Decorrelating the topology in full QCD

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We investigate the performance of the hybrid Monte Carlo algorithm 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, regardless of the number and type of fermions, with this or any similar algorithm. Simulated tempering is examined as a means of accelerating the decorrelation.

1. Introduction

All production runs in full QCD use molecular dynamics based algorithms. For integer multiples of four staggered or two Wilson fermions one has the exact hybrid Monte Carlo (HMC), while for other multiples there is the very similar hybrid molecular dynamics algorithm.

We examine here how effective the HMC is in decorrelating the topology for both full QCD with four staggered fermions and pure $SU(3)$ gauge theory. The latter we compare with an over-relaxed heat-bath algorithm. Although the only HMC algorithm with four staggered fermions has been investigated, the conclusions drawn are valid for any algorithm based on molecular dynamics.

An ensemble containing the correct topology is crucial for the $\eta'$ mass, for example. It can also become relevant for other quantities, for example the proton mass, at some level of accuracy. One criterion that the ensemble must fulfill is that the global topological charge averages to zero; we find that this is not so for a long run at our smallest quark mass.

Other simulations involving the topology in the presence of fermions have been presented in the literature, where the existence of long range correlations have been reported.

We have a large set of configurations generated with the HMC, originally prepared with the aim of studying the spin of the proton. As the operator involves the topology, the longest topological auto-correlation length determines the number of independent configurations. This is the auto-correlation of the global topological charge on cooled configurations.

The conclusions drawn here require only that our method sees the most slowly updated modes associated with the ‘topological’ content of the lattice configurations. For this purpose any reasonable definition of the global topological charge that is not affected by noise is adequate; we employed the field theoretic definition of $Q$, measured on cooled configurations.

2. Results

We use the $\Phi$ algorithm of reference, with 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 $SU(3)$. The two relevant units for comparing the auto-correlations are then fictitious molecular dynamics time in units of $\tau$, and wall clock time.

Let us begin with the results for quark mass $m = 0.01$. This yields a pion to rho mass ratio of $m_\pi/m_\rho \simeq 0.5$, so we are still quite far from the physical value. The lattice spacing is $a \simeq 0.14\text{fm}$ (from $m_\rho$), which gives a lattice volume of $V_3 \simeq (2.2\text{fm})^3$.

We performed a rather long simulation, with a total length after thermalisation of $\tau \simeq 500$ in units of fictitious time. Further details may be found in [8]. Fig. 1 shows the time history of the topological charge, where it is clear 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-

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\textsuperscript{2}We regard the topological modes to be those which, in the continuum limit, determine the topological properties of the lattice.
Figure 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.

The topological charge is 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 the over-relaxed heat-bath. One cycle of this algorithm consists of 5 microcanonical updates followed by a pseudo-heat-bath update.

In Table 1 we give the parameters used in our simulations and the estimates of the integrated auto-correlation time of the topological charge \( T_Q \). The estimates should be regarded as a lower limit for \( m = 0.01 \), and with a possible uncertainty of 10-20% for all other values.

There are three major results that have emerged from this work:

1. 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, then trajectories longer than one unit in molecular dynamics time seem to be slower.

2. For pure gauge theory at \( \beta = 6.0 \) the HMC algorithm is about two orders of magnitude slower in decorrelating \( Q \) than the local over-relaxed algorithm. For our ‘best’ set of HMC parameters we find that the plaquette decorrelates about 30 times more slowly, which agrees with the results of [9].

   The plaquette auto-correlation time in units of \( \tau \) is constant, though. However, \( Q \) decorrelates 60 times slower with the HMC than with the heat-bath over-relaxed for our ‘best’ parameters. Furthermore the auto-correlation of \( Q \) is far more sensitive to the choice of parameters than the plaquette.

3. The auto-correlation time \( T_Q \) rapidly increases with decreasing quark mass, in terms of both CPU time and molecular dynamics time. The auto-correlation time for the plaquette, on the other hand, re-

Table 1
Results from, and parameters used for the Hybrid Monte Carlo (HMC) runs, and, in the last row, 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 \( \tau_{\text{tra}} \). The last three columns give the integrated auto-correlation time of \( Q \) and the plaquette \( \Pi \) in units of fictitious time and wall clock hours on the 25 Gflops Quadrics.

| \( \beta \) | \( m \) | \( \tau_{\text{tra}} \) | \( T_Q(\tau) \) | \( T_Q(\text{hrs}) \) | \( T_{\Pi}(\tau) \) |
|---|---|---|---|---|---|
| 5.35 | 0.010 | 0.3 | \gtrsim 200 | \gtrsim 72 | 1.2 |
| 5.35 | 0.035 | 0.3 | 15 | 2 | 2.5 |
| 5.35 | 0.05 | 0.3 | 6 | 0.3 | 2.2 |
| 6.00 | \( \infty \) | 0.3 | 320 | 0.9 | 1.7 |
| 6.00 | \( \infty \) | 0.6 | 140 | 0.4 | 1.7 |
| 6.00 | \( \infty \) | 0.16 | 312 | 0.67 | 2.8 |
| 6.00 | \( \infty \) | 0.32 | 180 | 0.34 | 1.9 |
| 6.00 | \( \infty \) | 0.64 | 72 | 0.12 | 2.4 |
| 6.00 | \( \infty \) | 0.96 | 43 | 0.08 | 4.1(27s) |
| 6.00 | \( \infty \) | 1.50 | 69 | 0.12 | 4.9 |
| 6.00 | \( \infty \) | 2.00 | 83 | 0.15 | 5.6 |
| 6.00 | \( \infty \) | HBOR | 5.7 | \( \text{0.0014} \) | \( \text{0.9(0.9s)} \) |
mains similar in units of $\tau$. The time required appears to increase faster than the $T_Q \approx 1/m^2.5$ expected if one uses $1/m^2 = 1/m$ as the relevant physical quantity, a factor $1/m$ from the matrix inversion, and another $\approx 0.5$ from the change in step size and acceptance rate. Note that in our rather long HMC simulation at $m = 0.01$ ($\tau \approx 500$) the ensemble is not yet sufficient to determine the auto-correlation at all well; we cannot even estimate how long the run should have been to get $\langle Q \rangle \approx 0$.

### 3. Improvements

It may also be possible to improve the performance of the HMC algorithm at small masses via the use of simulated tempering \[12\]. In simulated tempering, usually the coupling becomes a dynamical parameter in the simulation. We are currently investigating promoting the quark mass to a dynamical variable in the simulation. This helps in decorrelating the topological charge both because there are more fluctuations when the mass is large, and because the HMC algorithm itself is faster for larger masses.

In simulated tempering one has an ordered set of masses, chosen such that the action histogram of adjacent masses has some overlap. The mass can then change to an adjacent mass if the configuration lies in this overlapping region, i.e., if the configuration is a representative member of the probability distribution for each of the masses.

We are currently investigating simulations using masses between 0.01 and 0.035. From these preliminary investigations we estimate that the improvements will more than compensate the additional overhead if the masses used range between $m \lesssim 0.01$ and 0.02.

Finally, we mention that algorithms that are 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.

### 4. Conclusions

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 much more rapidly than previously expected. 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 independent 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.

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