Speeding up the HMC: QCD with Clover-Improved Wilson Fermions

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We apply a recent proposal to speed up the Hybrid-Monte-Carlo simulation of systems with dynamical fermions to two flavor QCD with clover-improvement. For our smallest quark masses we see a speed-up of more than a factor of two compared with the standard algorithm.

1. Introduction

It is clear that simulation algorithms that are used today will not be able to reach physical values of the quark masses. The scaling behavior (see e.g. [1]) of the algorithms predict enormous costs for simulations at quark masses as light as the up- and down-quarks. To reach this physical point, extrapolations using \( \chi \)PT (chiral perturbation theory) have to be used. However contact to \( \chi \)PT seems to be happening at rather small values of the quark masses themselves. Any progress to reach overlap between \( \chi \)PT and lattice QCD, alternative approaches should be used. However contact to \( \chi \)PT seems to be happening at rather small values of the quark masses themselves. Any progress to reach overlap between \( \chi \)PT and lattice QCD, allowing for a safe extrapolation to physical quark masses.

Still the HMC (Hybrid-Monte-Carlo) algorithm [2] and its variants are the methods of choice in large scale simulations of lattice QCD with dynamical Wilson-fermions. One obstacle in going to light quarks is that the step size of the integration scheme has to be reduced to maintain a constant acceptance rate. In ref. [3] we proposed to split the fermion matrix into two factors and to introduce a pseudo-fermion field for both factors. The numerical study of the two dimensional Schwinger model showed that the step-size can be enlarged and thus the computational effort can be reduced substantially this way. In ref. [4] we presented first results for lattice QCD with two flavors of Wilson fermions and clover improvement [5]. Here we present new results for lattices up to \( 16^3 \times 24 \) at \( \beta = 5.2 \) and quark masses down to \( m_{PS}/m_V \approx 0.686 \).

2. The pseudo-fermion action

The partition function of lattice QCD with two degenerate flavors of dynamical fermions is given by

\[
Z = \int D[U] \exp(-S_G[U]) \det M[U]^2 ,
\]

where \( S_G[U] \) is the Wilson plaquette action. In our case, \( M[U] \) is the Wilson fermion matrix with \( O(a) \) (clover)-improvement. For the details see e.g. ref. [6]. An important feature of our proposal [6] is that it can be applied on top of standard preconditioning. Here, we use even-odd preconditioning as it is detailed in ref. [6]. The fermion matrix can be written as

\[
M = \begin{pmatrix}
1_{ee} + T_{ee} & -\kappa M_{eo} \\
-\kappa M_{oe} & 1_{oo} + T_{oo}
\end{pmatrix},
\]

where \( e \) refers to even sites and \( o \) to odd sites of the lattice. The determinant of the fermion matrix can now be written as

\[
\det M \propto \det(1_{ee} + T_{ee}) \det \hat{M} ,
\]

where \( \hat{M} = 1_{oo} + T_{oo} - M_{oe}(1_{ee} + T_{ee})^{-1}M_{eo} \). In the following, we shall consider the Hermitian matrix \( \hat{Q} = \tilde{c}_0 \gamma_5 \hat{M} \), where we have set \( \tilde{c}_0 = 1 \) in the simulations discussed below. The effective action for the standard HMC simulation reads [6]

\[
S_{eff}[U, \phi, \phi] = S_G[U] + S_{det}[U] + S_F[U, \phi, \phi] ,
\]

with \( S_{det}[U] = -2\text{Tr} \log(1 + T_{ee}) \) and \( S_F[U, \phi, \phi] = \phi \hat{Q}^{-2} \phi \). In our study we keep \( S_G[U] \) and \( S_{det}[U] \) in their standard form. However, \( S_F[U, \phi, \phi] \) is replaced by alternative expressions: We split the fermion matrix \( \hat{Q} \) into two factors. The determinant of each factor is...
estimated by an integral over pseudo-fermion fields:
\[
det \hat{Q}^2 = \det WW^\dagger \det [W^{-1} \hat{Q}][W^{-1} \hat{Q}]^\dagger \propto \int D\phi_1^\dagger D\phi_1 D\phi_2^\dagger D\phi_2 \exp (-S_{F1} - S_{F2}) \tag{5}
\]
where
\[
S_{F1} = \phi_1^\dagger (WW^\dagger)^{-1} \phi_1 \quad ,
S_{F2} = \phi_2^\dagger \left([W^{-1} \hat{Q}][W^{-1} \hat{Q}]^\dagger\right)^{-1} \phi_2 \quad . \tag{6}
\]
We considered two choices for \(W\):
\[
W = \hat{Q} + \rho \gamma_5 \quad , \tag{7}
\]
which is the original proposal of ref. \[3\]. Below we shall show only results for this choice. In addition we considered \(W = \hat{Q} + i\rho\), which was first tested in ref. \[4\]. Also in ref. \[4\], results for this choice are presented. It turns out that both choices for \(W\) give a similar performance improvement of the algorithm.

An important feature of our approach is that the variation of the modified pseudo-fermion action can be computed as easily as for the standard pseudo-fermion action. One only has to replace \(\hat{Q}\) by \(W\). For the second part of the pseudo-fermion action we get
\[
\delta S_{F2} = -X^\dagger \delta \hat{Q} Y - Y^\dagger \delta \hat{Q}^\dagger X
+ X^\dagger \delta W \phi_2 + \phi_2^\dagger \delta W^\dagger X \quad . \tag{8}
\]
with the vectors
\[
X = \left(\hat{Q} \hat{Q}^\dagger\right)^{-1} W \phi_2 \quad , \quad Y = \hat{Q}^{-1} W \phi_2 \quad . \tag{9}
\]

3. Numerical results

We have tested our modified algorithm at parameters that had been studied by UKQCD before \[3\]. We have performed simulations at \(\beta = 5.2\) and \(c_{SW} = 1.76\). Note that \(c_{SW} = 1.76\) was a preliminary result for the improvement coefficient, while the final analysis resulted in \(c_{SW} = 2.0171\) for \(\beta = 5.2\) \[4\]. We have studied \(\kappa = 0.137, 0.139, 0.1395\) and 0.1398. These values of \(\kappa\) correspond to \(m_\pi/m_\rho \approx 0.856, 0.792, 0.715\) and 0.686, respectively \[3\]. We applied periodic boundary conditions in all lattice directions, except for anti-periodic boundary conditions in time-direction for the fermion-fields.

In addition to the standard leap-frog scheme, we used a scheme with a reduced coefficient of the \(O(\delta \tau^2)\) corrections proposed by Sexton and Weingarten (see eq. (6.4) of ref. \[15\]). In order to eliminate the influence of the gauge action on the step size of the integration scheme, we used the split of time scale as proposed in ref. \[11\]. In particular, we have computed the variation of the gauge action four times as frequent as for the fermion action. As length of the trajectory we have always chosen \(\tau = 1\).

In our study, we applied the BiCGstab as solver. We have stopped the solver when the iterated residual \(r\) becomes smaller than a certain bound. To compute the action for the accept/reject step at the end of the trajectory we required \(r^2 < 10^{-20}\). Note that we take the absolute residual and not the relative. To compute the variation of the fermionic action, we required a less strict criterion \(r^2 < R^2\). It turns out that for \(R^2\) smaller than some threshold the acceptance rate virtually does not depend on \(R^2\), while it rapidly drops to zero as \(R^2\) becomes larger than this threshold. In the simulations reported below, \(R^2\) is chosen \(10^{-1}\) times the threshold or smaller.

In table 1 we show results for the acceptance rate for a \(8^3 \times 24\) lattice at \(\kappa = 0.137\). After equilibration we generated 200 trajectories for each parameter set. The standard pseudo-fermion action is given by \(\rho = 0\). First of all, for the same step size \(\delta \tau\) the acceptance with the modified pseudo-fermion action is higher than for the standard action. The maximum of the acceptance rate is rather shallow for both integration schemes. It is located at \(\rho \approx 0.5\). Next we performed longer simulations (with 6000 to 8000 trajectories each) for the standard pseudo-fermion action \((\rho = 0)\) and the optimal \(\rho = 0.5\) in the modified pseudo-fermion case. This time we tuned the step-size such that \(P_{acc} \approx 0.8\). For the standard pseudo-fermion action and the leap-frog scheme we get with \(\delta \tau = 0.025\) the acceptance rate \(P_{acc} = 0.793(3)\). The leap-frog scheme with the modified pseudo-fermion action at \(\rho = 0.5\)
Table 1
Acceptance rates $P_{\text{acc}}$ for the $8^3 \times 24$ lattice at $\beta = 5.2$, $\kappa = 0.137$ and $c_{\text{sw}} = 1.76$. Each run consists of 200 trajectories. The leap-frog runs (L) were performed with the step size $\delta \tau = 0.02$. The runs with the improved scheme (S) with $\delta \tau = 0.05$.

| $\rho$ | L, $P_{\text{acc}}$ | S, $P_{\text{acc}}$ |
|---|---|---|
| 0.0 | 0.856(7) | 0.876(10) |
| 0.1 | 0.914(8) |
| 0.3 | 0.940(5) | 0.968(4) |
| 0.5 | 0.948(5) | 0.973(2) |
| 0.6 | 0.944(4) | 0.973(2) |
| 0.7 | 0.934(4) | 0.969(3) |
| 1.0 | 0.938(7) | 0.957(3) |

gives $P_{\text{acc}} = 0.770(3)$ for $\delta \tau = 0.04$. Using the improved integration scheme, combined with the modified pseudo-fermion action even a step-size as large as $\delta \tau = 0.1$ gives $P_{\text{acc}} = 0.883(2)$. Note however that for the improved scheme the variation of the action has to be computed twice per time-step and for the leap-frog only once. For these more extended runs we have computed integrated autocorrelation times for the value of the plaquette and the number of iterations that are needed by the solver. It turned out that within error-bars the autocorrelation times are the same for all three runs reported above. Hence the modification of the pseudo-fermion action has no detectable effect on autocorrelation times (measured in units of trajectories).

In table 2 we give our results for the $16^3 \times 24$ lattice at our largest value of $\kappa$. Starting after equilibration, we performed 100 trajectories for each parameter set. Here the maximum of the acceptance rate has become sharper than for the $8^3 \times 24$ lattice at $\kappa = 0.137$. For the leap-frog scheme the largest acceptance rate is still reached at $\rho \approx 0.5$, while for the scheme of Sexton and Weingarten the optimum is shifted down to $\rho \approx 0.2$. It is interesting to note that the improved scheme profits much more from the modified pseudo-fermion action than the leap-frog scheme. In the case of the leap-frog scheme the step-size can only be doubled, while for the improved scheme the step-size can be more than tripled. In the last column of table 2 we give the total number of applications of $\hat{Q}^2$ per trajectory. This number is proportional to the numerical effort of the simulation. Comparing the leap-frog scheme at $\rho = 0$ with the improved scheme at $\rho = 0.2$, we find a reduction of the numerical cost by a factor of roughly 2.4.

Table 2
Results for a $16^3 \times 24$ lattice at $\beta = 5.2$, $c_{\text{sw}} = 1.76$ and $\kappa = 0.1398$. $\#\hat{Q}^2$ gives the total number of applications of $\hat{Q}^2$ per trajectory.

| scheme | $\rho$ | $\delta \tau$ | $P_{\text{acc}}$ | $\#\hat{Q}^2$ |
|---|---|---|---|---|
| L | 0.0 | 0.01 | 0.77(3) | 17000 |
| L | 0.05 | 0.02 | 0.62(3) | 11700 |
| L | 0.15 | 0.02 | 0.75(3) | 10700 |
| L | 0.3 | 0.02 | 0.76(2) | 10100 |
| L | 0.5 | 0.02 | 0.78(2) | 9500 |
| L | 1.0 | 0.02 | 0.64(4) | 9300 |
| S | 0.0 | 0.02 | 0.64(4) | 16500 |
| S | 0.05 | 0.066 | 0.35(4) | 7500 |
| S | 0.1 | 0.066 | 0.67(3) | 6500 |
| S | 0.15 | 0.066 | 0.72(3) | 6800 |
| S | 0.2 | 0.066 | 0.74(3) | 6900 |
| S | 0.4 | 0.066 | 0.49(3) | 6100 |
| S | 0.5 | 0.05 | 0.67(4) | 7700 |

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