Hybrid Monte Carlo and topological modes of full QCD

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We investigate the performance of the hybrid Monte Carlo algorithm, the standard algorithm used for lattice QCD simulations involving fermions, in updating non-trivial global topological structures. We find that the hybrid Monte Carlo algorithm has serious problems decorrelating the global topological charge. This represents a warning which must be seriously considered when simulating full QCD by hybrid Monte Carlo.

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1 Introduction

The present state of the art algorithm for lattice QCD with dynamical fermions, used in all production runs, is the hybrid Monte Carlo \([1–3]\) (HMC) algorithm (for four staggered or two Wilson fermions), or the hybrid molecular dynamics variant of this for fewer fermions. In this letter we investigate the effectiveness of the HMC algorithm, both with and without fermions, in updating the topological sector. For the former we use four flavours of staggered fermions. For the latter case we compare the HMC with over-relaxed heat-bath results.

We find that decorrelating the topology requires a dramatic increase in computer time as the quark mass decreases, over and above the increase naively expected. For the smallest mass, the algorithm requires days to decorrelate the topology, running on a powerful computer (25Gflop APE/QUADRICS). This implies that one cannot generate a set of configurations with the correct sampling of the topological sector using brute force.

The correct sampling of topological modes\(^2\) is clearly crucial for quantities such as the \(\eta'\) mass, which depend directly on the topology via the explicit breaking of the \(U_A(1)\) symmetry. It can also become relevant for other quantities, for example the proton mass, at some level of accuracy. Some attempts to study the topology in the presence of fermions have been presented in the literature \([4–6]\).

2 Topology

This investigation began as part of a calculation of the spin content of the proton \([7]\). This can be related to the matrix element of the topological charge density operator \(q(x)\) between on-shell proton states with small momentum transfer. To this end we prepared a large set of configurations using the HMC algorithm. We examined the longest auto-correlations in this set, namely the auto-correlation time of the global topological charge \(Q\). Any reasonable definition of \(Q\) is sufficient to determine the auto-correlations; we used the field theoretic definition of \(Q\), measured on cooled \([8]\) configurations.

The global topological charge \(Q\) is defined as

\[
Q = \sum_x \frac{-1}{24 \times 32\pi^2} \sum_{\mu\nu\rho\sigma}^{\pm 4} \epsilon_{\mu\nu\rho\sigma} \Tr [\Pi_{\mu\nu}(x)\Pi_{\rho\sigma}(x)] . \tag{1}
\]

where \(\Pi_{\mu\nu}(x)\) is the plaquette in the \(\mu\nu\) plane. A related quantity is the topological

\(^2\) We regard the topological modes to be those which, in the continuum limit, determine the topological properties of the lattice.
susceptibility $\chi$ defined as

$$\chi = \langle Q^2 \rangle / V_4$$

(2)

where $V_4$ is the lattice four-volume. The cooled configurations are obtained from each configuration generated by the HMC by minimizing locally the gauge part of the action.

Note that the conclusions drawn in this letter about the decorrelation of global topological charge by the HMC algorithm are independent of the definition of $Q$ used here. It is sufficient to assume that the cooling procedure is able to capture the most slowly updated modes associated with the ‘topological’ content of the lattice configurations, a perfectly reasonable assumption. Possible systematic errors in this procedure will not change our final conclusions.

As mentioned above, in order to extract physical results related to the topological properties, a Monte Carlo simulation must provide a set of configurations covering phase space. In particular, the global topological charge must average to zero. So the algorithm must be effective in changing topological modes. As we shall see, this efficiency appears unobtainable for values of $\beta$ large enough to have scaling when the quark mass is taken as small as currently feasible (eg., $m = 0.01$). Note that this dramatic slowing down is seen for quark masses still far from the chiral limit.

Although the existence of long auto-correlations has been observed in previous studies using the HMC algorithm, results on many quantities, some associated with the topology, have been reported. We believe that critical slowing down in the HMC has been under-estimated with respect to the topological modes. As we shall show in the following, this casts serious doubt on the possibility of performing any study involving topological properties in the relevant region of $\beta$ and $m$.

### 3 Results

We have used the Wilson action for the pure gauge sector, and four flavours of staggered fermions. Having four flavours allows the use of an exact algorithm, the so-called $\Phi$ algorithm described in detail in reference [2]. The molecular dynamics equations of motion are integrated in fictitious time $\tau$, using the leapfrog integration method, and beginning with a half-step in the gauge fields. The two relevant units for comparing the auto-correlations from different simulations are then fictitious time in units of $\tau$, and wall clock time. The production runs were done using a $16^3 \times 24$ lattice at a coupling $\beta = 5.35$ for full QCD, and a $16^3 \times 16$ lattice at $\beta = 6.00$ for pure SU(3).

Let us begin with the results for quark mass $m = 0.01$. This yields a pion to rho mass ratio of $m_\pi/m_\rho \simeq 0.5$ [3], so we are still quite far from the physical value. The lattice
Fig. 1. Time history, in units of molecular dynamics time $\tau$, of the topological charge $Q$ for the HMC simulation at $\beta = 5.35$ and $m = 0.01$ on a $16^3 \times 24$ lattice.

spacing is $a \simeq 0.14\text{fm}$ (from $m_\rho$), which gives a lattice volume of $V_3 \simeq (2.2\text{fm})^3$. The parameters used for the HMC simulation were

$$
\tau_{\text{traj}} = 0.3, \\
\Delta \tau = 0.004,
$$

where $\Delta \tau$ is the step size of the molecular dynamic evolution, and $\tau_{\text{traj}}$ the length of each trajectory. We performed a rather long simulation, with a total length after thermalisation of $\tau \simeq 500$ in units of fictitious time. Fig. 1 shows the Monte Carlo time-history of the topological charge, as determined after 25 cooling sweeps of a pseudo-heat-bath algorithm at $\beta = \infty$. These data show clearly that the HMC is unable to change the global topological modes efficiently, leading to very long auto-correlations. The value of the topological charge got stuck at around $Q \simeq -2$, and its value averaged over all configurations generated so far is decidedly non-zero: $\langle Q \rangle = -1.7(4)$. A very rough estimate of the integrated auto-correlation time $T_Q$ from a blocking analysis of the data gives $T_Q \gtrsim 2 \times 10^2$ in units of molecular dynamics time. The simulations were performed on the 25 Gflops APE tower, with around 50% efficiency. On this machine $T_Q \simeq 200$ corresponds to about three days of computer time, a considerable amount. Notice that most simulations at comparable values of $\beta$ and $m$ presented in the literature have $\tau \simeq 100$.

To further investigate the behaviour of the HMC, we have performed simulations with larger quark masses, $m = 0.035$ and $m = 0.05$, and in the quenched case, which represents the large quark mass limit of full QCD. Quenched simulations were performed at $\beta = 6.0$, and here HMC has been compared with one of the best available local algorithms, the
Table 1
Results from, and parameters used for the Hybrid Monte Carlo (HMC) runs, and, in the last line, the heat-bath over-relaxed (HBOR) run. The full QCD runs with four staggered fermions were performed on a $16^3 \times 24$ lattice, the pure SU(3) runs on a $16^3 \times 16$ lattice. The length of each trajectory in fictitious time is $\tau_{\text{traj}}$, the total length is $\tau_{\text{total}}$ in units of fictitious time and $\Delta \tau$ is the step size. The last three columns give the integrated auto-correlation time of $Q$ in units of fictitious time and wall clock hours on the 25 Gflops Quadrics, as well as the auto-correlations for the plaquette ($T_{\Pi}$). For the HBOR algorithm the auto-correlations are given in numbers of cycles and wall clock seconds.

| $\beta$ | $m$ | $\Delta \tau$ | $\tau_{\text{traj}}$ | $\tau_{\text{total}}$ | $\langle Q \rangle$ | $\chi \times 10^5$ | $T_{\Pi}(\tau)$ | $T_{Q}(\text{hrs})$ | $T_{Q}(\text{hrs})$ |
|--------|----|-------------|----------------|----------------|----------------|---------------|----------------|-----------------|----------------|
| 5.35   | 0.010 | 0.004 | 0.3 | 450 | -1.7(4) | $\gtrsim 200$ | $\gtrsim 72$ | 1.2 |
| 5.35   | 0.035 | 0.005 | 0.3 | 180 | -0.8(4) | 2.4(9) | 15 | 2 | 2.5 |
| 5.35   | 0.05 | 0.006 | 0.3 | 300 | -0.3(7) | 11(2) | 6 | 0.3 | 2.2 |
| 6.00   | $\infty$ | 0.01 | 0.3 | 2000 | 0.5(1.3) | 8.1(1.5) | 320 | 0.9 | 1.7 |
| 6.00   | $\infty$ | 0.01 | 0.6 | 4500 | -0.2(7) | 6.3(1.0) | 140 | 0.4 | 1.7 |
| 6.00   | $\infty$ | 0.016 | 0.16 | 8960 | -1.0(5) | 6.1(1.9) | 312 | 0.67 | 2.8 |
| 6.00   | $\infty$ | 0.016 | 0.32 | 3200 | -0.3(7) | 5.8(1.1) | 180 | 0.34 | 1.9 |
| 6.00   | $\infty$ | 0.016 | 0.64 | 23600 | 0.2(2) | 6.1(5) | 72 | 0.12 | 2.4 |
| 6.00   | $\infty$ | 0.016 | 0.96 | 9000 | 0.2(2) | 4.6(6) | 43 | 0.08 | 4.1(27s) |
| 6.00   | $\infty$ | 0.016 | 1.50 | 9000 | 0.1(2) | 6.9(7) | 69 | 0.12 | 4.9 |
| 6.00   | $\infty$ | 0.016 | 2.00 | 6000 | -0.1(3) | 6.5(5) | 83 | 0.15 | 5.6 |

over-relaxed heat-bath. One cycle of this algorithm consists of 5 microcanonical updates followed by a pseudo-heat-bath update. We mention that in pure gauge theory a local version of the HMC can be constructed \cite{10}, which performs better than the HMC algorithm, but which cannot be extended to fermions.

In Table 1 we give the parameters used in our HMC simulations and the corresponding estimates of the integrated auto-correlation time of the topological charge $T_{Q}$, given in molecular dynamics time units and in CPU hours. $T_{Q}$ has been estimated from a binning procedure, as well as directly where the statistics were sufficient to be able to calculate the integrated auto-correlation time. In these cases both agree. The binning estimates should be regarded as a lower limit for $m = 0.01$, and with a possible uncertainty of 10-20% for all other values. This is sufficient to our purpose. The results for the quenched case must be compared with the auto-correlation time of the local over-relaxed algorithm which is $T_{Q} \simeq 5.7$ cycles, or $T_{Q} \simeq 5.2$ seconds in CPU time.
There are three major results that have emerged from this work:

(i) In HMC simulations the integrated auto-correlation time of the global topological charge decreases as the length of the trajectory increases. If expressed in terms of computer time, however, there is a decrease in performance for trajectories longer than one unit in molecular dynamics time. The best step size in pure SU(3) seems to be one giving an acceptance rate around 70%.

(ii) The performance of the HMC is already poor for pure gauge theory, i.e. in the limit $m \to \infty$. At $\beta = 6.0$, it turns out to be about two orders of magnitude slower in decorrelating $Q$ than local over-relaxed algorithms. For our ‘best’ set of HMC parameters we find that the plaquette decorrelates about 30 times slower than the heat-bath over-relaxed algorithm, which agrees with the results of [11]. The plaquette auto-correlation time in units of $\tau$ is constant, though.

For our ‘best’ parameters in pure SU(3) $Q$ decorrelates 60 times slower with the HMC than with the heat-bath over-relaxed. Furthermore the auto-correlation of $Q$ is far more sensitive to the choice of parameters than the plaquette, increasing dramatically in units of $\tau$, and of course in real time as well, the more the parameters differ from optimal.

(iii) The auto-correlation time $T_Q$ rapidly increases with decreasing quark mass, in terms of both CPU time (which is also due to critical slowing down in the inversion of the fermion matrix) and molecular dynamic time. The increase in real time required appears to scale as $T_Q \approx 1/m^\alpha$ with $\alpha \approx 3$ to 5. This is considerably more than the $\alpha \approx 2.5$ expected from using $1/m^2 = 1/m$ as the relevant physical quantity [12] causing slowing down, a factor $1/m$ from the matrix inversion, and another $\approx 0.5$ from the change in step size and acceptance rate.

The auto-correlation time for the plaquette, on the other hand, remains similar in units of $\tau$. So the increase in real time required for the topology is considerably more than the increase in real time required for smaller quark masses that one has previously learnt to expect [11,13] based on studies of more local correlators like the plaquette.

In our rather long HMC simulation at $\beta = 5.35$ and $m = 0.01$ ($\tau \approx 500$ in molecular dynamic time unit) the sampling of the topological modes appears not to be correct, making the determination of $\chi$ impossible. We cannot even estimate how long the run should have been to get $\chi$. At $m = 0.035$ the sampling of $Q$ turned out to be sufficiently long to allow a calculation of $\chi$.

In conclusion we have shown that the HMC algorithm has serious problems decorrelating global topological modes, more serious than those associated with commonly studied quantities. For full QCD the algorithm appears to slow down as roughly $1/m^4$. We stress again that this warning must be seriously considered when simulating full QCD. It is especially important when studying quantities related to the topology, but may be less relevant in the calculation of the mass spectrum (with the exception of, for example, the $\eta'$ mass), since an effective decoupling from the topological modes is expected. Note also that this slowing down is independant of both the number of fermions and type of fermion
simulated, as the underlying dynamics of the algorithm are the same as the cases studied here.

It may also be possible to improve the performance of the HMC algorithm at small masses beyond gains coming from tuning the trajectory length and step size via the use of simulated tempering \[14\]. In this, the quark mass becomes a dynamical variable in the simulation. This helps in decorrelating the topological charge both because there are more fluctuations in the charge when the mass is large, and because the conjugate gradient inversion is faster for larger masses. This is presently under investigation. Finally, we mention that other algorithms, not based on equations of motion, (for example, Lüscher’s \[13\] multi-boson algorithm), may perform better with respect to the topological modes than the HMC algorithm. This is also being examined.

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