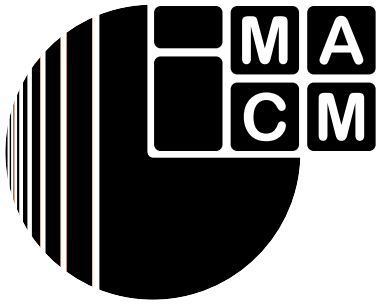

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Fachbereich Mathematik und Naturwissenschaften

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Michèle Wandelt and Michael Günther

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Abstract Lattice Quantum Chrome Dynamics (Lattice QCD) is a gauge theory formulated on a highly dimensional grid or lattice of points in space and time. It aims at determining observables such as the mass of elementary particles as accurate as possible, with computational costs as low as possible at the same time. Thus high performance computing tools are inevitable, as well as the construction of HPSC hardware tailored to the needs of Lattice QCD. In the Hybrid Monte Carlo (HMC) approach [1], Monte Carlo simulations involving a molecular dynamics step in its core are performed, which yield physical values provided with their statistical errors.

In this talk we concentrate on the Wilson Flow, a system of differential equations defined on the Lie group $SU(3)$. The Wilson Flow can be used, e.g., to determine the physical lattice spacing which influences the result of the HMC simulations. We focus on tailored Runge-Kutta Lie group integration methods with step size prediction. The numerical results confirm that our strategy is able to reduce the statistical errors of the simulation.

1 Introduction

Quantum Chromo Dynamics (QCD) is a quantum field theory that describes the strong interaction between fundamental constituents of matter inside subatomic particles. The discretized version of QCD is formulated on a 4-dimensional grid - or lattice - in space and time and called Lattice QCD. It aims at the computation of observables like the mass of elementary particles which is theoretically done via the computation of path integrals. Due to the fact that these integrals are very high

Michèle Wandelt and Michael Günther
Bergische Universität Wuppertal, Fachbereich C - Mathematik und Naturwissenschaften, Lehrstuhl für Angewandte Mathematik / Numerische Analysis, Gaußstr. 20, D-42119 Wuppertal, e-mail: {wandelt,guenther}@math.uni-wuppertal.de

dimensional, this calculation is done using Monte Carlo simulations. During these simulations, a sequence $[U]^0 \to [U]^1 \to [U]^2 \to \ldots$ of field configurations is computed which consists of a set of matrices being elements of the special unitary matrix Lie group $SU(3)$. Moreover, the observables are determined as expectation values of certain operators of the different configurations. As a byproduct of the Monte Carlo simulation, the so-called Wilson flow can be computed, see [2, 3]. It is a flow in the field space and can be used to investigate certain physical properties of the lattice as, for example, the physical lattice spacing. The Wilson flow is defined by a system of differential equations of the kind

$$\dot{V}(t) = Z([V(t)]) \cdot V(t) \,. \tag{1}$$

Since the variables $V(t)$ are elements of the matrix Lie group $SU(3)$ and the variables $Z([V(t)])$ elements of the appropriate matrix Lie algebra $\mathfrak{su}(3)$ we have a differential equation on the manifold $SU(3)$. This means, the solution has to be also in the Lie group. Thus, we have to choose a numerical method that ensures a solution in the Lie group like, for example, Munthe-Kaas Runge-Kutta (RK-MK) methods. Usually, the Wilson Flow is computed via Runge-Kutta methods for Lie groups of fixed convergence order.
In this paper, we concentrate on the numerical integration of the Wilson flow using step size prediction. In section 2, we start with a brief explanation of RK-MK schemes for differential equations of type (1). Then, we focus on step size prediction for RK-MK schemes in section 3. Afterwards, we show the numerical results for a RK-MK scheme of convergence order (2)3 in section 4. Here, we compute the Wilson flow and investigate the so-called Wilson energy as observable. Then, we adapt the step size prediction for the whole set of variables of a field configuration. Finally, we show some simulation results.

2 Runge Kutta Methods for Lie Groups

In the Wilson flow, a differential equation on a Lie group which is a differentiable manifold has to be solved. This differential equation has a special structure:

$$\dot{V} = Z \cdot V \tag{2}$$

with V being an element of a Lie group G and Z an element of the Lie algebra $\mathfrak{g}$. This kind of differential equation can be solved using the theorem of Magnus [4]. That means, the unknown Lie group element V can be replaced by a mapping

$$V = \exp(\Omega) V_0 \tag{3}$$

with unknown Lie algebra element Ω. Then, Ω is the solution of the differential equation

$$\dot{\Omega} = d\exp_{\Omega}^{-1}(Z) \tag{4}$$

in the Lie algebra with $\dot{\Omega}$ being the derivative of the inverse exponential mapping and initial value $\Omega(0) = 0$. At the end, the solution of (2) is given as the mapping (3) of the solution Ω of (4). Thereby, the derivative of the inverse exponential map can be rewritten as infinite series

$$d\exp_{\Omega}^{-1}(Z) = \sum_{k=0}^{\infty} \frac{B_k}{k!} ad_{\Omega}^{k}(Z)$$

with B_k being the k-th Bernoulli number and adjoint operator ad_{Ω}^{k} which is a mapping

$$ad_{\Omega}(A) := [\Omega, A] = \Omega \cdot A - A \cdot \Omega$$

in the Lie algebra $\mathfrak{g}$. For the numerical simulation, the infinite series of the derivative of the inverse exponential map has to be truncated. This truncation induces a model error which should be smaller or equal than the convergence order of the numerical method used for the detection of the solution Ω.

Munthe-Kaas describes a suitable truncation for Runge-Kutta methods [5, 6] as follows: for a Runge-Kutta method of convergence order p, the truncation index q has to be larger than $p-2$:

$$\dot{\Omega} = \sum_{k=0}^{q} \frac{B_k}{k!} ad_{\Omega}^{k}(Z) \quad , q \geq p-2 \tag{5}$$

A Runge-Kutta method for the differential equation (2) can be computed in three steps: Start with the mapping $V = \exp(\Omega)V_0$. Then, use an appropriate numerical integration scheme to solve the differential equation

$$\dot{\Omega} = d\exp_{\Omega}^{-1}(Z) = \sum_{k=0}^{q} \frac{B_k}{k!} ad_{\Omega}^{k}(Z)$$

with initial value $\Omega(0) = 0$, e.g the Munthe-Kaas Runge Kutta scheme. Finally, map the solution Ω via equation (3) from the Lie algebra to the Lie group.

The RK-MK for the computation of the solution of the differential equation (4) is given as:

$$\begin{aligned} \Omega_1 &= h\sum_i b_i K_i \quad \text{with} \quad K_i = f_q(Y_i, Z_i) \\ Y_i &= h\sum_k a_{ik} K_k, \qquad Z_i = Z(V_i), \qquad V_i = \exp(Y_i) \cdot V_0 \end{aligned}$$

Here, $f_q(Y_i, Z_i)$ is described by (5) as

$$f_q(Y_i, Z_i) = B_0 \cdot Z + B_1 \cdot [\Omega, Z] + \frac{B_2}{2} \cdot \big[\Omega, [\Omega, Z]\big] + \ldots + \frac{B_q}{q!} ad_{\Omega}^{q}(Z)$$

This means, the function f_q has to be suitably truncated according to the desired convergence order of the method. For example, a convergence order $p = 2$ can be achieved using $f_0 = B_0 \cdot Z$, and for $p = 3$ we would need $f_1 = B_0 \cdot Z + B_1 \cdot [\Omega, Z]$.

3 Step Size Control

Our aim is to solve the equation $\dot{V} = Z \cdot V$ using a step size control. Here, we use a common step size control as, for example, described in [7] and combine it with a Munthe-Kaas Runge-Kutta method. We proceed as follows: Start from initial values V_0 with a given step size and compute the solutions $\hat{V}_1$ of convergence order p and V_1 of convergence order $p+1$. Here, the RK-MK method is adapted for the step size control: start with $V_1 = \exp(\Omega_1) \cdot V_0$ and $\hat{V}_1 = \exp(\hat{\Omega}_1) \cdot V_0$ To reach the desired convergence order p of $\hat{V}_1$ and $p+1$ of V_1, the RK-MK algorithm is given as

$$
\begin{aligned}
\Omega_1 &= h \sum_i b_i K_i \quad \text{with} \quad K_i = f_{p-2}(Y_i, Z_i) \\
Y_i &= h \sum_j a_{ij} K_j, \qquad Z_i = Z(V_i), \qquad V_i = \exp(Y_i) \cdot V_0 \\
\hat{\Omega}_1 &= h \sum_i \hat{b}_i \hat{K}_i \quad \text{with} \quad \hat{K}_i = f_{p-1}(\hat{Y}_i, \hat{Z}_i) \\
\hat{Y}_i &= h \sum_j a_{ij} \hat{K}_j, \qquad \hat{Z}_i = Z(\hat{V}_i), \qquad \hat{V}_i = \exp(\hat{Y}_i) \cdot V_0 \, .
\end{aligned}
$$

The measure for the error is calculated as

$$
\text{err} = \sqrt{\frac{1}{n} \sum_{j=1}^{n} \Big(\frac{||\hat{\Omega}_1 - \Omega_1||_j}{ATOL + RTOL \cdot ||\hat{\Omega}_1||_j} \Big)^2} \, .
$$

As we work on a set of matrix Lie algebra elements, the computation of the error measure has to be adapted to a set of Lie algebra elements: The norms $||\hat{\Omega}_1 - \Omega_1||_j$ and $||\hat{\Omega}_1||_j$ have to be chosen as matrix norms like, for example, the Frobenius norm, row sum norm or the spectral norm. Afterwards, the optimal step size h_{opt} is computed as

$$
h_{\text{opt}} = h \cdot \sqrt[p+1]{\frac{1}{\text{err}}} \cdot \rho
$$

with safety factor ρ. Additionally, the step size should not increase or decrease too fast which is prevented by

$$
h_{\text{opt}} = \min\Big(\alpha \cdot h, \max\big(\beta \cdot h, h_{opt} \big) \Big) \, .
$$

If the error measure is small enough, i.e. err ≤ 1, the step is accepted and V_1 taken as initial value for the new step, otherwise the step is repeated. In any case, the new step size is set to h_{opt}.

Remark 1 (Step Size Control for the Wilson Flow). The Wilson Flow is a flow in the field space, i.e. for a lattice of n variables there are n differential equations

$$\dot{V}_j(t) = Z([V(t)]) \cdot V_j(t) \quad j = 1, \ldots, n$$

to be solved. The calculation for one Wilson Flow starts at one of the given configurations, e.g. $[U]^i$ which serves as initial values $[V]^0$. Here, we have to refresh our mind with the fact that the variables $V_j(t)$, $j = 1, \ldots, n$ are elements of the special unitary Lie group $SU(3)$. The function $Z([V(t)])$ maps an element $V_j \in SU(3)$ to its appropriate special unitary Lie algebra $\mathfrak{su}(3)$:

$$V_j \to Z_j = Z([V]) \quad , \qquad SU(3) \to \mathfrak{su}(3).$$

Thereby, the function Z does not just depend on V_j itself but of several adjacent variables V_k (considered to be constants at this moment). This dependence is induced by the notation $Z([V])$. Considering the elements $V_j \in SU(3), Z_j \in \mathfrak{su}(3)$ we have a system of the aforementioned differential equations on Lie groups with solution being as well in the Lie group.

4 Numerical Results and Outlook

We compute the Wilson flow for one single configuration that consists of n lattice points. Then, we measure the Wilson energy

$$E = \sum_p \text{Real Trace}(\mathbf{1} - U(p)) \tag{6}$$

whose formula is, for example, described in [2]. We have implemented a Munthe-Kaas Runge-Kutta method of convergence order (2)3 with Bogacki-Shampine coefficients given in table 1. This means, we have a Runge-Kutta method of four stages and have to compute

$$\Omega_1 = h \sum_{i=1}^{k=3} b_i K_i \quad \text{with } K_i = f_1(Y_i, Z_i) = f_0(Y_i, Z_i) + B_1[Y_i, Z_i]$$
$$\hat{\Omega}_1 = h \sum_{i=1}^{k=4} \hat{b}_i \hat{K}_i \quad \text{with } \hat{K}_i = f_0(Y_i, Z_i)$$

for all n points in the configuration. Then, the solutions V_1 of convergence order three and $\hat{V}$ of convergence order two are reached for all lattice points via

$$V_1 = \exp(\Omega_1) V_0 \quad \text{and} \quad \hat{V}_1 = \exp(\Omega_1) V_0 \, .$$

Table 1 Bogacki-Shampine coefficients

0					
1/2	1/2				
3/4	0	3/4			
1	2/9	1/3	4/9		
	2/9	1/ 3	4/9	0	$\leftarrow b$
	7/24	1/4	1/3	1/8	$\leftarrow \hat{b}$

Since the model error of $\hat{K}_i$ is larger than the one of K_i, we use the better approximation K_i instead of $\hat{K}_i$ if it is already available (this is the case in the first three stages). In figure 4, we compare the Wilson energy (6) computed (via the Wilson flow) with a RK method of order 2 with one computed with the aforementioned step size prediction. Here, the parameters for the step size control are set to ATOL=$1e-3$, RTOL=0, $\rho = 0.8$, facmin=0.5 and facmax=2. We see that a step size prediction works for the Wilson flow which consists of a set of matrices being Lie group elements.

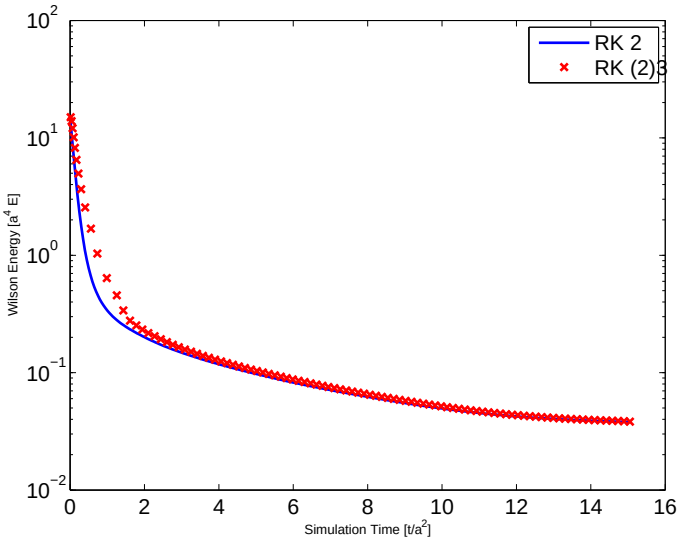

Fig. 1 Wilson energy computed with a Runge-Kutta method of convergence order 2 (blue) and with step size control (red).

Conclusion and Outlook

Usually, the Wilson flow is computed via a Runge-Kutta method with fixed step size and physicists are interested in the mean values of the observables computed from many configurations including their statistical errors. There are two advantages of the step size prediction explained here: first of all, the computational effort is reduced exploiting the dynamics of the system. Here, the parameters controlling the step size prediction have to be approved in a next step. Then, the step size prediction controls the numerical error such that the statistical errors can be reduced in a suitable manner. This has to be investigated in a next step.

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