Exact 2+1 Flavour RHMC Simulations

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We consider the Rational Hybrid Monte Carlo algorithm for performing exact 2+1 flavour fermion simulations. The specific cases of asqtad and domain wall fermions are considered. We find that in both cases the naive performance is similar to conventional hybrid algorithms.

1. Introduction

Traditionally, “2+1” flavour simulations have been performed using the R algorithm [1], but an exact algorithm is clearly desirable. There also exist exact Polynomial Hybrid Monte Carlo algorithms [2,3], which can be used for 2+1 simulations: however, such algorithms are expensive with regard to memory consumption and for the case of ASQTAD fermions such an algorithm would be impractical due to the very expensive force term calculation. We explore the use of the Rational Hybrid Monte Carlo (RHMC) algorithm applied to ASQTAD and domain wall 2+1 simulations.

2. Rational Hybrid Monte Carlo

The RHMC algorithm [4] is an exact algorithm which allows the simulation of theories where the fermionic determinant is raised to a non-integer power. As with conventional Hybrid Monte Carlo (HMC) [5], the determinant is replaced by an integral over the exponential of an action containing bosonic pseudofermion fields. The non-local fermion matrix is replaced by a rational approximation,

\[ \det M^\alpha = \int D\bar{\psi}D\psi e^{-\bar{\psi}M^{-\alpha}\psi} \]

\[ \approx \int D\bar{\psi}D\psi e^{-\bar{\psi}r(M)\psi}. \]

Such approximations are cheap to evaluate since they can be written in partial fraction form, allowing evaluation using a multi-shift solver.

Rational approximations have a great advantage over polynomial approximations of the same degree, because rational approximations typically have an error many orders of magnitude smaller. It is this important feature, which allows the use of a conventional Metropolis acceptance test (cost \( \propto V^{5/4} \)) as opposed to a noisy estimator (cost \( \propto V^2 \)).

When performing RHMC, we must ensure that the approximations used for the heatbath and the evaluation of the accept/reject Hamiltonian are exact (to machine precision), otherwise we would introduce a systematic error into our simulation. This requirement is not true for the molecular dynamics (MD) evolution, where any error introduced is corrected for by the acceptance test. As this error increases, a decrease in the acceptance probability will be observed. Typically this means that we have two approximations when performing our simulations, a high order approximation which is used for the heatbath and accept/reject evaluation, and a lower order approximation used for the MD evolution through phase space.

3. ASQTAD Simulations

ASQTAD simulations are popular at the moment, since they are computationally very cheap
compared to the chiral approaches favoured for theoretical reasons. As with conventional staggered fermions, ASQTAD fermions naturally describe a theory of four degenerate flavours, and we are forced to take the square root of the fermion matrix to obtain a theory which we may hope describes two degenerate flavours. Similarly, we can take a fourth root to obtain a single quark theory, which we take to be the strange quark contribution. For such a 2+1 theory, the fermionic action reads

\[ S_t = \bar{\psi} M(m_i = \bar{m})^{-1/2} \psi + \bar{\chi} M(m_i = m_s)^{-1/4} \chi, \]

where \( \bar{m} = (m_u + m_d)/2 \) and \( \bar{m} = m_s \). With such an action, we can use RHMC as described above with the two fields \( \psi \) and \( \chi \). The eigenspectrum of the ASQTAD operator is bounded from below by \( m_i \), so it trivial to ensure that the rational approximation encompasses all of the spectrum.

A complexity does arise when we consider the calculation of the force contribution when integrating Hamilton’s equations. When performing ASQTAD-type simulations using the R algorithm at typical quark masses, the computational cost is split roughly equally between the matrix inversion and the cost of the derivative of the matrix with respect to the gauge field. If we were to proceed naively using the same formulation, we would be evaluating this derivative \( \bar{m} + n_s \) times (where \( \bar{n} \) and \( n_s \) are the degrees of the MD rational approximations for the light and strange quark contributions, of \( O(10) \) for typical light masses), since each term in the partial fraction expansion requires a different field with a different shift. This would lead to an algorithm approximately \( \frac{1}{2} (\bar{n} + n_s) \) more expensive than the R algorithm.

The solution lies in how we calculate this derivative. The ASQTAD force term is composed of terms like \( U \ldots U XX^† U \ldots U \), where \( X = M^{-1} \phi \). When there are just one or two pseudofermion fields \( \phi \), it is most efficient to compute the \( U \ldots U X \) products first and then evaluate the outer product: indeed, this is how the R algorithm is implemented. However, it is crucial that the shift dependence is only present in the vectors which appear in the force term. This suggests that for the RHMC force term, where there are many vectors \( X_i \), if we perform the link matrix multiplication first, which is shift independent, and then include the outer product for each partial fraction contribution, we will vastly reduce the number of operations performed, i.e.,

\[ \sum_{i=1}^{n} (U \ldots UX_i ) (X_i^† U \ldots U) = U \ldots U \left( \sum_{i=1}^{n} X_i X_i^† \right) U \ldots U \]

The drawback of this approach is that we will still be doing more operations than if we were performing the R algorithm calculation. It turns out that the operations required scale with volume \( V \) as \( (782,424 + 720n)V \), where \( n \) is the degree of the approximation, compared to 196,920V for the R algorithm. This would imply an approximate four-fold overhead, but since the only mass dependence in the derivative appears in the vectors, we can combine the calculation of the derivative for the light and strange contributions, thus reducing the overhead by about a factor of two. Also, for the 2+1 case, the R algorithm requires that the ASQTAD operator be constructed three times within a single MD step (once for each heatbath, and once for the inversion), compared to only once for inversion with RHMC. Taking all of the above into account, we can see that the R algorithm scales for 2+1 like 828,288V, so the R algorithm is actually more expensive.

The current implementation of RHMC for ASQTAD fermions on the QCDOC is very competitive with the R algorithm implementation. Their respective efficiencies are very similar at around 36% of peak performance. It is difficult to compare the two algorithms since the R algorithm is an inexact algorithm, and strictly requires an extrapolation to zero step size.

4. Domain Wall Simulations

The case of Furman–Shamir domain wall simulations is quite different to ASQTAD type simulations. We now have a 2+1 action as follows

\[ S_t = \bar{\psi} \frac{M(m_i = 1)}{M(m_i = \bar{m})} \psi + \bar{\chi} \sqrt{\frac{M(m_i = 1)}{M(m_i = m_s)}} \chi. \]
For the two flavour contribution we can use conventional HMC evolution, the complication is only present for the strange quark contribution. We represent the square root which appears in the action by a rational approximation and proceed using conventional HMC for the degenerate light contribution and RHMC for the strange contribution. Unfortunately, it is not quite so simple because of the inclusion of the Pauli–Villars field in the numerator in the square root. Since $m_i$ does not appear as a multiple of the identity in the domain wall fermion matrix, it is not possible to write a rational approximation as a function of this ratio in terms of shifted matrices. This does not prevent evaluation of such an approximation, but it does preclude using a multi-shift solver for the evaluation, rendering the formulation expensive.

The solution to this problem is to split this ratio into separate fields. The action is then written as

$$S_f = \bar{\psi} \frac{M(m_i = 1)}{M(m_i = \bar{m})} \psi + \bar{\phi} \frac{M(m_i = 1)}{\frac{1}{2}} \phi + \bar{\chi} \frac{M(m_i = m_s)}{\frac{1}{2}} \chi,$$

where we have to perform RHMC on the last two fields. Although we are now including an extra field, with which we have to perform a matrix inversion, the additional cost is negligible since the mass is $O(100)$ times greater than that of the degenerate light pair. Indeed, the cost of including the effects of the strange quark are small compared to that of the light pair since it too is relatively heavy. This cost can be reduced by using a Sexton–Weingarten integration scheme [6], using a smaller step size for the light quark pair. With such an implementation, the overhead of performing 2+1 over regular 2 flavour is negligible. It should be noted that we are forced to perform a matrix inversion to include the bosonic Pauli–Villars field — a surprising result. Since the force calculation is trivial for domain wall fermions, the contribution to the force is performed naively as the extra cost is negligible.

We have implemented this algorithm and have tested simple observables to ensure its correctness. A more systematic study of algorithmic performance using domain wall fermions shall be forthcoming in a future publication.

5. Conclusions

We have demonstrated that RHMC can be used to generate gauge configurations efficiently when applied to 2+1 asqtad simulations. The naive cost is similar to the R algorithm for a given step size, but the latter requires extrapolation to zero step size.

Initial findings from performing an exact 2+1 domain wall simulation have been presented. These initial results indicate that RHMC is perfectly suited for this fermion formulation.

When performing simulations using RHMC we automatically are using multipseudofermions leading to a Hasenbusch-type force reduction, which can be utilised to allow an increase in the step size. This accelerates the performance of RHMC over that of the R algorithm and conventional HMC significantly. The effect of this acceleration, and how these 2+1 simulations behave on large volumes and small masses, shall be investigated in initial runs on the QCDOC.

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