The RHMC Algorithm for 2 Flavours of Dynamical Staggered Fermions

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We describe an implementation of the Rational Hybrid Monte Carlo (RHMC) algorithm for dynamical computations with two flavours of staggered quarks. We discuss several variants of the method, the performance and possible sources of error for each of them, and we compare the performance and results to the inexact R algorithm.

1. Introduction

Computations with two flavours of dynamical staggered quarks are quite popular at present. There are a number of possible problems with such calculations such as flavour symmetry breaking and non-locality of the square-root of the four-flavour action. In this investigation we shall ignore these and consider only the possible errors introduced through algorithmic approximations.

We propose the use of the Rational Hybrid Monte Carlo (RHMC) algorithm [1]. This method is stochastically exact, in the sense that it is free from molecular dynamics (MD) stepsize errors. It is comparable to the usual R algorithm [2] in performance, but without the need for extrapolation in the MD stepsize $\delta t$.

2. Two Flavour Algorithms

All Hybrid Molecular Dynamics (HMD) algorithms have the same underlying structure: a fictitious momentum field is introduced, and the gauge field is integrated along classical trajectories in fictitious time, interleaved with refreshment of the momenta from a Gaussian heatbath. When integrating Hamilton’s equations the evaluation of the fermionic contribution to the force acting on the gauge fields is the costliest part of generating full QCD gauge field configurations. Most algorithmic developments are techniques to calculate the fermionic force more efficiently.

The desired probability distribution for the gauge fields $U$ with $n_f$ flavours of staggered fermions is

$$P(U) \propto e^{-S_G(U)} \det[M(U)]^{n_f/4}, \quad (1)$$

where $M$ is the staggered fermion kernel and $S_G$ is the gauge action. Thus for $n_f = 2$ flavours of fermion we require the square root of the fermion determinant. Choosing a suitable normalisation the spectrum of the staggered fermion kernel $M$ is contained in the interval $[\varepsilon, 1]$, where $\varepsilon = (1 + \frac{16m^2}{m^2})^{-1} = \frac{m^2}{16} + O(m^4)$.

2.1. The $R$ algorithm

The identity $\det M^{n_f/4} = \exp \text{tr} \ln M^{n_f/4}$ allows us to express the determinant as a term in the action, and the number of flavours just appears as a factor in front of this term, $S_{PF} = -\frac{n_f}{4} \text{tr} \ln M$. In the $R$ algorithm [2] the evaluation of the force corresponding to this trace is performed stochastically, as computing it exactly would be prohibitively expensive. To do this without introducing $O(\delta t)$ errors we introduce an auxiliary field that is evaluated at time $(1 - \frac{n_f}{4})\frac{\delta t}{2}$ along each integration step. For two flavours this breaks time-reversal invariance, violates Liouville’s theorem, and leads to an irreversible and non area-preserving algorithm: as such, it cannot be made exact by the inclusion of a Metropolis step. A detailed analysis of the errors in the probability distribution produced by this algorithm was presented in [3].

3. Rational Hybrid Molecular Dynamics

RHMD [1] uses a uses a rational approximation to fractional powers $\alpha$ of a matrix. This is analogous to the use of polynomial approximations introduced in [4,5,6], but optimal (Chebyshev) rational approximations give a much closer approximation over a given interval than the cor-
| Relative Error | 1e-30 | 1e-24 | 1e-12 |
|----------------|-------|-------|-------|

Where

\[ \| \mathcal{M} \| \text{norm.} \]

The RHMD algorithm proceeds as follows

\[ \| \mathcal{M} \| = \| \mathcal{M} \| \text{norm.} \]

The Gaussian integral over a bosonic (pseudofermion) approximation used.

falls exponentially with the degree of the rational approximation used.

The maximum error \( \Delta \) for the MD integration as well (\( \bar{\Delta} = \Delta \)), although this is not logically required.

This leads to an algorithm which has finite step-size errors of \( O(\delta t^2) \) and errors of \( O(\Delta) \) incurred from the use of rational approximations.

Rational functions can be expressed as a product or as a partial fraction expansion,

\[
\tilde{r}(x) = \tilde{c}_0 \prod_{i=1}^d \frac{(x - \tilde{\gamma}_i)}{(x - \tilde{\beta}_i)} = \tilde{c}_0 + \sum_{i=1}^d \frac{\tilde{\alpha}_i}{x - \tilde{\beta}_i}.
\]

In partial fraction form \( \ref{eq:partial_fraction} \) the pseudofermionic force takes the form

\[
\frac{\partial \tilde{H}}{\partial \chi_i} = \phi_i \frac{\partial \tilde{r}(\mathcal{M})}{\partial \chi_i} \phi = -\sum_{i=1}^d \tilde{\alpha}_i \chi_i \frac{\partial \mathcal{M}}{\partial \chi_i} \chi_i,
\]

where \( \chi_i = (\mathcal{M} - \tilde{\beta}_i)^{-1} \phi \). A multishift solver \( \ref{eq:multishift_solver} \) can be used to compute all the \( \chi_i \) in a common Krylov space. The computational cost of generating the appropriate Krylov space depends upon the smallest shift, and the only extra cost is that of updating the extra \( d - 1 \) solution vectors.

4. Rational Hybrid Monte Carlo

The RHMC algorithm is similar to RHMD but with the addition of a Metropolis accept/reject step. The acceptance probability for this is given by

\[
P_{\text{ACC}} = \min \left( 1, e^{\delta H \frac{\det \mathcal{M}^{n/4} r(\mathcal{M})^2}{\det \mathcal{M}^{n/4} r(\mathcal{M}')^2}} \right) \tag{2}
\]

where \( H = \frac{1}{2} |\pi|^2 + S_G + \phi^\dagger r(\mathcal{M}) \phi \).

If we use a high enough degree rational approximation \( r \) such that \( \Delta \leq 1 \) ulp (unit of least precision for the floating point arithmetic used) in the computation of the pseudofermion heatbath and of \( \delta H \) we can ignore the explicit determinants in \( \ref{eq:partial_fraction} \) without introducing any systematic errors beyond the ever-present rounding errors. In practice we find that it is sufficiently cheap to use the same (machine accuracy) rational approximation for the MD integration as well (\( \tilde{\Delta} = \Delta \)), although this is not logically required.
5. Noisy Rational Hybrid Monte Carlo

RHMCN [1] allows the use of a lower degree rational approximation \( r \) while keeping the algorithm exact. The algorithm replaces the Metropolis step with a Kennedy-Kuti (KK) [9] noisy accept/reject step. A stochastic summation is used to estimate the determinant ratio in (2). The acceptance probability is defined as

\[
P_{\text{ACC}} = \lambda_+ + \lambda_- Q(U, U') \quad \text{for} \quad U > U'
\]

and

\[
P_{\text{ACC}} = \lambda_- + \lambda_+ Q(U, U') \quad \text{for} \quad U < U'
\]

respectively, where \( Q(U, U') \) is an unbiased (noisy) estimator of the determinant ratio occurring in (2) and \( \lambda_\pm \) are parameters used to ensure the resultant probability distribution lies in the range \([0, 1]\). When \( \lambda_+ = \lambda_- = \lambda \) the average acceptance rate is \( \langle P \rangle = 2\lambda \).

6. Comparison of RHMC and \( R \)

The use of multishift solvers in the implementation of the rational algorithms results in a lower computational cost than might otherwise be expected. On a \( 16^3 \times 32 \) lattice with \( \beta = 5.26 \), \( m = 0.01 \), and \( \delta t = 0.01 \) the time to perform one trajectory of length \( \tau = 0.5 \) on a single node Pentium 4 processor with no assembler optimisations is 274 minutes for the \( R \) algorithm. RHMC takes 318 minutes when a degree 10 rational function is used. Although a single \( R \) trajectory is faster, RHMC compares very favourably when it is remembered that an \( O(\delta t^2) \) extrapolation ought to be carried out when using the inexact \( R \) algorithm.

The computational cost of using RHMCN is unfavourable compared with RHMC. Although a lower degree rational approximation can be used this does not give a large benefit because of the efficacy of the multishift solver. To ensure negligible probability violations occur when \( \Delta > 1 \) ulp the KK acceptance test becomes increasingly expensive for large volumes and small quark masses. The cost of performing a single trajectory using the parameters given above with a degree 6 rational approximation and typical stochastic summation parameters is 385 minutes. We found that setting \( \lambda \) to give \( \langle P \rangle = 70\% \) gives as large an acceptance rate as feasible without incurring excessive violations, but for large \( V \) and small \( m \) it was found necessary to reduce this to about 50%.

7. Conclusion

We have found that it is easy and cheap to compute rational powers of the staggered fermion kernel to within machine accuracy using Chebyshev rational approximations expressed as partial fractions, and applied using a multishift solver. This form of the RHMC algorithm thus enables the exact HMC algorithm to be extended to the case of an arbitrary number of flavours. The ability to use Krylov space solvers makes RHMC faster than the PHMC algorithm [45]. In terms of computational cost there is very little to chose between the \( R \) and RHMC algorithms. Since this seems to be the only possible advantage of \( R \) over RHMC, we conclude that there is no reason for the continued use of the \( R \) algorithm.

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