5, \|V'\|_{W^6_\infty}, \|w\|_{H^3}\Big),$$

$$K_2\big(\cdot, \tfrac{\tau}{2}, A_*, S_1(\tau)\big) = I_{21}^{(-)}(S_1) + \big[I_{22}^{(-)}(S_1), A_*\big] + \big[\big[I_{23}^{(-)}(S_1), A_*\big], A_*\big],$$

$$K_2\big(t_0 + \tfrac{\tau}{2}, \tfrac{\tau}{2}, A_*, R\big) = I_{21}^{(-)}(R) + \big[I_{22}^{(-)}(R), A_*\big] + \big[\big[I_{23}^{(-)}(R), A_*\big], A_*\big],$$

$$\mathscr{K}_4\big(\cdot, \tfrac{\tau}{2}, A_*, S_1(\tau)\big)\, w = I_4^{(-)}(S_1)\, w + \mathscr{O}\Big(\tau^5, \|V'\|_{W^2_\infty}, \|w\|_{H^1}\Big),$$

$$\mathscr{K}_4\big(t_0, \tfrac{\tau}{2}, A_*, R\big)\, w = I_4^{(-)}(R)\, w + \mathscr{O}\Big(\tau^5, \|V'\|_{W^2_\infty}, \|w\|_{H^1}\Big).$$

Local error (Integral representation)

Local error. Obtain local error expansion

$$
\begin{aligned}
&\mathscr{S}(\tau)\, u(t_0) - u(t_0+\tau) \\
&= \mathrm{e}^{\frac{\tau}{2} A_*} \Big(I_{21}^{(+)}(S_2) - I_{21}^{(+)}(R) + \big[I_{22}^{(+)}(S_2) - I_{22}^{(+)}(R), A_* \big] + \big[\big[I_{23}^{(+)}(S_2) - I_{23}^{(+)}(R), A_* \big], A_* \big] \\
&\qquad + I_{21}^{(-)}(S_1) - I_{21}^{(-)}(R) + \big[I_{22}^{(-)}(S_1) - I_{22}^{(-)}(R), A_* \big] + \big[\big[I_{23}^{(-)}(S_1) - I_{23}^{(-)}(R), A_* \big], A_* \big] \\
&\qquad + I_{4}^{(+)}(S_2) - I_{4}^{(+)}(R) + I_{4}^{(-)}(S_1) - I_{4}^{(-)}(R) \\
&\qquad + \Big(I_{21}^{(+)}(S_2) + \big[I_{22}^{(+)}(S_2), A_* \big] + \big[\big[I_{23}^{(+)}(S_2), A_* \big], A_* \big] \Big) \\
&\qquad\qquad \times \Big(I_{21}^{(-)}(S_1) + \big[I_{22}^{(-)}(S_1), A_* \big] + \big[\big[I_{23}^{(-)}(S_1), A_* \big], A_* \big] \Big) \\
&\qquad\quad - \Big(I_{21}^{(+)}(R) + \big[I_{22}^{(+)}(R), A_* \big] + \big[\big[I_{23}^{(+)}(R), A_* \big], A_* \big] \Big) \\
&\qquad\qquad \times \Big(I_{21}^{(-)}(R) + \big[I_{22}^{(-)}(R), A_* \big] + \big[\big[I_{23}^{(-)}(R), A_* \big], A_* \big] \Big) \Big) \mathrm{e}^{\frac{\tau}{2} A_*} u(t_0) \\
&\quad + \mathscr{O}\Big(\tau^5, \| V' \|_{W^6_\infty}, \| u(t_0) \|_{H^3} \Big) .
\end{aligned}
$$

Local error (Integrals)

$$
\begin{aligned}
I_{21}^{(+)}(S_2) &= \int_0^{\frac{\tau}{2}} S_2(\tau)\, \mathrm{d}\sigma_1\,, \\
I_{21}^{(+)}(R) &= \int_0^{\frac{\tau}{2}} R\big(t_0 + \tfrac{\tau}{2} + \sigma_1\big)\, \mathrm{d}\sigma_1\,, \\
I_{22}^{(+)}(S_2) &= \int_0^{\frac{\tau}{2}} \sigma_1\, S_2(\tau)\, \mathrm{d}\sigma_1\,, \\
I_{22}^{(+)}(R) &= \int_0^{\frac{\tau}{2}} \sigma_1\, R\big(t_0 + \tfrac{\tau}{2} + \sigma_1\big)\, \mathrm{d}\sigma_1\,, \\
I_{23}^{(+)}(S_2) &= \tfrac{1}{2} \int_0^{\frac{\tau}{2}} \sigma_1^2\, S_2(\tau)\, \mathrm{d}\sigma_1\,, \\
I_{23}^{(+)}(R) &= \tfrac{1}{2} \int_0^{\frac{\tau}{2}} \sigma_1^2\, R\big(t_0 + \tfrac{\tau}{2} + \sigma_1\big)\, \mathrm{d}\sigma_1\,, \\
I_{4}^{(+)}(S_2) &= \int_0^{\frac{\tau}{2}} \int_0^{\sigma_1} S_2(\tau)\, S_2(\tau)\, \mathrm{d}\sigma_2\, \mathrm{d}\sigma_1\,, \\
I_{4}^{(+)}(R) &= \int_0^{\frac{\tau}{2}} \int_0^{\sigma_1} R\big(t_0 + \tfrac{\tau}{2} + \sigma_1\big)\, R\big(t_0 + \tfrac{\tau}{2} + \sigma_2\big)\, \mathrm{d}\sigma_2\, \mathrm{d}\sigma_1\,.
\end{aligned}
$$

Local error (Integrals)

$$I_{21}^{(-)}(S_1) = \int_{-\frac{\tau}{2}}^{0} S_1(\tau)\,\mathrm{d}\sigma_1\,,$$

$$I_{21}^{(-)}(R) = \int_{-\frac{\tau}{2}}^{0} R\big(t_0 + \tfrac{\tau}{2} + \sigma_1\big)\,\mathrm{d}\sigma_1\,,$$

$$I_{22}^{(-)}(S_1) = \int_{-\frac{\tau}{2}}^{0} \sigma_1\,S_1(\tau)\,\mathrm{d}\sigma_1\,,$$

$$I_{22}^{(-)}(R) = \int_{-\frac{\tau}{2}}^{0} \sigma_1\,R\big(t_0 + \tfrac{\tau}{2} + \sigma_1\big)\,\mathrm{d}\sigma_1\,,$$

$$I_{23}^{(-)}(S_1) = \tfrac{1}{2}\int_{-\frac{\tau}{2}}^{0} \sigma_1^2\,S_1(\tau)\,\mathrm{d}\sigma_1\,,$$

$$I_{23}^{(-)}(R) = \tfrac{1}{2}\int_{-\frac{\tau}{2}}^{0} \sigma_1^2\,R\big(t_0 + \tfrac{\tau}{2} + \sigma_1\big)\,\mathrm{d}\sigma_1\,,$$

$$I_{4}^{(-)}(S_1) = \int_{0}^{\frac{\tau}{2}}\int_{\frac{\tau}{2}-\sigma_1}^{\frac{\tau}{2}} S_1(\tau)\,S_1(\tau)\,\mathrm{d}\sigma_2\,\mathrm{d}\sigma_1\,,$$

$$I_{4}^{(-)}(R) = \int_{0}^{\frac{\tau}{2}}\int_{\frac{\tau}{2}-\sigma_1}^{\frac{\tau}{2}} R\big(t_0 + \tfrac{\tau}{2} - \sigma_1\big)\,R\big(t_0 + \tfrac{\tau}{2} - \sigma_2\big)\,\mathrm{d}\sigma_2\,\mathrm{d}\sigma_1\,.$$

Local error ()

Local error. In final step, replace R by Taylor polynomial

$$
\begin{aligned}
&\mathscr{S}(\tau)\, u(t_0) - u(t_0 + \tau) \\
&= \mathrm{e}^{\frac{\tau}{2} A_*} \Big(\underbrace{I_{21}^{(+)}(S_2) - I_{21}^{(+)}(R) + I_{21}^{(-)}(S_1) - I_{21}^{(-)}(R)}_{= \mathscr{O}\left(\tau^5, R^{(4)}\right)} + \big[\underbrace{I_{22}^{(+)}(S_2) - I_{22}^{(+)}(R) + I_{22}^{(-)}(S_1) - I_{22}^{(-)}(R)}_{= \mathscr{O}\left(\tau^5, R'''\right)}, A_* \big] \\
&\qquad + \big[\big[\underbrace{I_{23}^{(+)}(S_2) - I_{23}^{(+)}(R) + I_{23}^{(-)}(S_1) - I_{23}^{(-)}(R)}_{= \mathscr{O}\left(\tau^5, R''\right)}, A_* \big], A_* \big] \\
&\qquad + \underbrace{I_4^{(+)}(S_2) - I_4^{(+)}(R) + I_4^{(-)}(S_1) - I_4^{(-)}(R) + I_{21}^{(+)}(S_2)\, I_{21}^{(-)}(S_1) - I_{21}^{(+)}(R)\, I_{21}^{(-)}(R)}_{= c\tau^4 (R')^2} \Big)\, \mathrm{e}^{\frac{\tau}{2} A_*} u(t_0) \\
&\quad + \mathscr{O}\Big(\tau^5, \|V'\|_{W_\infty^6}, \|u(t_0)\|_{H^3}\Big).
\end{aligned}
$$