The potential of Padé approximations for molecular dynamics simulations

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Numerical Challenges in Lattice QCD 2022

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Molecular Dynamics step

Geometric Integration on Lie Groups

Munthe-Kaas approach

Decomposition Schemes for Lie Groups

Conclusion and Outlook

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Hybrid Monte Carlo Method (HMC)*

HMC Algorithm

1. Start with a gauge field of links $[U]_i$.
2. Draw a field of random and fictitious momenta $[P]_i$.
3. Perform a Molecular Dynamics (MD) Step
$$([U]_i, [P]_i) \to ([U]_{i+1}, [P]_{i+1}) = \Phi_h ([U]_i, [P]_i)$$
using a geometric integration scheme Φ_h.
4. Accept the new configuration with probability
$$\min (1, \exp(-\Delta\mathcal{H})),$$
with $\Delta\mathcal{H} = \mathcal{H} ([U]_{i+1}, [P]_{i+1}) - \mathcal{H} ([U]_i, [P]_i)$.
5. Proceed with step 2.

*Duane et al., "Hybrid Monte Carlo"

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Molecular Dynamics Step - Hamiltonian EoM

- separable Hamiltonian

$$\mathcal{H}\left([U],[P]\right) = E_{\text{kin}}\left([P]\right) + S_G\left([U]\right)$$

  with kinetic energy E_{kin} and Wilson gauge action S_G.

- Hamiltonian equations of motion

$$\dot{U}_{x,\mu} = \frac{\partial \mathcal{H}\left([U],[P]\right)}{\partial P_{x,\mu}} \quad \text{and} \quad \dot{P}_{x,\mu} = -\frac{\partial \mathcal{H}\left([U],[P]\right)}{\partial U_{x,\mu}}$$

- Lie group / Lie algebra problem

$$\dot{U}_{x,\mu} = iP_{x,\mu}U_{x,\mu} \qquad \text{(Lie group ODE)},$$
$$i\dot{P}_{x,\mu} = F\left([U]\right)_{x,\mu} \qquad \text{(Lie algebra ODE)}.$$

Special Unitary Group $\mathrm{SU}(N)$

- Links U situated in the Lie group

$$\mathrm{SU}(N) = \left\{ Y \in \mathbb{C}^{N \times N} \,|\, Y^\dagger Y = I,\, \det(Y) = 1 \right\}$$

  of unitary matrices $Y \in \mathbb{C}^{N \times N}$ with determinant 1.
- Momenta P are traceless and Hermitian.
- Scaled momenta iP situated in the corresponding Lie algebra

$$\mathfrak{su}(N) = \left\{ A \in \mathbb{C}^{N \times N} \,|\, A^\dagger + A = 0,\, \mathrm{tr}(A) = 0 \right\}$$

  of traceless and anti-Hermitian matrices $A \in \mathbb{C}^{N \times N}$.

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Lie Group / Lie Algebra Problem

- Initial value problem of constrained ordinary differential equations

$$\dot{Y}(t) = A(t) \cdot Y(t), \qquad Y(0) := Y_0,$$
$$\dot{A}(t) = F(Y(t)), \qquad A(0) := A_0,$$

  on the time interval $[0, T]$.
- First differential equation evolving on Lie group G.
- Second differential equation evolving on corresponding Lie algebra $\mathfrak{g} = T_I G$, the tangent space at the identity.

Desired Properties of the Integration Scheme

- **Closure Property.** Preserve the Lie group / Lie algebra structure, i.e., we demand

$$(Y_1, A_1) = \Phi_h\left(Y_0, A_0\right) \in G \times \mathfrak{g}.$$

- **Time-Reversibility.** We demand

$$\rho \circ \Phi_h \circ \rho \circ \Phi_h(Y_0, A_0) = (Y_0, A_0)$$

with $\rho := \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$.

- **Volume-Preservation.** We demand

$$\left| \det \frac{\partial \Phi_h\left(Y_0, A_0\right)}{\partial\left(Y_0, A_0\right)} \right| = 1.$$

Local Coordinates Approach*

Local Coordinates Approach

Consider $Y_0 \in G$, $\Omega_0 \in \mathfrak{g}$ and a local parameterization $\Psi : \mathfrak{g} \to G$ s.t. $Y_0 = \Psi(\Omega_0) Y_0$. One step $Y_0 \mapsto Y_1$ with step size $h := t_1 - t_0$ is defined as follows:

1. Define the auxiliary ODE for $\Omega(t)$ as
$$\dot{\Omega}(t) = d\Psi_{\Omega}^{-1}(A(Y(t))), \quad \Omega(t_0) = \Omega_0.$$
2. Compute $\Omega_1 \approx \Omega(t_1)$ numerically by a numerical integration scheme Φ_h with step size $h := t_1 - t_0$.
3. Define the numerical solution of the ODE
$$\dot{Y}(t) = A(t) \cdot Y(t)$$
at time point $t_1 = t_0 + h$ by $Y_1 = \Psi(\Omega_1) \cdot Y_0$.

*Hairer, Lubich, and Wanner, *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations; 2nd ed.*

Local Coordinates Approach*

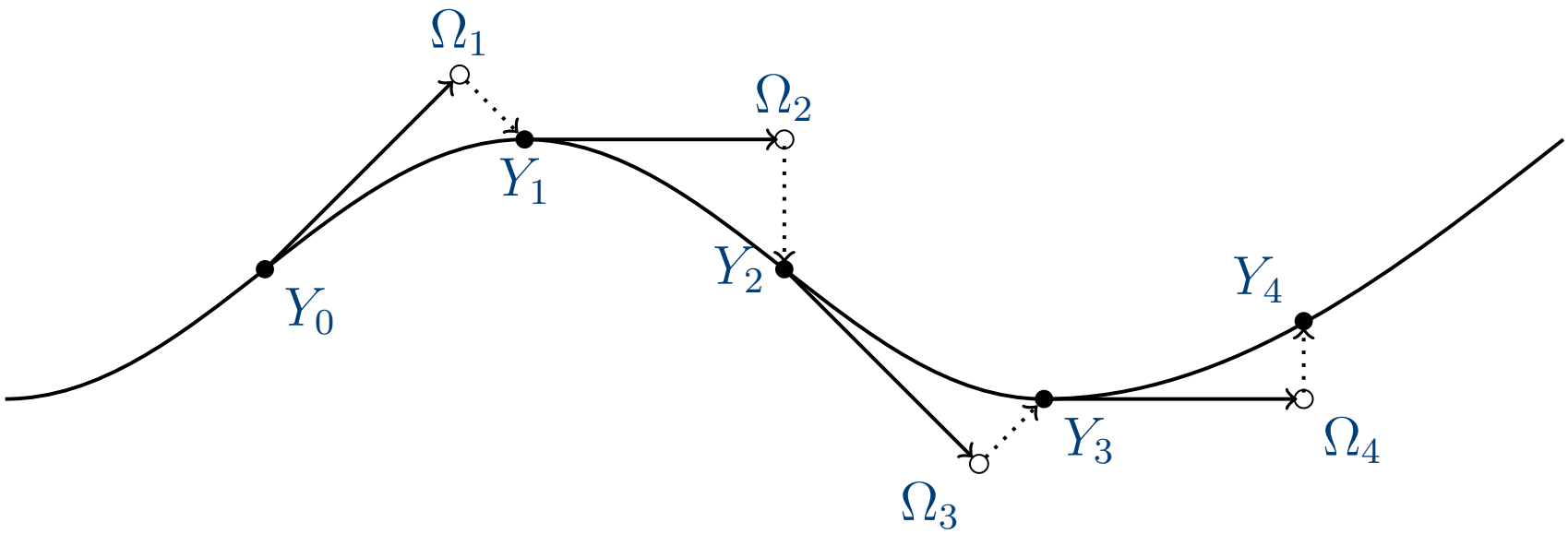

Figure: The numerical solution of differential equations on Lie groups via local coordinates. The Ω_i denote the result of the method Φ_h. The solid arrows denote the integration scheme Φ_h, whereas the dotted arrows denote the local parameterization Ψ.

*Hairer, Lubich, and Wanner, *Geometric Numerical Integration: Structure-Preserving Algorithms for Ordinary Differential Equations; 2nd ed.*

Choice of the local parameterization

Remark

As long as the local parameterization defines a mapping

$$\Psi : \mathfrak{g} \to G$$

and the initial value Ω_0 satisfies the consistency condition

$$\Psi(\Omega_0) = I,$$

the local coordinates approach defines an exact solution of the ODE

$$\dot{Y}(t) = A(t) \cdot Y(t).$$

Ψ is a local diffeomorphism near $\Omega = 0$.

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Munthe-Kaas Approach*

- special case of the local coordinates approach with $\Psi := \exp$
- The auxiliary ODE reads

$$\dot{\Omega}(t) = \sum_{k=0}^{\infty} \frac{B_k}{k!} \mathrm{ad}_{\Omega}^{k}(A(Y(t))), \quad \Omega(t_0) = \Omega_0 = 0,$$

  where B_k is the k-th Bernoulli number, and $\mathrm{ad}_{\Omega}(A) = [\Omega, A] = \Omega A - A\Omega$ is the adjoint operator.
- $B_0 = 1,\ B_1 = -\frac{1}{2},\ B_2 = \frac{1}{6},\ \ldots$
- $\mathrm{ad}_{\Omega}^{0}(A) = A,\ \mathrm{ad}_{\Omega}^{1}(A) = [\Omega, A],\ \mathrm{ad}_{\Omega}^{2}(A) = [\Omega, [\Omega, A]],\ \ldots$

*Munthe-Kaas, "Runge-Kutta methods on Lie groups".

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$$\dot{\Omega}(t) = \sum_{k=0}^{q} \frac{B_k}{k!} \mathrm{ad}_\Omega^k(A(Y(t))), \quad \Omega(t_0) = \Omega_0 = 0,$$

  where B_k is the k-th Bernoulli number, and $\mathrm{ad}_\Omega(A) = [\Omega, A] = \Omega A - A\Omega$ is the adjoint operator.
- $B_0 = 1$, $B_1 = -\frac{1}{2}$, $B_2 = \frac{1}{6}$, $\ldots$
- $\mathrm{ad}_\Omega^0(A) = A$, $\mathrm{ad}_\Omega^1(A) = [\Omega, A]$, $\mathrm{ad}_\Omega^2(A) = [\Omega, [\Omega, A]]$, $\ldots$
- Munthe-Kaas showed that $q \geq p - 2$ is necessary to obtain a method of convergence order p.

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- Munthe-Kaas showed that $q \geq p - 2$ is necessary to obtain a method of convergence order p.
- **Truncation of the infinite series introduces a model error.**

*Munthe-Kaas, "Runge-Kutta methods on Lie groups".

Runge-Kutta Munthe-Kaas (RKMK) methods†

- RKMK methods are suitable schemes for geometric integration on Lie groups
- Symmetric partitioned RKMK methods of order $p \geq 3$ are implicit due to the symmetry condition*

  $a_{i,j} = -a_{s+1-i,s+1-j}$.

  $\rightarrow$ RKMK methods of higher order are computationally infeasible.
- no conditions for volume-preserving schemes of order $p \geq 3$ found so far

*Wandelt, *Geometric Integration on Lie Groups and its Applications in Lattice QCD (PhD thesis)*

†Munthe-Kaas, "Runge-Kutta methods on Lie groups"

Improvement of RKMK schemes*

- idea: replace $\exp$ by the Cayley transform

$$\operatorname{cay}(A) := \left(I - \frac{1}{2}A\right)^{-1}\left(I + \frac{1}{2}A\right)$$

- resulting auxiliary ODE is given by

$$\dot{\Omega} = d\operatorname{cay}_{\Omega}^{-1}(A) = \left(I - \frac{1}{2}\Omega\right) A \left(I + \frac{1}{2}\Omega\right)$$

  $\rightarrow$ no infinite series, **no model error**
- for higher-order schemes ($p \geq 3$), we still have the problematic symmetry condition and no conditions for volume-preservation found so far
- non-optimized implementation of the Cayley transform as fast as the exponential map

*Schäfers, *Analysis of Partitioned GARK Methods for Geometric Integration on Lie Groups with focus on the Cayley Transform and Lattice QCD (Master thesis)*

Computation time of exp and cay in SU(2)

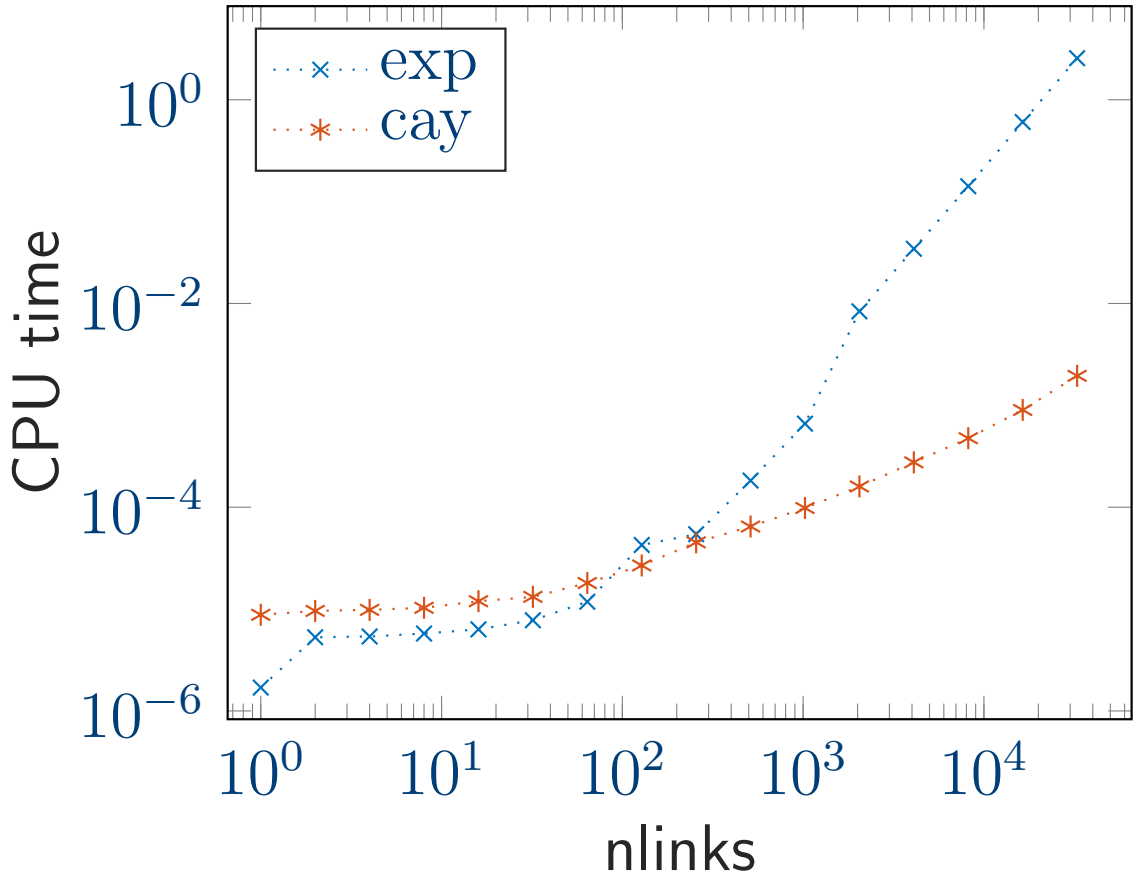

Figure: Comparison of the execution time of the exponential map $(\times)$ and the Cayley transform $(*)$ in SU(2) for different numbers of links. Implementation in MATLAB, execution time measured via function **timeit**.

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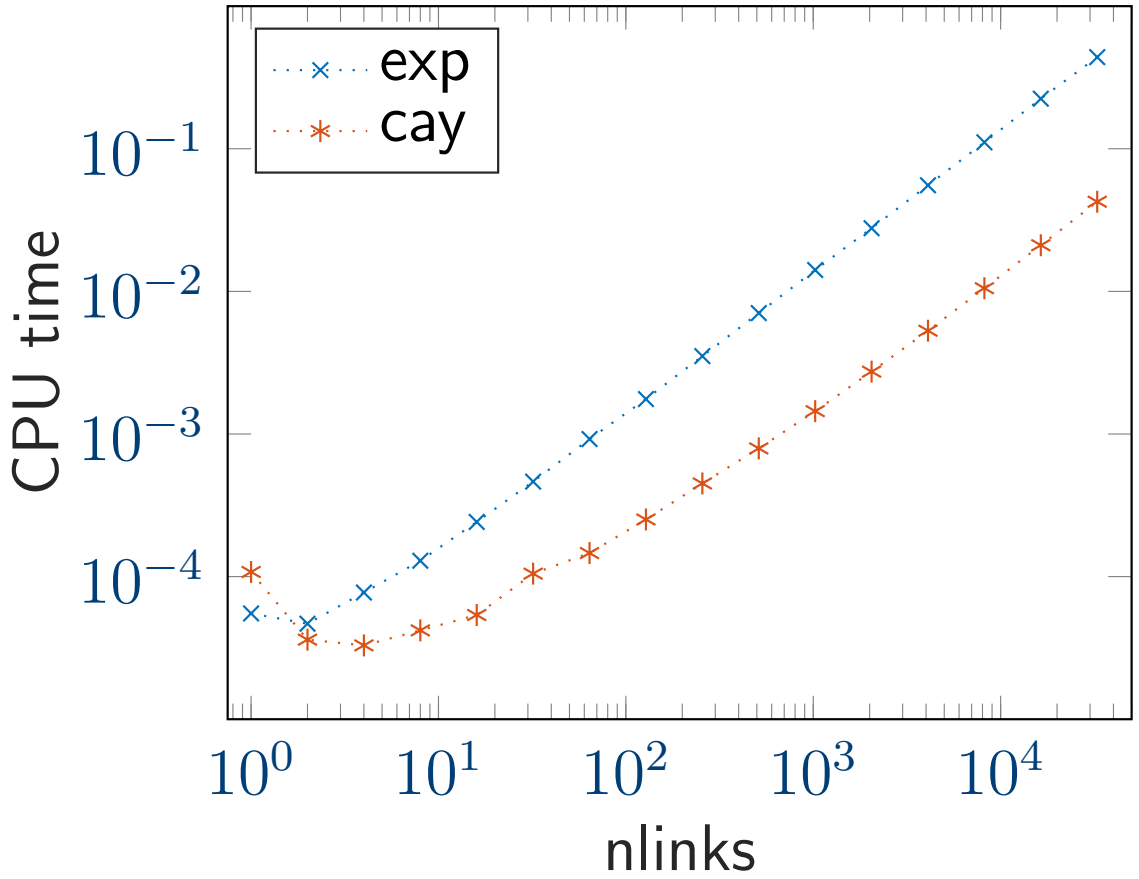

Figure: Comparison of the execution time of the exponential map $(\times)$ and the Cayley transform $(*)$ in SU(3) for different numbers of links. Implementation in MATLAB, execution time measured via function **timeit**. For $nlinks > 10^2$, cay is approx. 10 times faster.

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Decomposition Schemes*

- decomposition approach: factor out the exponential propagator on such suboperators which can be represented analytically or at least in quadratures
- achieved by splitting the full operator in its kinetic $\mathcal{A}$ and potential $\mathcal{B}$ parts
- then the total propagator can be decomposed as

$$e^{(\mathcal{A}+\mathcal{B})\Delta t+\mathcal{O}(\Delta t^{K+1})} = \prod_{p=1}^{P} e^{\mathcal{A}a_p\Delta t} e^{\mathcal{B}b_p\Delta t}$$

- extension to force-gradient integrators (FGIs)

$$e^{(\mathcal{A}+\mathcal{B})\Delta t+\mathcal{O}(\Delta t^{K+1})} = \prod_{p=1}^{P} e^{\mathcal{A}a_p\Delta t} e^{\mathcal{B}b_p\Delta t+\mathcal{C}c_p\Delta t^3}$$

where $\mathcal{C} = [\mathcal{B}, [\mathcal{A}, \mathcal{B}]]$.

*Omelyan, Mryglod, and Folk, "Symplectic analytically integrable decomposition algorithms: classification, derivation, and application to molecular dynamics, quantum and celestial mechanics simulations"

Model errors in state-of-the-art schemes?

Störmer–Verlet Method

$$
\begin{aligned}
A_{1/2} &= A_0 + \frac{h}{2} F(Y_0), \\
Y_1 &= \exp\left(h A_{1/2}\right) Y_0, \\
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- Time-reversible and volume-preserving numerical integration scheme of convergence order $p = 2$
- RKMK scheme, as well as decomposition scheme

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- Time-reversible and volume-preserving numerical integration scheme of convergence order $p = 2$
- RKMK scheme, as well as decomposition scheme
- **Solution of the auxiliary ODE is hidden as the argument inside the exponential map**
- Do we introduce a model error of order 2?

Problems of a possible model error

Composition Schemes

Let Φ_h be a one-step scheme of order p. If

$$\gamma_1 + \ldots + \gamma_s = 1 \quad \text{and} \quad \gamma_1^{p+1} + \ldots + \gamma_s^{p+1} = 0,$$

then the composition scheme $\tilde{\Phi}_h = \Phi_{\gamma_s h} \circ \ldots \circ \Phi_{\gamma_1 h}$ is at least of order $p+1$.

- common procedure to obtain symplectic and time-reversible Lie group integrators of higher order
- Example: using the Störmer–Verlet method as the basic scheme with $\gamma_1 = \gamma_3 = \frac{1}{2-\sqrt[3]{2}}$, $\gamma_2 = 1 - 2\gamma_1$ leads to Yoshida's scheme of order 4.
- integration error of order 4; if model error of order 2 $\rightarrow$ overall error of order 2 $\lightning$
- remedy: increase truncation index q suitably

Special property of decomposition schemes

- In decomposition schemes, the update of the Lie group elements consists of Lie-Euler steps.
- As every Lie-Euler step is an own local coordinates step, i.e., we always start with $\Omega_0 = 0$, the right-hand side $d\exp_{\Omega}^{-1}(A)$ of the auxiliary ODE will only be evaluated at time point t_0.
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- Thus, the auxiliary ODE reads

$$\dot{\Omega}(t) = A - \frac{1}{2}[\Omega_0, A] + \frac{1}{12}[\Omega_0, [\Omega_0, A]] + \dots$$

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- Thus, the auxiliary ODE reads

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- As the right-hand side becomes independent of Ω, there is **no model error** introduced.
- Hence composition schemes work.

Benefits of decomposition schemes

- Decomposition schemes and their compositions
  - only evaluating the auxiliary ODE at Ω_0
  - auxiliary ODE for $\Psi = \exp$ reduces to $\dot{\Omega}(t) = d\exp_{\Omega_0}^{-1}(A) = A$
- Lie group methods of Runge-Kutta type
  - usually include evaluations of the auxiliary ODE at internal stages $\bar{\Omega}_i \neq 0$
  - for $\Psi = \exp$, we need a suitable truncation of the auxiliary ODE
  - to obtain a scheme of order $p \geq 3$, commutators have to appear in the truncated ODE

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$\Rightarrow$ **Decomposition schemes are benefitial.**

Padé approximations for decomposition schemes

- As there is no model error, the use of Padé approximations can be motivated by possible speed-up
- It holds $d\mathrm{cay}^{-1}_{\Omega_0}(A) = A$ and $\mathrm{cay}(tA) - \exp(tA) = \mathcal{O}(t^3)$
  $\rightarrow$ in all schemes up to order 2, we can just replace the exponential map by the Cayley transform

Störmer-Verlet with exp and cay

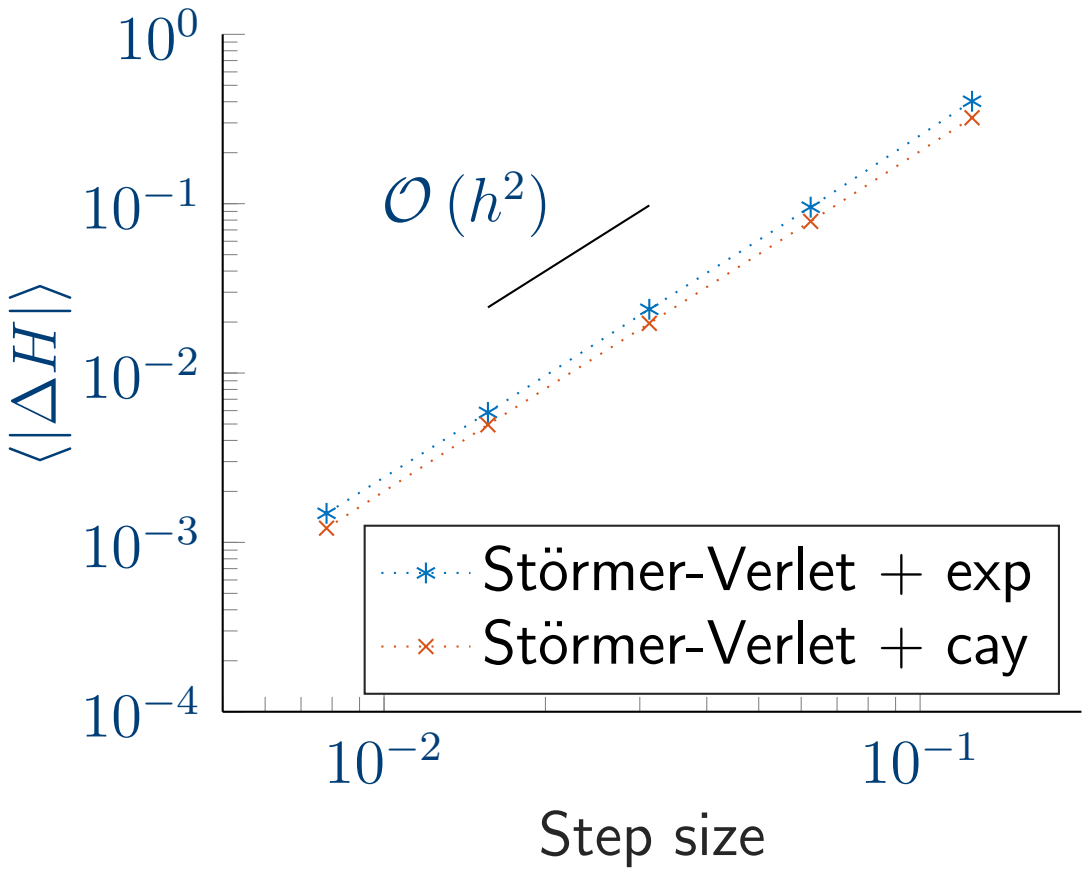

Figure: Numerical approximation error of $\langle |\Delta \mathcal{H}| \rangle$ for the Störmer-Verlet method using exp ($*$) and cay ($\times$) for different step sizes. $\langle |\Delta \mathcal{H}| \rangle$ along a trajectory with length 1 is computed from pure gauge field simulations in SU(3) that are comprised of 5000 trajectories on a lattice of size 32×32.

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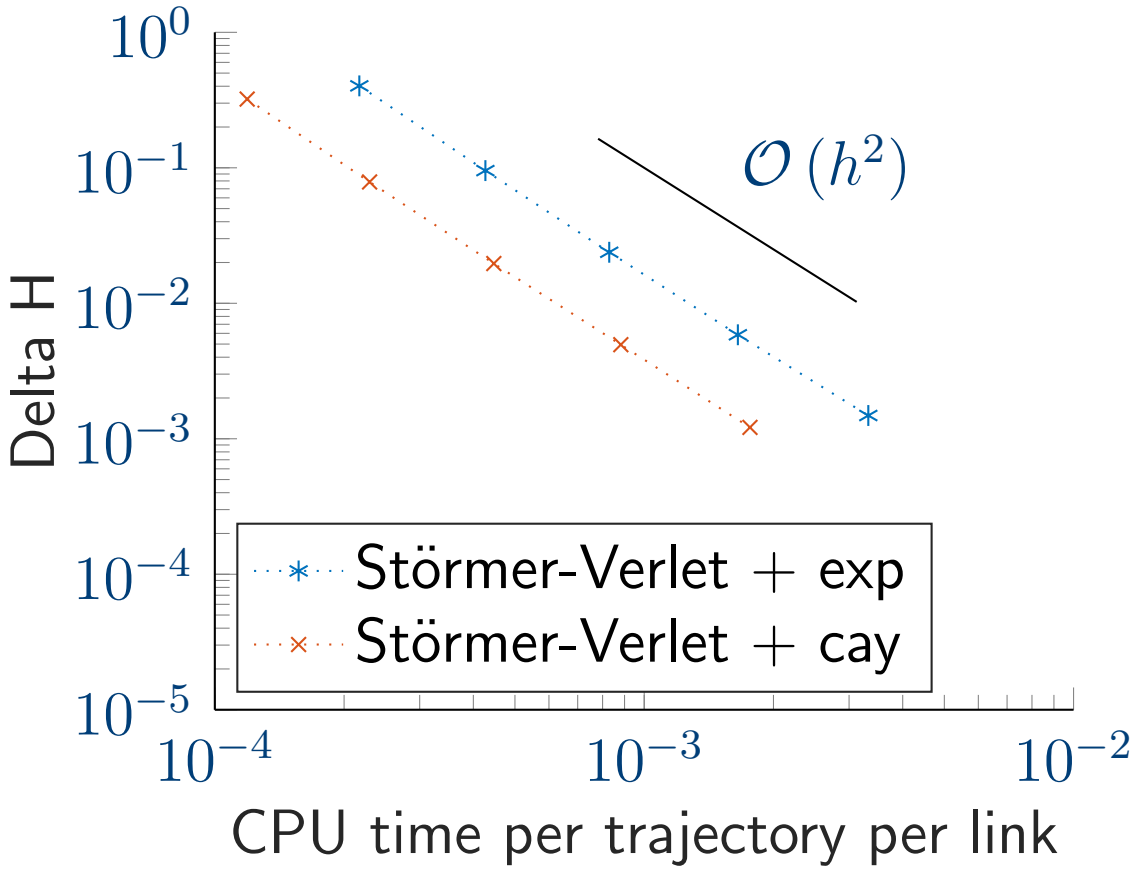

Figure: CPU time versus accuracy for Störmer–Verlet using exp ($*$) and cay ($\times$). These values are measured in pure gauge field simulations in SU(3) on a lattice of size 32×32.

Padé approximations for decomposition schemes

- Force-gradient integrators cannot use the Cayley transform as the force-gradient term changes
- Remedy: the Padé approximation of index $(2, 2)$

$$\mathrm{pade2}(A) := \left(I - \frac{1}{2}A + \frac{1}{12}A^2\right)^{-1}\left(I + \frac{1}{2}A + \frac{1}{12}A^2\right)$$

has the same force-gradient term s.t. the use of this local parameterization works for all FGIs of order 4

5-stage force-gradient scheme*

$$\Delta_{5C}(h) = e^{\frac{1}{6}h\hat{\mathcal{B}}} e^{\frac{1}{2}h\hat{\mathcal{A}}} e^{\frac{2}{3}h\hat{\mathcal{B}} - \frac{1}{72}h^3\mathcal{C}} e^{\frac{1}{2}h\hat{\mathcal{A}}} e^{\frac{1}{6}h\hat{\mathcal{B}}}$$

with force-gradient term $\mathcal{C} = \{\mathcal{B}, \{\mathcal{A}, \mathcal{B}\}\}$ with $\{,\}$ defining Lie brackets.
We approximate $\mathcal{C}$ via Taylor expansion as proposed by Yin and Mawhinney†.

†Yin and Mawhinney, "Improving dwf simulations: The force gradient integrator and the möbius accelerated dwf solver"

*Omelyan, Mryglod, and Folk, "Symplectic analytically integrable decomposition algorithms: classification, derivation, and application to molecular dynamics, quantum and celestial mechanics simulations"

FGI of order 4 - exp vs. pade2

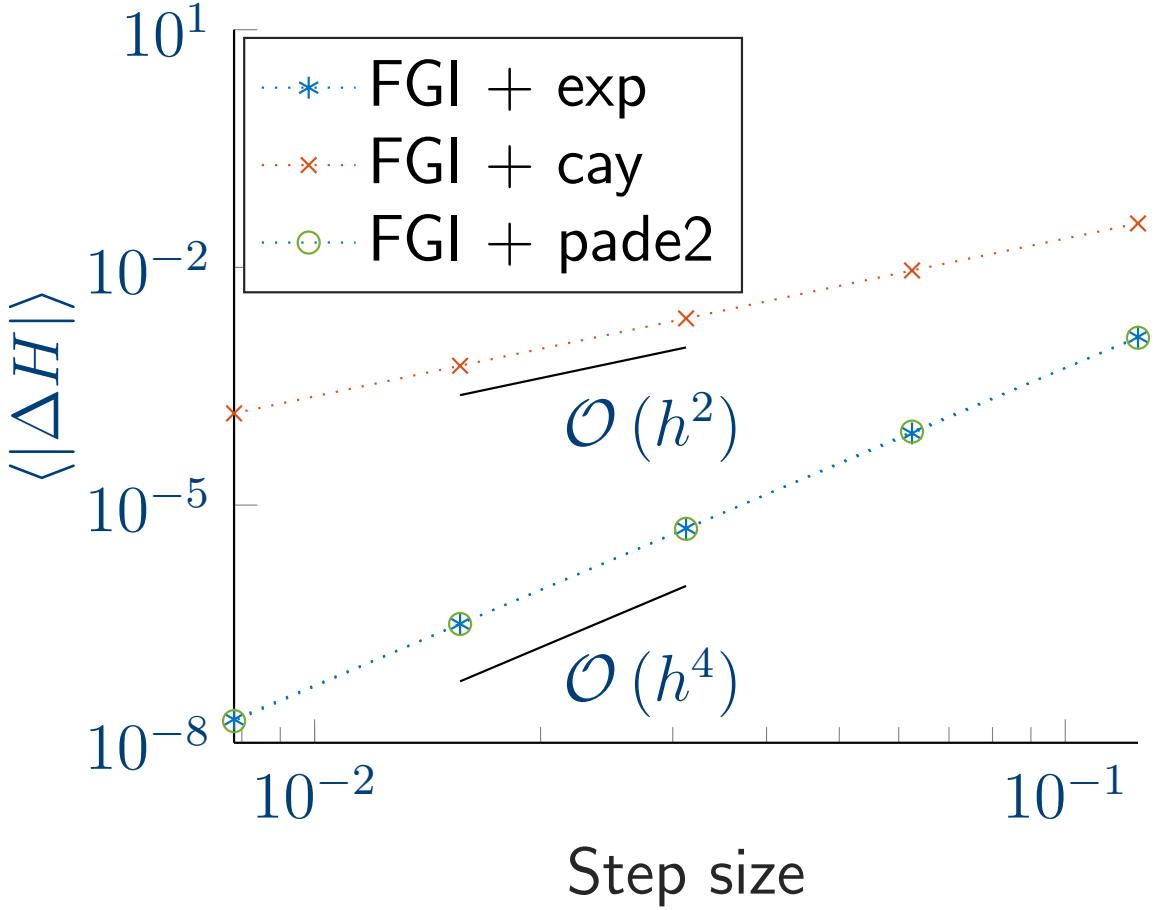

Figure: Numerical approximation error of $\langle|\Delta\mathcal{H}|\rangle$ for the Störmer-Verlet method using exp ($*$), cay ($\times$) and pade2 ($\circ$) for different step sizes. $\langle|\Delta\mathcal{H}|\rangle$ along a trajectory with length 1 is computed from pure gauge field simulations in SU(3) that are comprised of 1000 trajectories on a lattice of size 32×32.

Solving problems of Padé approximations for $\mathrm{SU}(3)$

- Problem: Padé approximations only define local parameterizations

$$\Psi : \mathfrak{su}(3) \to \mathrm{U}(3),$$

  i.e., it only holds $|\det(\Psi(A))| = 1$ for $A \in \mathfrak{su}(3)$.
- Way out using modification

$$\tilde{\Psi}(A) := \frac{1}{\sqrt[3]{\det \Psi(A)}} \cdot \Psi(A)$$

  which is equivalent to

$$\tilde{\Psi}(A) := e^{i\theta} \cdot \Psi(A)$$

  with

$$\theta := \frac{2}{3} \tan^{-1} \left(\frac{\Re(\det(\Psi(A))) - 1}{\Im(\det(\Psi(A)))} \right).$$

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Conclusion

- Decomposition schemes are consistent with the theorem of Munthe-Kaas
- (De-)composition schemes suitable tool for construction of explicit geometric integration methods for Lie groups that do not introduce a model error
- Padé approximations of the exponential map lead to a possible speed-up of (de-)composition schemes

Outlook

- Acceleration of the MD step by using Padé approximations of the exponential map
- Investigate force-gradient integrators using Padé approximations of the exponential map
- Parameter tuning of (non-gradient and force-gradient) decomposition schemes w.r.t. different objective functions
- Investigation of alternative approaches
  - Crouch-Grossman methods*
  - Celledoni-Marthinsen-Owren methods†
  - Bazavov commutator-free Lie group integrators‡

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*Crouch and Grossman, "Numerical integration of ordinary differential equations on manifolds"

†Celledoni, Marthinsen, and Owren, "Commutator-free Lie group methods"

‡Bazavov, "Commutator-free Lie group methods with minimum storage requirements and reuse of exponentials"