Accelerating Fermionic Molecular Dynamics

M. A. Clark\textsuperscript{a} and A. D. Kennedy\textsuperscript{a}

\textsuperscript{a}School of Physics, The University of Edinburgh, Edinburgh EH9 3JZ, United Kingdom

We consider how to accelerate fermionic molecular dynamics algorithms by introducing \( n \) pseudofermion fields coupled with the \( n \)th root of the fermionic kernel. This reduces the maximum pseudofermionic force, and thus allows a larger molecular dynamics integration step size without hitting an instability in the integrator.

1. Introduction

For over fifteen years the algorithm of choice for generating lattice field theory configurations including the dynamical effect of fermions has been Hybrid Monte Carlo (HMC) \cite{1}. Unfortunately the cost of this algorithm increases rapidly as the fermion mass \( m \) decreases; in order to keep the HMC acceptance rate \( P_{\text{acc}} \) constant the molecular dynamics integration step size \( \delta \tau \) has to be reduced, and for molecular dynamics trajectories of length \( \tau = 1 \) this corresponds directly to an increased number of molecular dynamics integration steps and hence larger cost.

This required decrease in step size is because of the breakdown of symmetric symplectic integrators. For light dynamical fermions there is an instability for a few isolated light fermion modes, whose frequency is well separated from the bulk of the modes. This instability is seen to be directly responsible for the exponential decrease of HMC acceptance with integration step size above some critical value.

We introduce a method for reducing the severity of this problem by reducing the highest “effective frequency” of the fermionic modes, or equivalently of decreasing the magnitude of the fermionic contribution to the force acting on the gauge fields. The basic idea follows the suggestion of Hasenbusch \cite{2} to split the fermionic action into two parts, and to introduce separate pseudofermion fields for each part. Our approach can be easily generalised to an arbitrary number of pseudofermion fields.\footnote{Hasenbusch’s method also allows an arbitrary number of pseudofermion fields to be used, but the parameters in the action have to be tuned to ensure that the contributions to the force are divided up equally.}

2. Non-linearity of CG

We observe that the force due to the fermion kernel \( \mathcal{M}^{-1} \) is dominated by the smallest eigenvalues of \( \mathcal{M} \). The condition number \( \kappa(\mathcal{M}) \) is the ratio of the largest eigenvalue to the smallest eigenvalue, and to a first approximation controls the rate of convergence of iterative Krylov space solvers. The largest eigenvalue remains approximately constant as the fermion mass \( m \) is decreased, and the smallest eigenvalue is typically of the order \( m^{\alpha} \) where \( \alpha = 1 \) or 2, so we expect \( \kappa(\mathcal{M}) \propto m^{-\alpha} \).

Consider the numerical solution of the linear system \( \mathcal{M}\chi = \phi \), where \( \mathcal{M} > 0 \) and has condition number \( \kappa(\mathcal{M}) \). The cost of solving these linear equations is proportional to \( m^{-\alpha} \). On the other hand we could equivalently solve the set of coupled linear equations \( \sqrt{\mathcal{M}}\psi = \phi \) and \( \sqrt{\mathcal{M}}\psi = \phi \), each of which has condition number \( \kappa(\sqrt{\mathcal{M}}) = \sqrt{\kappa(\mathcal{M})} \), leading to a cost of order \( 2m^{-\alpha/2} \) in this case, which is cheaper for sufficiently small \( m \). This reflects the essential non-linearity of Krylov space solvers. Indeed, we may even be more adventurous and solve the set of \( n \) coupled systems \( \sqrt{\mathcal{M}}\psi_j = \psi_{j+1} \), where \( \psi_0 = \chi \) and \( \psi_n = \phi \), for which we have to perform \( n \) solves each with condition number \( \kappa(\mathcal{M}^{1/n}) = \kappa(\mathcal{M})^{1/n} \), leading to a total cost of order \( n\kappa(\mathcal{M})^{1/n} \).

Unfortunately we cannot take advantage of this non-linearity, the problem being that it is
not straightforward to apply $\sqrt{\mathcal{M}}$ to a vector when $\mathcal{M}$ is not serendipitously a manifest square. There are efficient techniques for evaluating matrix functions, such as computing the optimal polynomial or rational Chebyshev approximation to the function over the spectrum of the matrix $\mathcal{M}$ [3]. For the rational case the approximations may be found using the Remez algorithm, and they usually converge exponentially in the degree of the rational function. In practice only a relatively low degree rational function is needed to achieve machine floating-point precision [4]. Furthermore, if we take a rational approximation then we can express it as a partial fraction, and apply all the terms simultaneously (in the same Krylov space) using a multi-shift solver. This reduces the cost of solving $\mathcal{M}^{1/n} x = b$ to about the same cost as solving $\mathcal{M} x = b$. This in turn is expected to be proportional to the condition number $\kappa(\mathcal{M})$. Sadly, this means that the cost of the proposed method is of order $n \kappa(\mathcal{M})$ rather than $n \kappa(\mathcal{M})^{1/n}$, and we are worse off than when we started. Although this method is clearly useless to accelerate the convergence of Krylov space solvers, it still does significantly reduce the condition number of each of the $n$ solves, and this is what we shall make use of to decrease the pseudofermionic force. Indeed, we expect the force to be of order $n \kappa(\mathcal{M})^{1/n} \delta \tau$, which is small compared to $\kappa(\mathcal{M}) \delta \tau$ for large $\kappa(\mathcal{M})$. A naïve calculation minimising $n \kappa(\mathcal{M})^{1/n} / \kappa(\mathcal{M})$ leads to the conclusion that the optimal number of pseudofermion fields should be $^3 n_{\text{opt}} = \ln \kappa(\mathcal{M})$.

3. Pseudofermion Sampling

Recall that we represent the fermion determinant as a pseudofermion Gaussian functional integral, $\det \mathcal{M} \propto \int d\phi d\phi^\dagger \exp(-\phi^\dagger M^{-1} \phi)$, and then select a single equilibrium pseudofermion configuration using a Gaussian heatbath. We expect, therefore, that the variance of this stochastic estimate of the fermion determinant will lead to statistical fluctuations in the fermionic force: in other words the pseudofermionic force may be larger than the exact fermionic force, which is the functional derivative $\partial U \ln \det \mathcal{M}(U)/\partial U$ with respect to the gauge field $U$. This means that the pseudofermionic force may trigger the instability in the symplectic integrator even though the exact fermionic force would not.

An obvious way of ameliorating this effect is to use $n > 1$ pseudofermion fields (which shall call multipseudofermions) to sample the functional integral representing the fermion determinant, and this is achieved simply by writing

$$\det \mathcal{M} = [\det \mathcal{M}^{1/n}]^n \propto \prod_{j=1}^n d\phi_j d\phi_j^\dagger \exp(-\phi_j^\dagger M^{-1/n} \phi_j);$$

that is, introducing $n$ pseudofermion fields $\phi_j$ each with kernel $M^{-1/n}$.

We may now follow a similar argument to that in §2 to estimate the optimal value for $n$. We must keep the maximum force fixed so as to avoid the instability in the integrator, so we may increase the integration step size to $\delta \tau'$ such that $n \kappa(\mathcal{M})^{1/n} \delta \tau' = \kappa(\mathcal{M}) \delta \tau$. At constant trajectory length, and hence constant autocorrelation time, the cost of an HMC trajectory is proportional to the step size, and thus is minimised by choosing $n$ so as to minimise $\delta \tau'/\delta \tau = (\kappa(\mathcal{M}))^{1-1/n}/n$, which leads to the condition $n_{\text{opt}} \approx \ln \kappa(\mathcal{M})$, corresponding to cost reduction by a factor of $\delta \tau/\delta \tau' \approx e \ln \kappa(\mathcal{M})/\kappa(\mathcal{M})$.

4. RHMC Acceleration

Our method is to apply the RHMC algorithm [4] to generate gauge field and pseudofermion configurations distributed according to the probability density

$$P(U, \phi_1, \ldots, \phi_n) = \frac{1}{Z} \exp[-S_B(U) - S_F(\mathcal{M})],$$

where $S_B$ is the bosonic (pure gauge) action and $S_F(\mathcal{M}) = \sum_{j=1}^n \phi_j^\dagger M^{-1/n} \phi_j$. Optimal rational approximations are used to evaluate these matrix functions, and we proceed as we would for conventional HMC [1]. Using a multi-shift solver the computational cost is very similar to HMC, with the additional overhead of having to perform a matrix inversion to evaluate the heatbath.
Figure 1. Efficiency $E$ as a function of integration step size $\delta \tau$, for QCD with 4 flavours of naive staggered quarks of mass $m = 0.025$ at $\beta = 5.26$ on an $8^4$ lattice with trajectory length $\tau = 1$.

We have performed tests of the algorithm using small lattices with four flavours of naive staggered fermions. As well as being the least computationally demanding simulations to perform, the improvement for such systems should be a lower bound on the improvement for large volume and/or Wilson type fermion simulations, where the fermion matrix is less well-conditioned.

The $n = 1$ case runs were performed using conventional HMC, and the $n > 1$ runs using RHMC. We define an efficiency measure $E \equiv \langle P_{\text{acc}} \rangle / N_{\text{inv}}$, where $N_{\text{inv}}$ is number of Krylov solves performed per trajectory. For HMC this is given by $1 + \tau / \delta \tau$ and for RHMC by $(2 + \tau / \delta \tau)n$, where $\tau$ is the trajectory length and $\delta \tau$ the step size. The additional inversion per field for RHMC is for the pseudofermion heatbath.

Figure 1 is a plot of the efficiency against step size for various value of $n$. The conjecture that there is some optimal value of $n$ is confirmed, and it can be seen that $n = 2$ is the value for this particular lattice. It represents an increase in efficiency of 33% ($n = 2$ peak divided by $n = 1$ peak). We have conducted the same test with a mass parameter of $m = 0.01$, which shows the same optimal value of $n$, but with a substantial efficiency increase of 60%. This confirms that the improvement factor increases as less well-conditioned systems are studied.

5. Conclusions

We have demonstrated that our method for accelerating the Monte Carlo acceptance test improves the efficiency over conventional HMC. This is clearly still a very preliminary study, and shall be extended to large scale systems for both ASQTAD and domain wall simulations using QCDOC. On such systems, we would expect the improvement in efficiency to increase, and it will be interesting to see how much improvement can be gained. It would also be interesting to compare our method with that proposed by Hasenbusch in [2].

Acknowledgements

ADK would like to thank Brian Pendleton and Artan Boriçi for useful discussions and encouragement.

REFERENCES

1. S. Duane, A. D. Kennedy, B. J. Pendleton, and D. Roweth, Phys. Lett. 195B, 216 (1987).
2. M. Hasenbusch, Phys. Lett. B519, 177 (2001), hep-lat/0107019.
3. A. D. Kennedy, Nuclear Physics (Proceedings Supplements), B128, 107–116 (2004), hep-lat/0402037.
4. M. A. Clark and A. D. Kennedy, Nuclear Physics (Proceedings Supplements), B129, 850–852 (2004), hep-lat/0309084.