Can we do better than Hybrid Monte Carlo in Lattice QCD?
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The Hybrid Monte Carlo algorithm for the simulation of QCD with dynamical staggered fermions is compared with Kramers equation algorithm. We find substantially different autocorrelation times for local and nonlocal observables. The calculations have been performed on the parallel computer CRAY T3D.

1. INTRODUCTION

Overcoming critical slowing down in Monte Carlo simulations of lattice field theories is imperative to approach the continuum limit. Collective mode algorithms have improved the quality of numerical studies for systems with bosonic degrees of freedom substantially during the last years. Besides many other things the important role played by autocorrelation functions has been recognized and in particular strong finite size effects present in the decay of autocorrelation functions have been observed.

On the other hand it is fair to say, that the improvements of fermionic simulation algorithms for lattice field theories since the introduction of the Hybrid Monte Carlo (HMC) algorithm ten years ago have not been overwhelming. The theoretical analysis of the HMC algorithm has been possible in the free field case while the practical analysis to compare the performance of variants of the HMC algorithm and other dynamical fermion algorithms for lattice QCD has only be done for Wilson fermions.

The work reported here is a first step to obtain reliable estimates for integrated autocorrelation times of different operators in lattice QCD with dynamical staggered fermions using two different simulation algorithms.

2. AUTOCORRELATION FUNCTIONS

In lattice quantum field theory one evaluates expectation values of observables $A(\phi)$

$$\langle A(\phi) \rangle = \frac{1}{Z} \int \prod_{x \in \Lambda} d\phi_x e^{-S(\phi)} A(\phi)$$

with $S(\phi)$ the action and $\phi_x$ a field on a lattice $\Lambda$ by a dynamic Monte Carlo algorithm.

The dynamics of the numerical algorithm is a stochastic process which is realized on a computer by a Markov process. The transition probability matrix $P(\phi \rightarrow \phi')$ leaves the equilibrium distribution invariant.

Detailed balance is equivalent to the selfadjointness of $P$ as an operator on $L^2(\mu)$ with real spectrum $(\lambda_{\text{min}}, \lambda_{\text{max}})$, and the stationarity condition

$$\int \prod_{x \in \Lambda} d\phi_x e^{-S(\phi)} P(\phi \rightarrow \phi') = 1 \cdot e^{-S(\phi')}$$

may be read as an eigenvalue equation with eigenvalue $\lambda = 1$ and eigenvector $e^{-S(\phi')}$. All other eigenvalues $\lambda$ have the upper bound $1$.

The exponential autocorrelation time $\tau_{\text{exp}}$ parameterizes the gap between $\lambda = 1$ and the subleading (unwanted) modes. The expected error $\sigma_A$ of an observable $A(\phi)$ is

$$\sigma_A^2 = \frac{1}{n} \sum_{t = -(n-1)}^{n-1} \left( 1 - \frac{|t|}{n} \right) C_{AA}(t)$$

$$\approx \frac{1}{n} 2 \tau_{\text{int},A} \cdot C_{AA}(0), \quad \text{for } n \gg \tau_{\text{exp}}$$

with the autocorrelation function

$$C_{AA}(t) = \langle (A(i) - \bar{A})(A(i+t) - \bar{A}) \rangle$$
and the integrated autocorrelation time
\[ \tau_{\text{int},A} = \frac{1}{2} \sum_{t=-\infty}^{\infty} \frac{C_{AA}(t)}{C_{AA}(0)}. \]

The performance of dynamic Monte Carlo algorithms for a finite system with linear size \( L \) and correlation length \( \xi \) is described by empirical dynamical scaling laws
\[ \tau_{\text{int},A} \sim \min(L, \xi)^z. \]

3. GENERALIZED HMC ALGORITHM

Introduce a set of “fictitious momenta” \( \pi \) and a Hamiltonian
\[ H(\phi, \pi) = \frac{1}{2} \pi^2 + S(\phi) \]
then the HMC alternates two Markov steps: momentum refreshment and Monte Carlo molecular dynamics which contains molecular dynamics and a global Metropolis step to correct for the discretization errors in Hamilton’s equations.

The first step is momentum refreshment, where momenta \( \pi \) are replaced by new values chosen at random from a Gaussian distribution.

Horowitz [5] suggested a generalized momentum refreshment (Kramers equation) by adding a Gaussian noise
\[ \pi' = e^{-\gamma \delta \tau} \cdot \pi + \sqrt{1 - e^{-2\gamma \delta \tau}} \cdot \eta \]
with
\[ P(\eta) = \frac{1}{Z} e^{-\eta^2/2} \]
where \( 0 \leq \gamma \leq \infty \). For \( \gamma = \infty \) one obtains full momentum refreshment, while \( \gamma = 0 \) gives exact generalization of the second order Langevin algorithm. Detailed balance will be satisfied if the new phase space configuration is accepted with probability
\[ P[(\phi, \pi) \rightarrow (\phi', \pi')] = \min(1, e^{H(\phi', \pi') - H(\phi, \pi')}). \]

4. NUMERICAL RESULTS

All our results are for lattice QCD with four flavours of dynamical staggered fermions and gauge group \( SU(2) \).

In the HMC algorithm there are two free parameters: the integration step size \( \delta \tau \) and the trajectory length \( \tau_0 = n \delta \tau \), where \( n \) is the number of integration steps. \( \delta \tau \) must be adjusted to keep \( P_{\text{acc}} \) reasonably large. Optimal choice for \( \tau_0 \) is less clear. In the Gaussian model with \( L \gg \xi \) the dynamical critical exponent \( z \) is \( z = 2 \) for \( \tau_0 \) constant, and \( z = 1 \) if \( \tau_0 \propto \xi \). For constant \( \tau_0 \) the dynamical critical exponent \( z \) becomes \( z = 2 \) for \( \xi \gg L \).

For dynamical fermions with \( m = 0.1 \) we measured autocorrelation times for the plaquette, Polyakov loop, and the chiral order parameter with trajectory length \( 1/4 \leq \tau_0 \leq 2 \) on various lattices with sample sizes of \( \approx 1000 \tau_{\text{int}} \).

In Fig. 1 we show the autocorrelation function of the plaquette on a lattice of size \( 8^4 \) for both algorithms. For the Kramers equation algorithm \( k = 12 \) (see below) and on the horizontal axis \( t \) is given in units of molecular dynamics time. The straight lines are fixed exponentials to guide the eye.

For the Kramers equation algorithms the second exponential in the decay of the autocorrelation function seemed to be stronger coupled. This
observation has been found for local as well as nonlocal observables.

**4.1. Generalized HMC algorithm**

Through the generalized momentum refreshment a new tunable parameter $\gamma$ is introduced.

Detailed balance requires that the momenta must have their sign flipped after every rejected step.

The Monte Carlo molecular dynamics step can be performed $k$ times. For dynamical fermions with $m = 0.1$ we measure autocorrelation times $\tau_{\text{int,A}}$ for the plaquette, Polyakov loop and the chiral order parameter with $0.03 \leq \delta \tau \leq 0.12$, and $k = 4, 8$ and $12$.

![Figure 2. Comparison of the HMC and Kramers.](image)

For more details we refer to [6].

In Fig. 2 we compare the cost in molecular dynamics time for the Polyakov loop operator as a function of stepsize for both algorithms. Data with $k = 4$ and $k = 8$ are included and compared with HMC using a trajectory length $\tau_0 = 1$. We consider the pattern of this plot similar to the findings of [2] in their figure 2.

**4.2. HMC on the CRAY T3D**

The computational demands of our study let us move to the massively parallel processing CRAY T3D with a peak rate of 150 Mflops in 64 bit arithmetic per node. We decided to implement the shared memory routines because they show less overhead than Parallel Virtual Machine or Message Passing Interface. We found the expected speedup within a few percents for 4 PEs up to 128 PEs on a $16^4$ lattice. For our present implementation of the HMC algorithm 5 PEs on a T3D are equivalent to one YMP processor indicating the improvement of the performance to cost ratio [7].

**5. CONCLUSIONS**

We find that reasonable high statistics are absolutely necessary to obtain reliable error bars for the integrated autocorrelation times. We consider the different decay behaviour of the integrated autocorrelation functions for the observables studied so far as an indication for different efficiency. Up to now we did not find a competitive set of parameters for the Kramers equation algorithm.

**6. ACKNOWLEDGEMENT**

One of us (S.M) enjoyed the kind hospitality of SCRI, Florida State University and of IWR, University of Heidelberg while the work described has been performed. It is a great pleasure to thank Kahl Bitar, Urs Heller, Karl Jansen and in particular Tony Kennedy for discussions and comments. We thank CRAY Research and in particular Dr.R. Fischer for support.

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