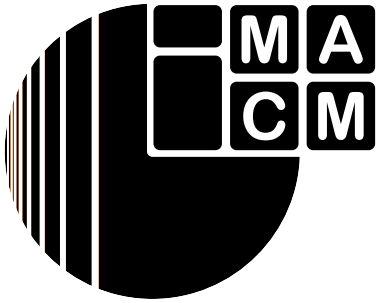

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Geometric integration on Lie groups using the Cayley transform with focus on Lattice QCD

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Abstract

This work deals with geometric numerical integration on a Lie group using the Cayley transformation. We investigate a coupled system of differential equations in a Lie group setting that occurs in Lattice Quantum Chromodynamics. To simulate elementary particles, expectation values of some operators are computed using the Hybrid Monte Carlo method. In this context, Hamiltonian equations of motion in a non-Abelian setting are solved with a time-reversible and volume-preserving integration method. Usually, the exponential function is used in the integration method to map the Lie algebra to the Lie group. In this paper, the focus is on geometric numerical integration using the Cayley transformation instead of the exponential function. The geometric properties of the method are shown for the example of the Störmer-Verlet method. Moreover, the advantages and disadvantages of both mappings are discussed.

Keywords: Numerical Analysis, Geometric Integration, Differential Equations on Lie Groups, Cayley Transform, Störmer-Verlet Scheme, Hybrid Monte Carlo, Lattice QCD

1. Introduction

This paper investigates the usage of the Cayley transform for matrix Lie groups inside the Störmer-Verlet scheme in the context of Lattice Quantum Chromo Dynamics (LQCD). For Lattice QCD computations, the Störmer-Verlet scheme defines a geometric integration method adapted to the Lie group structure. It uses the exponential function as local parameterization inside the Lie group. Since, in

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general, the computation of matrix exponential functions is very costly, the Cayley transform is surveyed as alternative local parameterization inside the Störmer-Verlet method. Both parameterizations are described in several publications, for example, in [1]-[9] and some applications can be found in [10]-[12].

Concerning Lattice QCD, the geometric properties – time-reversibility and volume-preservation – of the numerical integration scheme are of importance in order that they are also investigated in this work. For a numerical test, the geometric numerical integration schemes are applied on the Hamiltonian equations of motion in Lattice QCD, see, for example, [13] or [15]. More precisely, we simulate lattice gauge fields using Hybrid Monte Carlo (HMC) simulations [16] such that a Markov chain of configurations of lattice gauge fields is produced. Finally, these results are used for the computation of expectation values of some operators, for example for the mass of elementary particles. For this work, it is important that the Hybrid Monte Carlo method is composed of a Molecular Dynamics and an acceptance step. In the Molecular Dynamics part, Hamiltonian equations of motion occur which are coupled differential equations on a Lie group and a Lie algebra. They have to be solved with a time-reversible and volume-preserving numerical scheme to assure that the Markov chain tends towards the correct fixed point, i.e. the expectation values are computed correctly.

This paper opens with the recapitulation of some information about ordinary differential equations on Lie groups in section 2. It includes the local parameterizations used in numerical methods for Lie group equations and states the Lie-Euler and Störmer-Verlet schemes. Afterwards, the Cayley transform is introduced in section 3. In this part, the Störmer-Verlet method is adapted to the Cayley transform and finally, the geometric properties time-reversibility and volume-preservation are proven. Next, a brief introduction in Lattice QCD is followed in section 4. Here, the focus is put on the differential equations that have to be solved in the Hybrid Monte Carlo method. Also the Hamiltonian needed for the acceptance step is described in this part. Afterwards, the simulation of lattice gauge fields and its numerical results are described in section 5 leading to the conclusion in section 6.

2. Ordinary Differential Equations on Lie Groups

In this section, the concept of solving ordinary differential equations on Lie groups via local parameterizations is presented following the line of sections IV.5-IV.8 of [5]. Let G be a matrix Lie group and $\mathfrak{g}$ its associated Lie algebra. Then, the differential equation

$$\dot{Y}(t) = A(t) \cdot Y(t) \tag{1}$$

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with $Y(t) \in G$ and $A(t) \in \mathfrak{g}$ is a differential equation on a Lie group, i.e. its solution has to be in the Lie group. This result can be obtained via the connection of Lie groups and Lie algebras via differentiable manifolds as described in section IV.5 in [5] which is also the basis for the next paragraph.

Local parameterization. Differential equations on Lie groups are solved via the usage of a local parameterization

$$\Psi : \mathfrak{g} \mapsto G, \qquad Y(t) = \Psi(\Omega(t)) \tag{2}$$

from the Lie algebra $\mathfrak{g}$ to the Lie group G. Here, a new unknown $\Omega(t) \in \mathfrak{g}$ is introduced which is the result of the differential equation

$$\dot{\Omega} = \left(\mathrm{d}\,\Psi_{\Omega}^{-1}\right)(A) \tag{3}$$

in the Lie algebra, i.e. the expression $\mathrm{d}\,\Psi_{\Omega}^{-1}$ is applied on the Lie algebra element A such that the result $\dot{\Omega}$ is also in the Lie algebra. This is advantageous because the Lie algebra is a linear space such that the new differential equation $\dot{\Omega}$ can be solved using any numerical integration scheme for the Abelian case. Afterwards, the result is mapped back via the local parameterization (2) to the Lie group.

One difficulty is the detection of the expression $\mathrm{d}\,\Psi_{\Omega}^{-1}$. This can be achieved using the definition

$$\left(\frac{\mathrm{d}}{\mathrm{d}\,\Omega}\Psi(\Omega)\right)(H) = \left(\mathrm{d}\,\Psi_{\Omega}(H)\right) \cdot \Psi(\Omega) \tag{4}$$

where $\frac{\mathrm{d}}{\mathrm{d}\,\Omega}\Psi(\Omega)$ and $\mathrm{d}\,\Psi_{\Omega}$ are applied on a Lie algebra element H. Here, first the expression $\Psi(\Omega)$ has to be fixed. Then, the derivative $\frac{\mathrm{d}}{\mathrm{d}\,\Omega}\Psi(\Omega)$ applied on H follows using simple matrix calculus. Afterwards, the expression for $\mathrm{d}\,\Psi_{\Omega}(H)$ is the only unknown in equation (4) and can be computed which leads to its inverse $\mathrm{d}\,\Psi_{\Omega}^{-1}(H)$.

Exponential function as local parameterization. One possibility for the local parameterization is the exponential function as described in paragraphs IV.7 and IV.8 of [5]. It has the advantage that it can be used for any matrix Lie group such that it is applied as standard parameterization. The theorem of Magnus presents one way of solving the differential equation in the Lie group using the exponential function.

Theorem 1 (Magnus, [5], [17]). *The solution of the matrix differential equation* (1) *can be written as*

$$Y(t) = \exp(\Omega(t))\, Y_n \tag{5}$$

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with initial value $Y_n \in G$ and $\Omega(t)$ defined by

$$\dot{\Omega}(t) = \mathrm{d}\exp_{\Omega}^{-1}(A(t)), \quad \Omega(t_n) = \Omega_n = 0. \tag{6}$$

As long as $||\Omega(t)|| < \pi$ the convergence of the $d\exp_{\Omega}^{-1}$ expansion

$$\mathrm{d}\exp_{\Omega}^{-1}(A) = \sum_{k\geq 0}^{\infty} \frac{B_k}{k!} \mathrm{ad}_{\Omega}^{k}(A) \tag{7}$$

with Bernoulli numbers B_k and adjoint operator $\mathrm{ad}_{\Omega}(A) = [\Omega, A]$ is assured.

The Bernoulli numbers B_k and the adjoint operator ad_{Ω}^{k} are stated in the following definitions.

Definition 1 (Bernoulli Numbers, [5], [18]). *The Bernoulli numbers B_k are defined by*

$$\sum_{k\geq 0}^{\infty} \frac{B_k}{k!} x^k = \frac{x}{\exp(x) - 1}. \tag{8}$$

The first few Bernoulli numbers are $B_0 = 1, B_1 = -\frac{1}{2}, B_2 = \frac{1}{6}, B_3 = 0$.

Definition 2 (Adjoint Operator, [5], [19]). *The adjoint operator $\mathrm{ad}_{\Omega}(A)$ is a linear operator*

$$\mathrm{ad} : \mathfrak{g} \mapsto \mathfrak{g}, \qquad A \mapsto \mathrm{ad}_{\Omega}(A) = [\Omega, A] \tag{9}$$

for a fixed Ω and matrix commutator $[\Omega, A] = \Omega \cdot A - A \cdot \Omega$.

The adjoint operator can be used iteratively, such that ad_{Ω}^{k} denotes the k-th iterated application of the linear operator ad_{Ω}. It holds $\mathrm{ad}_{\Omega}^{k+1} = \left[\Omega, \mathrm{ad}_{\Omega}^{k}\right]$. By convention, $\mathrm{ad}_{\Omega}^{0}(A)$ is set to A.

The theorem of Magnus reveals how to replace the initial value problem (1) in the Lie group with an initial value problem (6) in the Lie algebra using the local parameterization

$$\exp : \mathfrak{g} \to G, \qquad \Omega(t) \mapsto Y(t) = \exp(\Omega(t)) \cdot Y_n \ . \tag{10}$$

So, the differential equation (6) can be solved with any Runge-Kutta method for the Abelian case. Afterwards, its numerical approximation Ω_{n+1} is mapped back to the Lie group via equation (10). Nevertheless, the usage of the exponential function suffers from one big disadvantage: the inverse of the derivative of the exponential function is an infinite series as stated in equation (7). In general, there is no closed form for $(\mathrm{d}\exp_{\Omega})^{-1}$, with the result that this series has to be truncated somehow in the numerical method. This procedure is known as Munthe-Kaas method.

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Algorithm 1 (Munthe-Kaas schemes, [5], [20]). *The Lie group problem* (1) *with initial values* $Y(t_n) := Y_n \in G$ *and* $A(t_n) := A_n \in \mathfrak{g}$ *can be solved as follows:*

1. *Consider the differential equation*

$$\mathrm{d}\exp_\Omega^{-1}(A) \approx \dot{\Omega} = \sum_{k\geq 0}^{q} \frac{B_k}{k!} \operatorname{ad}_\Omega^k(A) =: f_q(\Omega, A) \tag{11}$$

   with initial value $\Omega(t_n) = \Omega_n = 0$.
2. *Apply a Runge-Kutta method with initial values* $\Omega_n = 0$ *to reach the numerical approximation* $\Omega_{n+1} \approx \Omega(t_n + h)$.
3. *Define the numerical solution by*

$$Y_{n+1} = \exp(\Omega_{n+1})\, Y_n. \tag{12}$$

At this place, a model error is introduced because the considered differential equation (11) differs from the original differential equation (7) as discussed, e.g, in [21]. The model error should be smaller than the desired convergence order such that it does not influence the result. Munthe-Kaas describes a criterion for the truncation index q such that the model error is small enough related to a desired convergence order of the Runge-Kutta scheme as follows:

Theorem 2 (Truncation index, [5], [20]). *The method of algorithm 1 is of order* p *if the truncation index in* (11) *satisfies* $q \geq p - 2$ *and the underlying Runge–Kutta method is also of (classical) order* p.

The proof of this theorem can be found in section IV.8.2 of [5].

Lie-Euler scheme. The explicit Euler is the most simple example for a Munthe-Kaas Runge-Kutta scheme. It has convergence order $p = 1$ such that (according to theorem 2) the truncation index used in equation (11) would be $q = p-2 = -1$. Since values of q smaller than zero are not defined, $q = 0$ is used such that the differential equation $\dot{\Omega} = A$ with initial value $\Omega_n = 0$ has to be solved in the Lie algebra. Then, the explicit Euler scheme leads to the numerical approximation

$$\Omega_{n+1} = \Omega_n + h\, \dot{\Omega}(t_n) = h f_0(\Omega_n, A) = h\, A_n. \tag{13}$$

Finally, the result is mapped via equation (10) in the Lie group:

$$\Omega_{n+1} \mapsto Y_{n+1} = \exp(\Omega_{n+1}) \cdot Y_n. \tag{14}$$

Often, the combination of these two steps is mentioned as Lie-Euler method

$$Y_{n+1} = \exp(hA_n) \cdot Y_n. \tag{15}$$

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This is a special case of Munthe-Kaas as well as Crouch-Grossmann Runge-Kutta schemes of convergence order $p = 1$ using the exponential function as local parameterization in the Lie group [5].

Coupled differential equation in a Lie group and its associated Lie algebras. We are concerned with geometric integration schemes for a coupled system of differential equations on a matrix Lie group G and its associated matrix Lie algebra $\mathfrak{g}$. More precise, the system is given by

$$\dot{Y}(t) = A(t) \cdot Y(t) \tag{16a}$$

$$\text{and} \quad \dot{A}(t) = F(Y(t)) \tag{16b}$$

with matrix Lie group element $Y(t) \in G$, matrix Lie algebra element $A(t) \in \mathfrak{g}$ and matrix Lie algebra-valued function $F : G \mapsto \mathfrak{g}$. The first equation (16a) a differential equation on a Lie group G as equation (1) and can be treated in the same way. The second equation (16a) is solved on a Lie algebra $\mathfrak{g}$ which is a linear space. This means, it can be solved with any numerical method applicable for the Abelian case.

Störmer-Verlet scheme for Lie groups and Lie algebras. The most simple geometric, i.e. time-reversible and volume-preserving numerical integration scheme for such a system is the Leapfrog or Störmer-Verlet scheme. It solves the initial-value problem (16) with initial values $Y(t_0) = Y_n \in G$ and $A(t_0) = A_n \in \mathfrak{g}$ and reads

$$A_{n+\frac{1}{2}} = A_n + \tfrac{h}{2} F(Y_n), \tag{17a}$$

$$\Omega_{n+1} = h A_{n+\frac{1}{2}}, \tag{17b}$$

$$Y_{n+1} = \exp(\Omega_{n+1}) Y_n, \tag{17c}$$

$$A_{n+1} = A_{n+\frac{1}{2}} + \tfrac{h}{2} F(Y_{n+1}). \tag{17d}$$

Here, the parameterization $\Psi = \exp$ is used such that $\dot{\Omega} = \mathrm{d}\exp_\Omega^{-1}$ has to be solved numerically as explained for the explicit Lie-Euler scheme.

3. Cayley Transform

The Cayley transform can be used as alternative parameterization for quadratic Lie groups $G = \{Y | Y^\top P Y = P\}$ with given constant matrix $P \neq 0$ as mentioned in section IV.8.3 of [5]. It reads

$$\mathfrak{g} \mapsto G : \quad \Omega \mapsto \mathrm{cay}(\Omega) = \big(I - \Omega(t)\big)^{-1} \big(I + \Omega(t)\big). \tag{18}$$

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So, differential equations on Lie groups can be solved using the parameterization $\Psi = \mathrm{cay}$ such that the differential equation $\dot{\Omega} = \mathrm{d}\,\mathrm{cay}_\Omega^{-1}$ with

$$\mathfrak{g} \mapsto \mathfrak{g}: \qquad \mathrm{d}\,\mathrm{cay}_\Omega^{-1}\big(A(t)\big) = \frac{1}{2}\big(I - \Omega(t)\big)A(t)\big(I + \Omega(t)\big) \tag{19}$$

has to be solved in the Lie algebra. Here, no infinite series has to be truncated such that just two matrix multiplications have to be performed. On the other hand, the Cayley transform is feasible for quadratic Lie groups and, moreover, also the inverse of $I - \Omega(t)$ must exist and be computable in an easy and numerically stable way.

Inverse of $I - \Omega(t)$. In this work, we focus on the Hamiltonian equations of motion used in Lattice QCD which are defined for the Lie group $SU(N, \mathbb{C})$ and its associated Lie algebra $\mathfrak{su}(N, \mathbb{C})$. In this case, it is sufficient to show that the eigenvalues of $\Omega(t)$ are purely imaginary. The matrix $\Omega(t)$ is an element of the Lie algebra $\mathfrak{su}(N, \mathbb{C})$ such that it is traceless and anti-hermitian. This means, $\Omega(t) + \Omega^H(t) = 0$. The eigenvalues λ of $\Omega(t)$ are computed via $\Omega(t)x = \lambda x$. It follows $(\Omega(t)x)^H = \bar{\lambda}x^H$ with complex conjugate eigenvalue $\bar{\lambda}$ such that it holds

$$0 = x^H\Big(\Omega(t) + \Omega^H(t)\Big)x = |\bar{\lambda} + \lambda|\, x. \tag{20}$$

This implies that the real part of the eigenvalues λ of $\Omega(t)$ must be zero such that they are purely imaginary. Thus, the matrix $I - \Omega(t)$ is a regular matrix.

Numerical Schemes. Starting from an initial value $\Omega_n = 0$, the numerical approximation Ω_{n+1} is computed as

$$\Omega_{n+1} = \Omega_n + h \cdot \mathrm{d}\,\mathrm{cay}_\Omega^{-1} = \tfrac{h}{2}A_n. \tag{21}$$

according to equation (19). Then, the explicit Cayley-Lie-Euler scheme reads

$$Y_{n+1} = \mathrm{cay}(\Omega_{n+1})Y_n = \mathrm{cay}(\tfrac{h}{2}A_n)Y_n, \tag{22}$$

with result in the Lie group. Finally, we are interested in the Cayley-Leapfrog or Cayley Störmer-Verlet method for Lie groups:

$$A_{n+\frac{1}{2}} = A_n + \tfrac{h}{2}F(Y_n), \tag{23a}$$
$$\Omega_{n+1} = \Omega_n + \tfrac{h}{2}A_{n+\frac{1}{2}}, \tag{23b}$$
$$Y_{n+1} = \mathrm{cay}(\Omega_{n+1})Y_n, \tag{23c}$$
$$A_{n+1} = A_{n+\frac{1}{2}} + \tfrac{h}{2}F(Y_{n+1}). \tag{23d}$$

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This method is similar to the aforementioned scheme (17). Just the numerical approximation for the differential equation on the Lie group is adapted: the local parameterization in equation (23c) is changed from the exponential function (equation (17c)) to the Cayley transform. That requires an additional change from $\Omega_{n+1} = hA_{n+\frac{1}{2}}$ (see equation (17b)) in the standard Störmer-Verlet scheme towards $\Omega_{n+1} = h \cdot 0.5A_{n+\frac{1}{2}}$ to meet the same convergence order. This means for the Störmer-Verlet scheme, the operators $\mathrm{d}\exp_{\Omega}^{-1}$ and $\mathrm{d}\,\mathrm{cay}_{\Omega}^{-1}$ differ by a factor 0.5.

For the usage in HMC simulations it must be ensured that the numerical integration method is time-reversible and volume-preserving. The standard Störmer-Verlet scheme for coupled Lie group / Lie algebra problems as defined in equation (17) is known to have these qualities. Next, it is proven that the Cayley-Leapfrog method for Lie groups is also time-reversible and volume-preserving.

Volume-preservation. The Störmer-Verlet scheme computes the numerical approximation $(Y_{n+1}, A_{n+1}, \Omega_{n+1})$ from the initial values (Y_n, A_n, Ω_n). So, we observe the phase space $G \times \mathfrak{g} \times \mathfrak{g}$ which corresponds to the canonical volume form on $\mathbb{R}^{N\times N} \times \mathbb{R}^{N\times N} \times \mathbb{R}^{N\times N}$. The volume-preservation of the scheme is assured if the value of the determinant of the Jacobian of the overall step

$$\Theta := \frac{\partial(Y_{n+1}, A_{n+1}, \Omega_{n+1})}{\partial(Y_n, A_n, \Omega_n)} \tag{24}$$

takes the value ± 1.

It holds that an overall scheme is volume-preserving if it is composed of volume-preserving schemes. The Leapfrog method is composed of four subsequent single updates:

$$\begin{pmatrix} Y_n \\ A_n \\ \Omega_n \end{pmatrix} \xrightarrow{\alpha} \begin{pmatrix} Y_n \\ A_{n+\frac{1}{2}} \\ \Omega_n \end{pmatrix} \xrightarrow{\beta} \begin{pmatrix} Y_n \\ A_{n+\frac{1}{2}} \\ \Omega_{n+1} \end{pmatrix} \xrightarrow{\gamma} \begin{pmatrix} Y_{n+1} \\ A_{n+\frac{1}{2}} \\ \Omega_{n+1} \end{pmatrix} \xrightarrow{\delta} \begin{pmatrix} Y_{n+1} \\ A_{n+1} \\ \Omega_{n+1} \end{pmatrix}$$

Thus, it has to be shown that the determinant of the Jacobians of the single updates α, β, γ and δ have the values ± 1. The Jacobians read

$$\alpha := \left(\frac{\partial(Y_n, A_{n+1/2}, \Omega_n)}{\partial(Y_n, A_n, \Omega_n)}\right), \quad \beta := \left(\frac{\partial(Y_n, A_{n+1/2}, \Omega_{n+1})}{\partial(Y_n, A_{n+1/2}, \Omega_n)}\right),$$

$$\gamma := \left(\frac{\partial(Y_{n+1}, A_{n+1/2}, \Omega_{n+1})}{\partial(Y_n, A_{n+1/2}, \Omega_{n+1})}\right), \quad \delta := \left(\frac{\partial(Y_{n+1}, A_{n+1}, \Omega_{n+1})}{\partial(Y_{n+1}, A_{n+1/2}, \Omega_{n+1})}\right)$$

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and take the values

$$\alpha = \begin{pmatrix} I & 0 & 0 \\ \frac{h}{2}F'(Y_n) & I & 0 \\ 0 & 0 & I \end{pmatrix}, \quad \beta = \begin{pmatrix} I & 0 & 0 \\ 0 & I & 0 \\ 0 & \frac{h}{2}I & I \end{pmatrix},$$

$$\gamma = \begin{pmatrix} \operatorname{cay}(\Omega_{n+1}) & 0 & \operatorname{dcay}_{\Omega}(\Omega_{n+1})Y_n \\ 0 & I & 0 \\ 0 & 0 & I \end{pmatrix}, \quad \delta = \begin{pmatrix} I & 0 & 0 \\ \frac{h}{2}F'(Y_{n+1}) & I & 0 \\ 0 & 0 & I \end{pmatrix}.$$

The determinants of each Jacobian α, β and δ are obviously equal to one. For the determinant of γ it holds

$$\det(\gamma) = \det\big(\operatorname{cay}(\Omega_{n+1})\big).$$

Here, we know that the Cayley transform maps an element of the Lie algebra to the Lie group. Thus, for Lie groups characterized through a determinant with value one, it holds $\det\big(\operatorname{cay}(\Omega_{n+1})\big) = 1$. This is valid, for example for the special orthogonal or special unitary Lie groups $SO(N)$ and $SU(N, \mathbb{C})$ arising in the Lattice QCD setting in sections 4 and 5.

Time-reversibility. A method

$$\Phi_h : (Y_n, A_n) \to (Y_{n+1}, A_{n+1}) \tag{25}$$

is time-reversible if it holds

$$\Phi_h \circ \rho \circ \Phi_h = \rho \quad \text{with} \quad \rho = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}. \tag{26}$$

If the scheme is symmetric, i.e., $\Phi_h = \Phi_{-h}^{-1}$, then time-reversibility is equivalent to

$$\rho \circ \Phi_h = \Phi_{-h} \circ \rho. \tag{27}$$

Symmetry for a scheme is given if exchanging the subscripts $n \leftrightarrow n+1$ and step size $h \leftrightarrow -h$ leaves the method unaltered. This property can easily be verified for the Cayley-Leapfrog scheme described in equation (23). In addition, it can easily be shown that this scheme is also time-reversible. We just compute $\rho \circ \Phi_h(Y_n, A_n)$ and $\Phi_{-h} \circ \rho(Y_n, A_n)$ and compare these values. Starting with $\rho \circ \Phi_h$ gives

$$\rho \circ \Phi_h(Y_n, A_n) = \begin{pmatrix} \operatorname{cay}\left(\frac{h}{2}(A_n + \frac{h}{2}F(Y_n))\right)Y_n \\ -\Big(A_n + \frac{h}{2}F(Y_n) + \frac{h}{2}F\big(\operatorname{cay}\left(\frac{h}{2}(A_n + \frac{h}{2}F(Y_n))\right)Y_n\big)\Big) \end{pmatrix}^{\top}.$$

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The second equation leads to

$$\Phi_{-h} \circ \rho(Y_n, A_n) = \begin{pmatrix} \operatorname{cay}\Big(-\frac{h}{2}\big(-A_n - \frac{h}{2}F(Y_n)\big)\Big)Y_n \\ -A_n - \frac{h}{2}F(Y_n) - \frac{h}{2}F\Big(\operatorname{cay}\Big(-\frac{h}{2}\big(-A_n - \frac{h}{2}F(Y_n)\big)\Big)Y_n\Big) \end{pmatrix}^{\top}.$$

Thus, this shows that the condition for time-reversibility (27) is fulfilled.

4. Lattice QCD and Geometric Integration

We apply the Störmer-Verlet scheme on the Hamiltonian equations of motion occurring in Lattice Quantum Chromo Dynamics (LQCD), which investigates subatomic particles via simulations on an equidistant lattice. More precisely, the subatomic particles build the protons and neutrons inside the nucleus of an atom. They are called quarks and gluons; the quarks are are represented as complex vectors with a spin and color index whereas the gluons are modeled as elements of the special unitary Lie group $SU(3, \mathbb{C})$ which consists of complex and unitary matrices of size 3×3 and determinant one. For the simulations, the quarks and gluons are put on a 4-dimensional lattice such that the quarks are situated on the sites of the lattice and the gluons on the interconnecting lines between them. For our purposes of investigating the Cayley transform as local parameterization in the most simple geometric integration method, it is sufficient to work with a lattice gauge field of gluons which are also called link matrices or just links. In our simulations, we consider just the gluons, the quarks are left out.

Simulations of lattice gauge fields aim at computing expectation values of some operators using a Markov chain Monte Carlo method. Here, the Hybrid Monte Carlo method alternating a Molecular Dynamics and an acceptance step is frequently used. Inside the Molecular Dynamics step, a geometric integration scheme Φ is applied on Hamiltonian equations of motion such that a new test configuration is achieved. Afterwards, the probability for the new configuration is compared to the probability of the old configuration in the acceptance step. This is based on the difference of the Hamiltonians before and after a Molecular Dynamics step. Finally, either the old or the new configuration is added to the Markov chain and used as initial configuration for the next step. We focus on the Hamiltonian equations of motion inside the Molecular Dynamics step which have to be solved using a time-reversible and volume-preserving numerical integration scheme as described in [16]. Then, a Markov chain of configurations is produced according to the probability distribution of the Wilson action S_G. For the HMC, the Hamiltonian

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$H([U],[P])$ as well as its Hamiltonian equations of motion

$$\dot{U}_{x,\mu} = \frac{\partial H([U],[P])}{\partial P_{x,\mu}} \quad \text{and} \quad \dot{P}_{x,\mu} = -\frac{\partial H([U],[P])}{\partial U_{x,\mu}} \tag{28}$$

are of importance. The links $[U]$ represent the set of gluons whereas the momenta $[P]$ are purely fictitious but traceless and hermitian matrices of size $N \times N$.

The Hamiltonian equations of motion occur for each pair $(U_{x,\mu}, P_{x,\mu})$ at position (x,μ) on the grid and read in general

$$\dot{U}_{x,\mu} = iP_{x,\mu}U_{x,\mu} \quad \text{and} \quad i\dot{P}_{x,\mu} = F(U_{x,\mu}). \tag{29}$$

Here, $U_{x,\mu}$ is an element of the Lie group $SU(N,\mathbb{C})$, $iP_{x,\mu}$ an element of the Lie algebra $\mathfrak{su}(N,\mathbb{C})$ and F a linear mapping from the Lie group to the Lie algebra. (Compared to the formulation given in (28), the second equation is multiplied with i to work in the Lie algebra.) The Hamiltonian equations of motion (29) have the same shape as the coupled Lie group / Lie algebra problem (16). Thus, equation (16a) is a differential equation on a Lie group and requires a solution in the Lie group whereas equation (16b) is a differential equation on a Lie algebra and solved there. The numerical schemes have to be time-reversible and volume-preserving such that the Markov chain tends towards the correct equilibrium distribution.

The d-dimensional lattice itself consists on L^d grid points numbered from $x = 1,\ldots,L^d$ and d dimensions labeled with the Greek letters $\mu,\nu = 1,\ldots,d$ as explained, for example, in paragraph 2.1.1 of [14]. The links are situated on the dL^d interconnecting lines between the grid points. The indices (x,μ) denote all links $U_{x,\mu}$ in direction μ. More precisely, $U_{x,\mu}$ denotes the link between the grid points x and $x + a\hat{\mu}$ with lattice distance a and unit vector $\hat{\mu}$ in direction μ. The links are unitary such that a link in opposite direction $-\mu$ is denoted with $U_{x,\mu}^{-1}$. Usually, d is set to $d = 4$ or smaller. In our example, we work with $d = 2$ such that $2L^2$ coupled differential equations have to be solved in each step.

As mentioned before, the Hamiltonian has to be computed in the acceptance step of the Hybrid Monte Carlo algorithm. The Hamiltonian

$$H([U],[P]) = E_K([P]) + S_G([U]) \tag{30}$$

is composed of the Wilson gauge action

$$S_G([U]) = \sum_x \sum_{\mu\neq\nu} \beta \left(1 - \frac{1}{2N} Tr\Big(U_{x,\mu\nu}\Big)\right) \tag{31}$$

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(with N being the dimension of the matrices of the Lie group $SU(N, C)$ and coupling constant β) and the kinetic energy

$$E_K([P]) = \frac{1}{2} \sum_{x,\mu} Tr\left(P_{x,\mu}^2\right) \tag{32}$$

as defined in [15]. The kinetic energy is composed of all fictitious momenta $[P]$ such that it has no actual physical meaning but it ensures that the Hamiltonian is a conserved quantity. It is the sum of the traces of all squared momenta. Concerning the Wilson action S_G, the first sum runs over all possible plaquettes $U_{x,\mu\nu}$. The plaquette

$$U_{x,\mu\nu} = U_{x,\mu} \cdot U_{x+a\hat{\mu},\nu} \cdot U_{x+a\hat{\nu},\mu}^{-1} \cdot U_{x,\nu}^{-1} \tag{33}$$

used in equation (31) can be visualized as the shortest closed loop starting and ending at site x in the (μ, ν) plane and is a product of link matrices in clockwise or anti-clockwise direction. The summation in equation (31) means that all plaquettes at points $x = 1, \ldots, L^d$ corresponding to the different existing (μ, ν) planes for $\mu, \nu = 1, \ldots, d$ are computed.

5. Numerical Results

The Cayley-Leapfrog method for Lie groups is tested for the Hamiltonian equations of motion occurring in lattice gauge theory. More precisely, the Wilson action S_G is simulated in an $SU(2, \mathbb{C})$ Yang-Mills theory using the Hybrid Monte Carlo method. So, we work with a pure gauge field which consists of gluons and fictitious momenta of size 2×2. The gluons are complex special matrices with determinant one and the momenta $P_{x\mu}$ are traceless and hermitian. The simulations run on a small 2-dimensional lattice with periodic boundary conditions using Matlab. The lattice in our example has size 8×8.

We compute subsequent configurations of lattice gauge fields using the Hybrid Monte Carlo method. Here, the Hamiltonian equations of motion are computed with a Störmer-Verlet method with varying step sizes h and trajectory length $\tau = 1$. This means, there are always $n = \tau/h$ integration steps performed before each acceptance step. For the results shown here, 5000 trajectories are computed and the first 1000 are left out for thermalization reasons. Usually, for such a small lattice, the system is thermalized with less steps but we did not investigate this fact and want to be on the safe side. At this place, we state the Hybrid Monte Carlo algorithm and the details of the computation such that the results are reproducible. The HMC works as follows:

Algorithm 2. *HMC*

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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 Step*

$$([U]_i, [P]_i) \to ([U]_j, [P]_j) = \Phi([U]_i, [P]_i) \tag{34}$$

   using a geometric integration scheme Φ.
4. *Accept the new configuration with probability*

$$\min\Big(1, \exp(-\Delta H)\Big), \qquad \Delta H = H([U]_j, [P]_j) - H([U]_i, [P]_i) \tag{35}$$

5. *Proceed with step 2.*

Representation of the elements of the Configurations. For our simulations, we have chosen a 2-dimensional lattice with gauge field $[U]$ consisting of elements of special unitary Lie group $SU(2, \mathbb{C})$. It is stated in section 1.4.4 of [15] that the matrices $U_{x,\mu}$, $x = 1, \ldots, L^2$, $\mu = 1, 2$ can be build from the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{36}$$

which are traceless and hermitian such that it holds $\sigma_j = \sigma_j^\dagger$ for $j = 1, 2, 3$. Every matrix $U \in SU(2, \mathbb{C})$ can be represented by the basis $\{\sigma_1, \sigma_2, \sigma_3, I_2\}$ as

$$U = i \sum_{j=1}^{3} x_j \sigma_j + x_4 \cdot I_2 \tag{37}$$

with $i = \sqrt{-1}$, identity matrix $I_2 \in \mathbb{R}^2$ and a vector $x \in \mathbb{R}^4$ with length $||x||_2 = 1$. The values x_j, $j = 1, 2, 3, 4$ are drawn as uniformly distributed random numbers with $x_j \in [-1, 1]$. The corresponding fictious momenta $P_{x,\mu}$, $x = 1, \ldots, L^2$, $\mu = 1, 2$ are traceless and hermitian such that they can be build from a linear combination of the Pauli matrices σ_1, σ_2, σ_3 as

$$P_{x,\mu} = \frac{i}{\sqrt{2}} \sum_{j=1}^{3} y_j \sigma_j \tag{38}$$

with Gaussian distributed values $y \in \mathbb{R}^3$. A multiplication with i leads to the special unitary Lie algebra $\mathfrak{su}(2, \mathbb{C})$.

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Molecular Dynamics Step. For the Molecular Dynamics step, the numerical scheme Φ is applied on the Hamiltonian equations of motion

$$\dot{U}_{x,\mu} = iP_{x,\mu}U_{x,\mu} \quad \text{and} \quad i\dot{P}_{x,\mu} = \frac{\beta}{N}\{U_{x,\mu}\Sigma_{x,\mu}\}_{TA}. \tag{39}$$

Here, $\Sigma_{x,\mu}$ is the so-called staples

$$\Sigma_{x,\mu} = U_{x+a\hat{\mu},\nu} \cdot U^{-1}_{x+a\hat{\nu},\mu} \cdot U^{-1}_{x,\nu} + U^{-1}_{x+a(\hat{\mu}-\hat{\nu}),\nu} \cdot U^{-1}_{x-a\hat{\nu},\mu} \cdot U_{x-a\hat{\nu},\nu} \tag{40}$$

embracing the link $U_{x,\mu}$ and $\{\cdot\}_{TA}$ denotes the traceless anti-hermitian operator

$$\{M\}_{TA} := \frac{1}{2}(M - M^H) - \frac{1}{2N}Tr(M - M^H) \cdot I_2. \tag{41}$$

N is the size of the matrices, i.e. $N = 2$ and β the coupling constant chosen at the beginning of the simulation. In our simulations, the value is set to $\beta = 2.0$.

Acceptance Step. For the acceptance step, the Hamiltonian is computed before and after the numerical integration according to formula (30). If the new value H_j is smaller than the old value H_i, the new configuration is directly accepted. Otherwise, a uniformly distributed random number $r \in [0, 1]$ is drawn and compared to $\exp(-\Delta H)$. If r is larger than $\exp(-\Delta H)$, the new value is rejected and the old one added to the Markov chain of configurations.

Numerical Results. We investigate the convergence as well as the computational cost for the Cayley-Störmer-Verlet scheme compared to the standard Störmer-Verlet scheme.

Concerning the convergence, we expect that the convergence behaviour of the Cayley-Störmer-Verlet scheme is the same as for the standard Störmer-Verlet method. Here, we investigate the mean absolute difference of the Hamiltonian before and after one Molecular Dynamics step of both schemes including statistical errors. The statistical errors also include auto-correlation effects which are computed according to [22]. In figure 1, the convergence is shown. The numerical error is of order $\mathcal{O}(h^2)$ which implies a convergence order two for a single step as expected. This test is more or less just a reference that the code works correctly.

Finally, we inspect the computational cost of both schemes. We show the CPU time for one HMC integration of trajectory length $\tau = 1$ versus the absolute value of the mean energy difference ΔH. This means, we always compute τ/h steps for one trajectory. The matrix exponential $\exp(A)$ is computed via the

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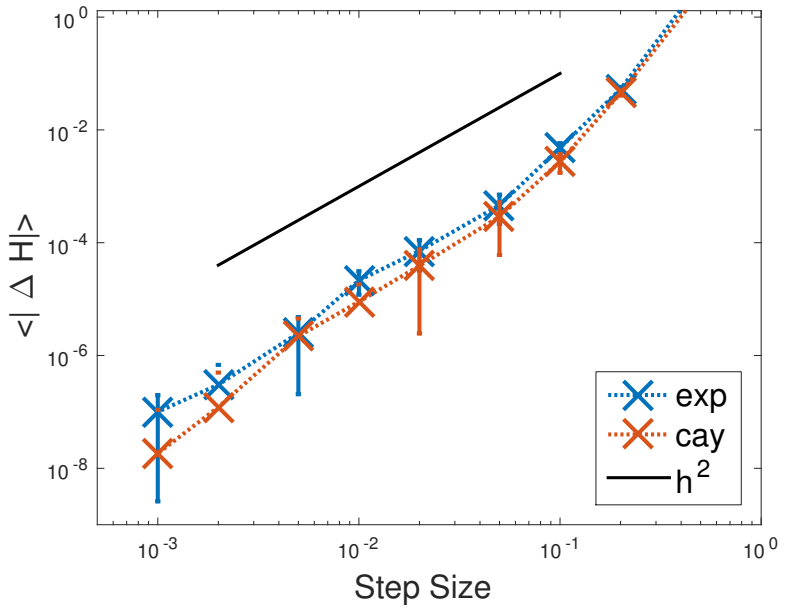

Figure 1: Convergence order of the standard Leapfrog (blue crosses) and the Cayley-Leapfrog (red crosses) scheme

matrix decomposition method described by Moler and Van Loan in [23] based on a similarity transformation $A = UDU^{-1}$. Finally, the exponential function is computed via $\exp(A) = U \exp(D) U^{-1}$. For our example of the Lie group $SU(2)$, we conclude that the Störmer-Verlet scheme using the Cayley transformation is ≈ 4.5 times faster than the exponential function. We also checked the acceptance rate of both methods: on this small lattice, it takes values of $\approx 100\%$ for step sizes lower than 0.1.

6. Conclusion

We examined the usage of the Cayley transform as local parameterization for the numerical approximation of differential equations on Lie groups. In this context, we focus on the geometric properties of the scheme and consider the Störmer-Verlet scheme applied on Lie group / Lie algebra problems using the Cayley transform. We prove that the Cayley-Störmer-Verlet scheme is time-reversible for any quadratic Lie group and volume-preserving for Lie groups with determinant one. Furthermore, we apply the scheme on the Hamiltonian equations of motion occurring in the Hybrid Monte Carlo method used in Lattice QCD, i.e. in the matrix Lie group $SU(2, \mathbb{C})$. Concerning this Lie group, we see that the scheme works better than the standard Störmer-Verlet scheme which is widely used in that field.

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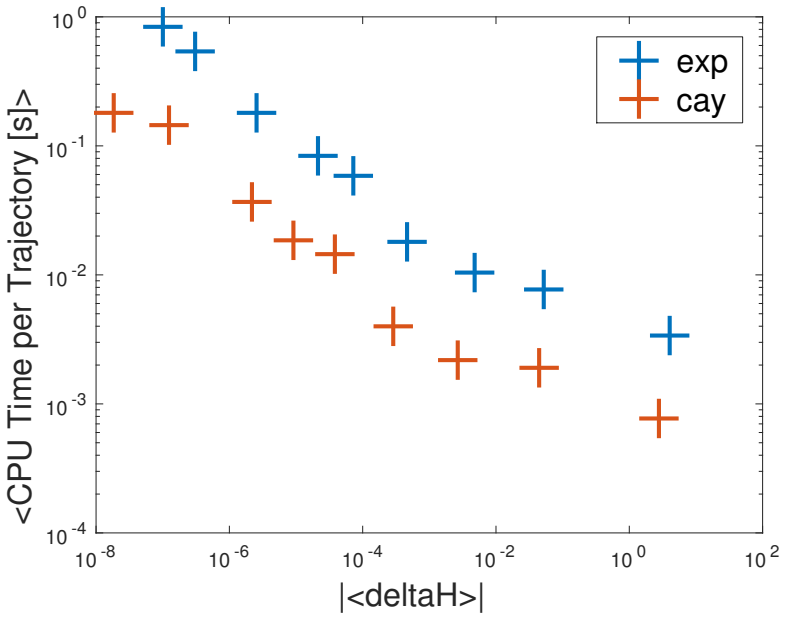

Figure 2: Computational cost of the Cayley-Leapfrog (red crosses) and the standard Störmer-Verlet scheme (blue crosses).

The Cayley-Störmer-Verlet scheme has two advantages. First, it hold for $SU(2,\mathbb{C})$ that the computation of the Cayley transform is approximately 4.5 times faster than the most rapid tested matrix exponential function. Second, no model error is introduced using this parameterization. Compared to the exponential function, the only disadvantage is that the Cayley transform is just feasible for quadratic Lie groups and that the inverse of $I - \Omega(t)$ must exist. Concerning Lattice QCD, the disadvantage does not come into play since all differential equations on Lie groups are modeled with special unitary Lie groups which are quadratic.

In a next step, the Cayley transform can be used for the development of higher-order partitioned Munthe-Kaas Runge-Kutta methods. The usage of the standard exponential function leads to difficulties because more and more Lie brackets have to be included for higher convergence orders. This is prevented using the Cayley transform. Concerning simulations in Lattice QCD, the Cayley transform can be tested on larger lattices for more elaborated simulations. If it really saves as much computing time as shown here, it would be very beneficial to replace the exponential function with the Cayley transform.

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