Cluster dynamics for first-order phase transitions in the Potts model

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Abstract

An algorithm for Monte Carlo simulations is proposed in which the parameter controlling the strength of the transition becomes a dynamical variable and in which efficient transitions are achieved by cluster steps. Numerical results for the Potts model demonstrate the advantages of the method.
To overcome slowing down is crucial in computer simulations of phase transitions. For second-order phase transitions in a number of systems critical slowing down can be drastically reduced by cluster algorithms as introduced by Swendsen and Wang [1]. There the acceleration is achieved by the nonlocal update of larger structures.

In the case of first-order transitions one encounters a different problem. On finite lattices one has an exponentially fast suppression of the tunneling between metastable states of the system with increasing lattice size. To reduce this type of slowing down the multicanonical Monte Carlo algorithm has been proposed [2, 3] which uses enhancement of the suppressed configurations. The canonical distribution is then obtained by an appropriate reweighting [4].

The application of cluster algorithms to first-order transitions leads only to little improvement [3, 8]. The obvious reason for this is that clusters can lead to some acceleration related to extended structures at not too large $q$, however, not with respect to the tunneling between order and disorder.

To overcome slowing down in systems with a rough free-energy landscape the method of simulated tempering [4] has been proposed and applied to the random-field Ising model. In this method temperature values are related to a dynamical variable and the fact is utilized that at lower $\beta$ the free-energy barriers are lower.

In the present paper we propose to make the parameter which controls the strength of a first order transition a dynamical variable. This allows to proceed from a state at large strength to ones at lower strength where the transitions become easier. If in particular there is a range where the transition gets of second order, in this way the tunneling and the related suppression can be completely circumvented. It is crucial then to avoid also the critical slowing down related to extended structures. This is achieved by combining the procedure with cluster updates.

We demonstrate in the case of the Potts model [8] in two dimensions, using a square lattice with periodic boundary conditions, that this general scheme works very efficiently. The parameter which has to become dynamical in this case is $q$, the number of the degrees of freedom of the spins.
Figure 1 shows the distribution $P(E, q)$ for energies and values $q$ which is obtained for $\beta_L$ (defined below). It is useful to illustrate the principle of our approach. Instead of tunneling across the valley we allow travelling along the peaks.

Starting at an ordered state at large strength of the transition the cluster updates will mainly induce transitions between ordered states. Travelling down to lower strength they will increasingly break up larger structures. From low strength then an easy way is open to disorder at large strength. Further, also all the steps between different values of the strength variable will contribute to decorrelation.

Before describing our update scheme it appears appropriate to formulate the general principle of making a parameter dynamical. A probability distribution $\mu_q(\sigma)$ of spin configurations $\{\sigma\}$ which depends on a parameter $q$ can be reinterpreted as the conditioned probability $\hat{\mu}(q; \sigma)$ for getting a configuration $\{\sigma\}$ given a value of $q$. Then prescribing a distribution $\bar{\mu}(q)$ one obtains the joint distribution $\mu(q, \sigma) = \bar{\mu}(q)\hat{\mu}(q; \sigma)$ for which the updates are to be performed.

Our update scheme has three steps. The first one generates bond configurations $\{n\}$ according to Swendsen and Wang \[1\] and is described here by the conditioned probability $A(\sigma, q; n)$. The second step is a Metropolis update for the marginal distribution $\bar{\mu}(q, n) = \sum_{\{\sigma\}} \mu(q, \sigma)A(\sigma, q; n)$ realizing the conditioned probability $T(n, q; q')$ for arriving at a new value $q'$. In the third step the new spins are obtained with the conditioned probability $\bar{A}(n, q'; \sigma') = \mu(q', \sigma')A(\sigma', q'; n)/\bar{\mu}(q', n)$ which corresponds to the special choice of Swendsen and Wang where the new cluster spins are independent of the old ones. The generalized transition matrix thus becomes

$$W(\sigma, q; \sigma', q') = \sum_{\{n\}} A(\sigma, q; n)T(n, q; q')\bar{A}(n, q'; \sigma'). \tag{1}$$

It leaves $\mu$ invariant if $T$ leaves $\bar{\mu}$ invariant, and it satisfies detailed balance with $\mu$ if $T$ does so with $\bar{\mu}$, which follows immediately from the definitions.

In our update scheme cluster generation in addition to reducing critical slowing down also has the important virtue to allow technically simple steps between different $q$-values. The reason for this is that spins are not involved and the dependences
on the bond configurations are simple in $\tilde{\mu}(q, n)$. Using $\mu(q; \sigma) \equiv \mu_q(\sigma) = Z^{-1} e^{-\beta H}$ with $H = - \sum_{\langle ij \rangle} \delta_{\sigma_i, \sigma_j}$ and $Z = \sum_{\( \sigma \)} e^{-\beta H}$, one gets its explicit form

$$\tilde{\mu}(q, n) = \bar{\mu}(q) Z^{-1}(q) (e^{\beta(q)} - 1)^{N_b(n)} q^{N_c(n)}$$

where $N_b$ is the number of bonds and $N_c$ the number of clusters of the bond configuration $\{n\}$.

The simulations have been performed for two sets of $q$-values, $q = 4, \ldots, 7$ and $q = 2, \ldots, 10$. Detailed balance for the Metropolis steps described by $T(n, q; q')$ has been guaranteed using the symmetric proposal matrix $T_p(q; q') = 1/2 (\delta_{q+1, q'} + \delta_{q, q'+1} + \delta_{q_{\min}, q_{\min}'} + \delta_{q_{\max}, q_{\max}'})$ and the acceptance matrix $\min(1, \bar{\mu}(n, q')/\bar{\mu}(n, q))$.

The distribution $\bar{\mu}(q)$ has been chosen to be (approximately) constant within the sets of $q$-values considered. In this context also the $q$-dependence of $Z^{-1}(q)$ in (2) is to be known. By requiring the number of sweeps to be the same for each of the $q$-values in the respective set it has been determined numerically in an iterative way. Table 1 shows the relative values of $Z^{-1}(q)\bar{\mu}(q)$ obtained for the set $q = 4, \ldots, 7$ requiring constancy of $\bar{\mu}(q)$ better than 4%.

For the values of $\beta(q)$ two choices have been considered. The first one, denoted by $\beta_L(q)$ here corresponds to equal height of the two peaks in the distribution of energies for $q > 4$ or to the maximum of the specific heat which is used for $q \leq 4$. Table 2 gives the values of $\beta_L(q)$ used for the set $q = 4, \ldots, 7$. The second $\beta$-value considered is the infinite-volume critical value $\beta_c = \text{ln}(\sqrt{q} + 1)$.

The observables measured for all $q$ are the energy $E$ and the order parameter $M = (q \max_a(N_a) - 1)/(q - 1)$ with $N_a = V^{-1} \sum_i \delta_{\sigma_i, a}$. For both of them in each case also exponential and integrated autocorrelation times have been determined. Further, for comparison also simulations for other algorithms have been performed and in addition tunneling times determined. The statistics collected has been in the range of $3 \times 10^6$ to $2 \times 10^7$ sweeps for each $q$ and all algorithms investigated.

There are results on other algorithms in literature for $q = 7$ [8, 11, 13] and for $q = 10$ [3, 8, 15]. We performed simulations for the heat bath algorithm (H), the
method of Swendsen and Wang (SW), and the multicanonical heat-bath algorithm (MH) ourselves to get autocorrelation times for a precise comparison (rather than to have to rely on tunneling times only available in most cases). Because the Metropolis algorithm has been found \[5\] to be rather slow it has not been considered here. SW turns out to be slightly superior to H if one accounts for CPU times, too.

Tunneling times \[5, 10\] are only useful at larger \(q\) where they get dominant in the autocorrelation times. We observe that they depend on the particular definition and differ from the autocorrelation times, which for MH and DQ persists even at larger \(L\).

Table 3 gives the average stay times for each \(q\) (the average number of sweeps spent at a particular \(q\) before leaving it) obtained for \(\beta_L\) and the set \(q = 4, \ldots, 7\). It is seen that the travelling goes relatively fast. For \(\beta_c\) and for the set \(q = 2, \ldots, 10\) the stay times are very similar.

In Table 4 the exponential autocorrelation times for \(\beta_L\) and the set \(q = 4, \ldots, 7\) are shown. The errors are statistical ones. In the cases of \(\beta_c\) and of the set \(q = 2, \ldots, 10\) the results are very similar. The results obtained for the order parameter within errors agree well with those for \(E\) (listed in the Table). Thus the measurement of both observables provides a valuable check.

Figures 2 and 3 give the exponential autocorrelation times for \(q = 7\) and \(q = 10\), respectively, which we obtained for the heat bath algorithm (H), the method of Swendsen and Wang (SW), the multicanonical heat-bath algorithm (MH), and our approach with dynamical \(q\) (DQ) for the sets \(q = 4, \ldots, 7\) and \(q = 2, \ldots, 10\). The time scale is in sweeps of the respective algorithm in each case.

For a comparison firstly the CPU times related to these scales are to be considered. Because the fraction of time for the Metropolis step is small (of the order of 4%) as compared to that of the cluster steps in DQ, these scales for SW and DQ are about the same. For H and MH the underlying sweeps are about a factor 2 slower.

To compare secondly one has to discuss that in DQ time is also spent at the other
values of \( q \). With the extreme view that only one of the \( q \)-values is of interest – and all other results obtained at no extra cost are ignored – one could multiply by 4 and by 9 in the cases of the sets \( q = 4, \ldots, 7 \) and \( q = 2, \ldots, 10 \), respectively (noting that according to the choice of \( \bar{\mu}(q) \) equal times are spent at different \( q \)). Even then one gets an improvement as compared to MH of up to factors 7 and 3 for \( q = 7 \) and \( q = 10 \), respectively, in the range considered \[14\]. With the more realistic view that all results are of interest the gain is more than an order of magnitude.

For \( q = 7 \) by MH as compared to H there is only a modest gain \[10\] of about a factor of 2. Recently by a multicanonical demon algorithm \[11\] some improvement upon MH has been achieved on larger lattices. For DQ on the set \( q = 4, \ldots, 7 \) we find an improvement with respect to both of these multicanonical algorithms which even after a multiplication by 4 as mentioned above is still about a factor 6. Thus by DQ in any case one improves more than an order of magnitude as compared to the conventional case.

For \( q = 10 \) MH gets more efficient, gaining more than an order of magnitude in the range considered here as compared to H. However, DQ remains still superior even after the multiplication by 9 mentioned above. In addition, the multiplication factor can be reduced by using the set \( q = 4, \ldots, 10 \) instead of the set \( q = 2, \ldots, 10 \). This is suggested by the stay times indicating that it is not worthwhile to go down to \( q = 2 \). This feature is also apparent from the comparison of the results for DQ for \( q = 7 \) obtained on the sets \( q = 4, \ldots, 7 \) and \( q = 2, \ldots, 10 \) where the advantage of not going down amounts to a factor of about 2.

In this context it should be noted that there are a number of possibilities for further improvements. Some have already been briefly tested with positive results. For example, instead of \( q \)-steps by one one can use steps by two. To accelerate certain transitions one can make \( \beta \) dynamical, too. Instead of keeping \( \bar{\mu}(q) \) constant it may be adjusted to get more favorable stay times. Modification of the Metropolis step offers various optimizations.

For \( q = 4 \) and 3, where the phase transition gets of second order, comparing with
integrated autocorrelation times obtained for SW \[12\] one observes still reductions by factors of about 4 and 3, respectively. For \(q = 2\) comparing with exponential autocorrelation times for SW \[13\] one gets a corresponding factor of about 1.4. To these reductions the additional tunneling possible at not too large \(L\) contributes which does not persist at very large \(L\).

From Figures 2 and 3 it is seen that for DQ there is some small exponential-like contribution present in the autocorrelation times. The obvious reason for this is that at not too large \(L\) there are still sizable additional contributions from tunneling which die out at larger \(L\). At very large \(L\) only travelling along the peaks is possible and the true asymptotic behavior occurs.

At the upper end of the range considered for DQ the increase of autocorrelation times is smaller than for MH which gives first hints about the ultimate asymptotic behavior. However, to conclude about the ultimate behavior much larger lattices are needed and it is to be noted that then details as, for example, the appropriate adjustment of \(\tilde{\mu}(q)\) become important. From the practical point of view on the lattices which can be reached there remains in any case substantial gain for DQ.

The proposed concept has been realized here with the simplest choices of details in order to check its working in practice. Clearly the next task is to optimize these choices. In any case the present results demonstrate that the concept works surprisingly well such that it deserves further development and also application to other systems.

One of us (W.K.) wishes to thank Claudio Rebbi and the Physics Department of Boston University for their kind hospitality during a sabbatical leave. This work has been supported in part by the Deutsche Forschungsgemeinschaft through grants Ke 250/7-1 and 250/9-1. The computations have been done on the SN I 400/40 of the Universities of Hessen at Darmstadt and on the Convex C230 of Marburg University.
References

[1] R.H. Swendsen and J.-S. Wang, Phys. Rev. Lett. 58, 86 (1987).

[2] B.A. Berg and T. Neuhaus, Phys. Lett. B267, 249 (1991).

[3] B.A. Berg and T. Neuhaus, Phys. Rev. Lett. 68, 9 (1992).

[4] A.M. Ferrenberg and R.H. Swendsen, Phys. Rev. Lett. 61, 2635 (1988).

[5] A. Billoire, R. Lacaze, A. Morel, S. Gupta, A. Irbäck, and B. Petersson, Nucl. Phys. B358, 231 (1991).

[6] W. Janke, HLRZ Preprint 50/92, Jülich (1992).

[7] E. Marinari and G. Parisi, Europhys. Lett. 19, 451 (1992).

[8] R.B. Potts, Proc. Camb. Phil. Soc. 48, 106 (1952); for a review see F.Y. Wu, Rev. Mod. Phys. 54, 235 (1982).

[9] A. Billoire, R. Lacaze, and A. Morel, Nucl. Phys. B370, 773 (1992).

[10] W. Janke, B.A. Berg, and M. Katoot, Nucl. Phys. B382, 649 (1992).

[11] R. Rummukainen, CERN Preprint CERN-TH.6654/92 (1992).

[12] X.-J. Li and A.D. Sokal, Phys. Rev. Lett. 63, 827 (1989).

[13] W. Kerler, Nucl. Phys. B (Proc. Suppl.) 26, 626 (1992); Phys. Rev. D 47, R1285 (1993).

[14] It is to be noted that for MH the autocorrelation time does not enter the error in the usual way. Comparing on the basis of variances, MH looses an additional factor of up to 2.3 in the range considered, which is not included in the numbers given.
Table 1

Values of \((Z^{-1}(q)\bar{\mu}(q))/(Z^{-1}(7)\bar{\mu}(7))\).

| \(L\) | \(q = 6\)        | \(q = 5\)        | \(q = 4\)        |
|-------|------------------|------------------|------------------|
| 12    | \(7.23 \times 10^{-1}\) | \(5.43 \times 10^{-1}\) | \(5.346 \times 10^{-1}\) |
| 16    | \(4.748 \times 10^{-1}\) | \(2.629 \times 10^{-1}\) | \(1.925 \times 10^{-1}\) |
| 24    | \(1.726 \times 10^{-1}\) | \(3.669 \times 10^{-2}\) | \(1.677 \times 10^{-2}\) |
| 34    | \(2.857 \times 10^{-2}\) | \(1.18 \times 10^{-3}\) | \(1.95 \times 10^{-4}\) |
| 50    | \(5.17 \times 10^{-4}\) | \(5.38 \times 10^{-7}\) | \(1.52 \times 10^{-8}\) |

Table 2

Numerical values for \(\beta_L\).

| \(L\) | \(q = 7\) | \(q = 6\) | \(q = 5\) | \(q = 4\) |
|-------|------------|------------|------------|------------|
| 12    | 1.2725     | 1.2158     | 1.1495     | 1.0708     |
| 16    | 1.2806     | 1.2238     | 1.1582     | 1.0792     |
| 24    | 1.2872     | 1.2309     | 1.1656     | 1.0879     |
| 34    | 1.29005    | 1.23407    | 1.16915    | 1.0918     |
| 50    | 1.29178    | 1.23607    | 1.17145    | 1.0947     |
Table 3

Average stay times for $\beta_L$ (with errors smaller than 1%).

| $L$ | $q = 7$ | $q = 6$ | $q = 5$ | $q = 4$ |
|-----|---------|---------|---------|---------|
| 12  | 2.48    | 1.27    | 1.32    | 2.70    |
| 16  | 2.70    | 1.39    | 1.47    | 3.08    |
| 24  | 3.22    | 1.69    | 1.88    | 4.02    |
| 34  | 4.19    | 2.24    | 2.66    | 5.85    |
| 50  | 6.84    | 3.81    | 5.04    | 12.8    |

Table 4

Exponential autocorrelation times for $\beta_L$.

| $L$ | $q = 7$   | $q = 6$   | $q = 5$   | $q = 4$   |
|-----|-----------|-----------|-----------|-----------|
| 12  | 15.1(2)   | 11.5(1)   | 9.04(6)   | 8.18(6)   |
| 16  | 21.2(4)   | 15.8(2)   | 12.5(1)   | 10.9(1)   |
| 24  | 36.8(6)   | 26.7(3)   | 20.4(2)   | 16.6(2)   |
| 34  | 64.0(6)   | 44.7(5)   | 31.8(3)   | 24.1(3)   |
| 50  | 126(2)    | 79(1)     | 50(1)     | 37.0(4)   |
Figure Captions

FIG. 1. Distribution $P(E, q)$ for $\beta_L$ (shown for $L = 34$).

FIG. 2. Comparison of exponential autocorrelation times for $q = 7$ and the algorithms H, MH, DQ on set $q = 4, \ldots, 7$, and DQ on set $q = 2, \ldots, 10$.

FIG. 3. Comparison of exponential autocorrelation times for $q = 10$ and the algorithms SW, H, MH, and DQ on set $q = 2, \ldots, 10$. 