Konrad-Zuse-Zentrum
für Informationstechnik Berlin

Takustraße 7
D-14195 Berlin-Dahlem
Germany

ERNST-MICHAEL ILGENFRITZ[1], WERNER KERLER[2],
HINNERK STÜBEN

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[1]Institute for Theoretical Physics, Kanazawa University, Kanazawa 920–1192, Japan
[2]Institut für Physik, Humboldt Universität zu Berlin, 10115 Berlin, Germany

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Decorrelation of the topological charge in tempered Hybrid Monte Carlo simulations of QCD*

E.-M. Ilgenfritz[a], W. Kerler[b] and H. Stüben[c]

[a]*Institute for Theoretical Physics, Kanazawa University, Kanazawa 920–1192, Japan*

[b]*Institut für Physik, Humboldt Universität zu Berlin, 10115 Berlin, Germany*

[c]*Konrad-Zuse-Zentrum für Informationstechnik Berlin, 14195 Berlin, Germany*

Abstract

We study the improvement of simulations of QCD with dynamical Wilson fermions by combining the Hybrid Monte Carlo algorithm with parallel tempering. As an indicator for decorrelation we use the topological charge.

1 Introduction

Decorrelation of the topological charge in Hybrid Monte Carlo (HMC) simulations of QCD with dynamical fermions is a long standing problem. For staggered fermions an insufficient tunneling rate of the topological charge Q_t has been observed [1, 2]. For Wilson fermions the tunneling rate is adequate in many cases [3, 4]. However on large lattices and for large values of κ near the chiral limit the distribution of Q_t is not symmetric even after more than 3000 trajectories (see Figure 1 of [3] and similar observations by CP-PACS [5]).

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The idea of parallel tempering is to improve transitions in parameter regions where tunneling is suppressed by opening ways through parameter regions with little suppression. In QCD the method has been applied successfully for staggered fermions [6]. In [7] parallel tempering has been used to simulate QCD with O(a)-improved Wilson fermions without finding any gain, however, with only two ensembles which does not take advantage of the main idea of the method.

Here we use parallel tempering in conjunction with HMC to simulate QCD with (standard) Wilson fermions in a parameter range close to the critical region, where the method is expected to be most advantageous. The gain achieved is demonstrated by studying time series and histograms of the topological charge.

2 Parallel tempering

In standard Monte Carlo simulations one deals with one parameter set λ and generates a sequence of configurations C. The set λ here includes β, κ, the leapfrog time step and the number of time steps. C comprises the gauge field and the pseudo fermion field.

In the parallel tempering approach [8, 9] one simulates N ensembles $(\lambda_i; C_i)$, $i = 1, \ldots, N$ in a single combined run. Two steps alternate: (1) update of N configurations in the standard way, (2) exchange of configurations by swapping pairs. Swapping of a pair of configurations means

$$((\lambda_i; C_i), (\lambda_j; C_j)) \to \begin{cases} ((\lambda_i; C_j), (\lambda_j; C_i)), & \text{if accepted} \\ ((\lambda_i; C_i), (\lambda_j; C_j)), & \text{else} \end{cases}$$

with the Metropolis acceptance condition

$$P_{\text{swap}}(i,j) = \min\left(1, e^{-\Delta H}\right) \tag{1}$$

$$\Delta H = H_{\lambda_i}(C_i) + H_{\lambda_j}(C_j) - H_{\lambda_i}(C_j) - H_{\lambda_j}(C_i).$$

Since after swapping both ensembles remain in equilibrium, the swapping sequence can be freely chosen. Swapping neighboring pairs and proceeding in parameter direction towards criticality has turned out to be most advantageous.

3 Simulation details

We used the standard Wilson action for the gauge and the fermion fields and worked on an 8^4 lattice. Our HMC program applied the standard conjugate gradient inverter with even/odd preconditioning. The trajectory length was always 1. The time steps were adjusted to get acceptance rates of about 70%. In all cases we generated 1000 trajectories (plus 50–100 trajectories for thermalization).

Q_t was measured by the field-theoretic method after 50 cooling steps of Cabibbo-Marinari type.

4 Results

We have run several tempered HMC simulations in the quenched approximation (tempering in β) and with dynamical fermions (tempering in κ, at fixed $\beta = 5.5$ and $\beta = 5.6$). For comparison also standard HMC simulations have been performed.

Figure 1 shows a typical comparison of results. We find that with tempering considerably more topologically nontrivial configurations occur and the histograms of Q_t become more symmetrical.

In standard runs Q_t frequently stayed for quite some time near 1 or near -1, while with tempering this never occurred. The standard run at $\kappa = 0.156$ shown in Figure 1, where Q_t gets trapped in this way for about 200 trajectories, provides an example of this. Such observations have also been made on large lattices [3, 5].

While a correlation analysis cannot be carried out with the size of our samples, some quantitative account of the improvement by tempering is possible using the mean of the absolute change of Q_t, called mobility in [3],

$$D_1 = \frac{1}{N_{\text{traj}}} \sum_{i=1}^{N_{\text{traj}}} |Q_t(i) - Q_t(i-1)| \ . \tag{2}$$

We give results for D_1 in Table 1. The κ-values of our tempered runs include the ones used by SESAM [3]. The considerable gain by tempering is obvious from Figure 1 and Table 1.

For comparisons in Table 1 one should, in addition to the individual errors at each of the κ-values (which are not small), take the overall behavior within the particular runs into account. Comparing the tempering results for 7 and 6 ensembles it appears that adding intermediate points (not shown in Table 1) in this case leads to less improvement than extending the range to lower κ-values does. The comparison of the results for 21 and 6 ensembles possibly indicates that extending the range to very large κ-values (with no transitions in standard simulations) affects the results at lower κ. In any case our data show that by a clever choice of range and distances of the parameter values the number of parameter points can be strongly reduced.

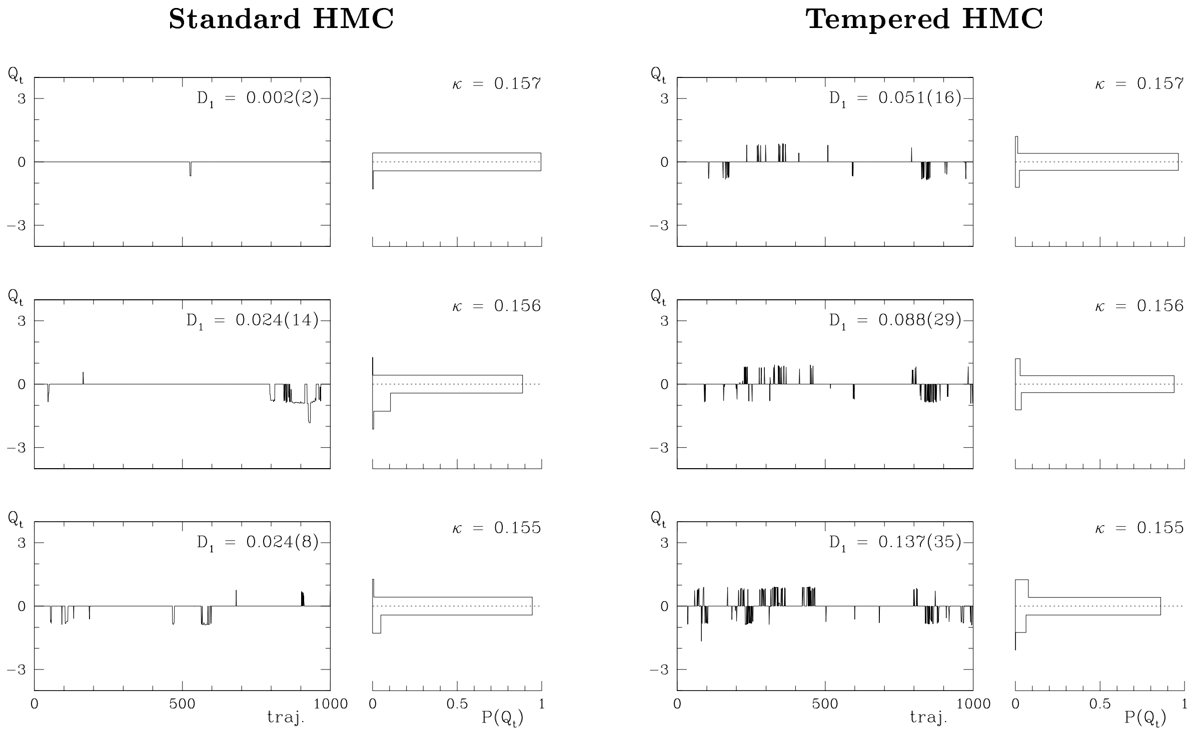

Figure 1: Comparison of standard with tempered HMC. The tempering data shown are from the run with 6 ensembles in Table 1.

κ	Standard HMC	Tempered HMC		
		7 ensembles $0.156 \leq \kappa \leq 0.1575$ $\Delta\kappa = 0.00025$	6 ensembles $0.155 \leq \kappa \leq 0.1575$ $\Delta\kappa = 0.0005$	21 ensembles $0.15 \leq \kappa \leq 0.16$ $\Delta\kappa = 0.0005$
0.1500	0.285(34)			0.668(41)
0.1550	0.024(8)		0.137(35)	0.106(26)
0.1555			0.141(35)	0.093(24)
0.1560	0.024(14)	0.053(22)	0.088(29)	0.076(19)
0.1565		0.032(13)	0.079(23)	0.057(17)
0.1570	0.002(2)	0.018(6)	0.051(16)	0.035(11)
0.1575		0.003(2)	0.033(11)	0.026(10)
0.1580	0.002(2)			0.013(6)
0.1600	0			0

Table 1: Mobilities D_1 (see (2)) on the 8^4 lattice at $\beta = 5.6$. The swap acceptance rates (1) achieved were about 82% for $\Delta\kappa = 0.00025$ and about 63% for $\Delta\kappa = 0.0005$.

5 Conclusions

Parallel tempering considerably enhances tunneling between different sectors of topological charge and generates samples with more symmetrical charge distributions than can be obtained by standard HMC. The histograms also get slightly broader or even become nontrivial thanks to this technique.

The enhancement of tunneling indicates an improvement of decorrelation also for other observables. More satisfactory histograms are important for topologically sensitive quantities. Both of these features make parallel tempering an attractive method for large-scale QCD simulations. The method is particularly economical when several parameter values have to be studied anyway.

A potential problem which remains to be studied is that for a given parameter set the swap acceptance rate (1) decreases for increasing lattice volume [7]. In this context possibly the choice of range and distances of the parameter values gets more important. We therefore plan to extend our investigations to larger lattices.

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References

[1] M. Müller-Preussker, Proc. of the XXVI Int. Conf. on High Energy Physics, Dallas, Texas (1992), 1545.

[2] B. Allés et al., Phys. Lett. B 359 (1996) 107.

[3] B. Allés et al., Phys. Rev. D 58 (1998) 071503.

[4] R. Burkhalter, this conference.

[5] R. Burkhalter, private communication.

[6] G. Boyd, Nucl. Phys. B (Proc. Suppl.) 60A (1998) 341.

[7] B. Joó et al., Phys. Rev. D 59 (1999) 114501.

[8] K. Hukushima et al., `cond-mat/9512035`.

[9] E. Marinari, `cond-mat/9612010`.