MULTICANONICAL CLUSTER ALGORITHM
AND THE 2-D 7-STATE POTT'S MODEL

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Abstract

I present a hybrid-like two-step algorithm, which combines a microcanonical update of a spin system using demons, with a multicanonical demon refresh. The algorithm is free from the supercritical slowing down, suffered by canonical methods: the exponential increase of the tunnelling time between the metastable states in the first-order phase transitions, when the volume of the system is increased. The demons act as a buffer between the multicanonical heat bath and the spin system, allowing the spin system to be updated with any microcanonical demon procedure, including cluster methods. The cluster algorithm is demonstrated with the 2-dimensional 7-state Potts model, using volumes up to $128^2$. The tunnelling time is found to increase as $L^{1.82}$, where $L$ is the linear dimension of the system.
1 Introduction

If a system has a first-order phase transition, at the transition temperature it can exist in a mixed state, where two different bulk phases are separated by an interface. The free energy carried by the interface is the interface tension $\sigma$. Because at the transition temperature the free energy densities of the bulk phases are equal, the free energy of the mixed state is higher than either of the pure phases by an amount of $F_s = \sigma A$, where $A$ is the area of the interface. In numerical simulations using the canonical ensemble at the transition temperature, the configurations containing the mixed phase are suppressed by the Boltzmann factor $e^{-F_s/T}$. When the volume of the system is increased, the suppression of the mixed state increases exponentially with the area of the interface – hence also the time it takes for the system to tunnel from one pure phase to another increases exponentially.

Recently, Berg and Neuhaus [1] introduced a powerful new method, the multicanonical algorithm, which avoids the exponential slowing down by artificially enhancing the probability of the configurations with an interface. The tunnelling time increases only polynomially with the increasing linear size $L$. In this method the individual spin updates generally depend on the total energy of the system in a non-linear fashion. This effectively prevents the use of vector or parallel coding (except if one runs many lattices in parallel) and cluster update algorithms.

In the microcanonical demon Monte Carlo approach, developed a decade ago by M. Creutz [2], one uses additional variables, demons, to transfer energy around the system. The total energy of the system plus the demons is absolutely conserved. However, by periodically updating the demon energies according to the Boltzmann distribution the method reduces to the canonical procedure.

In this work I present an algorithm which combines these two methods: first, a system is updated microcanonically with a set of demons, and second, the demons are refreshed with a multicanonical heat bath. The demons act as a buffer, isolating the actual system from the multicanonical heat bath, thus enabling one to choose an optimal microcanonical update step for a particular problem. The update can be a highly vectorizable and parallelizable local update or a cluster update, or some combination of these. As an example, I apply the cluster version of the algorithm to the 2-dimensional 7-state Potts model.

The Potts models have become standard tools for high-precision Monte Carlo studies of the first-order phase transitions. The 2-dimensional $q$-state (2dqs) Potts model \[4, 5\] is defined by the partition function

$$Z(\beta) = \sum_{\{s\}} \exp[-\beta E(s)]$$  \hspace{1cm} (1)
When \( q > 4 \), the transition is of first order. The infinite volume transition temperature is \( \beta_c = 1/T_c = \log(1 + \sqrt{q}) \). Beside the fact that many infinite volume quantities are exactly known, rigorous finite-size scaling (FSS) predictions by C. Borgs et al. offer a quantitative method for studying the approach to the asymptotic regime. I chose the 2d7s Potts model for comparison with the recent standard multicanonical calculation by W. Janke et al. and the canonical one by A. Billoire et al. The lattice sizes in this work were \( V = L^2 = 20^2, 32^2, 64^2 \) and \( 128^2 \); for the largest volume, two separate simulations were performed.

This article is divided into three parts: in the first section I discuss how the standard multicanonical approach is generalized to the two-step demon algorithm, and how it can be used to obtain an estimate of the density of states, and, through this, of all thermodynamical quantities. The next section describes the actual update algorithms: the microcanonical cluster update and the multicanonical demon refresh. I present a method which enables the ‘slow’ part of the multicanonical update to be performed in \( \propto \sqrt{V} \) steps. The results of the 2d7s Potts model simulations are reported in the third section. The tunnelling time was found to increase like \( L^{1.82(3)} \), which is better than the standard multicanonical method \( (L^{2.65}) \). Where appropriate, the thermodynamical measurements of the 128\(^2\) lattices fully agree with the rigorous FSS predictions of ref. \[6\], and all the measurements are consistent with the multicanonical MC data of ref. \[7\].

2 The Multicanonical Demon Algorithm

Close to the transition temperature the canonical probability distribution \( p_\beta(E) \) develops a double-peak structure, and one definition for the transition temperature \( T_c = 1/\beta_c \) itself is the temperature when the two peaks have equal height (fig. 1). Following refs. \[1, 7\], the peak locations are denoted by \( E_{1,2}^L \), and the probability density is normalized to \( p_\beta^L(E_{1,2}^L) = 1 \). Denoting the minimum of \( p_\beta^L \) between the peaks by \( p_{\text{min}}^L \), the interface tension is \[3\]:

\[
\sigma = - \lim_{L \to \infty} \frac{\log p_{\text{min}}^L}{2L}.
\]

Because of the periodic boundary conditions, the configurations corresponding to the minimum of the probability distribution have two interfaces separated by \( \sim L/2 \); hence the factor 2 in eq. \[3\]. In the following the \( L \)-dependence of the above quantities is mostly suppressed from the notation.

In the standard ‘direct’ multicanonical method, one usually aims at a roughly constant probability density in the domain between the peaks: \( p_W(E) = 1, E_1 \leq E \leq E_2 \). This can
be achieved by substituting the Boltzmann weight with a weight function \( W(E) \):

\[
p_W(E) \propto n_S(E) e^{-W(E)},
\]

(4)

where \( n_S(E) \) is the number of states at energy \( E \). The requirement that the probability density is constant implies that \( W(E) \propto \log n_S(E) = S(E) \) when \( E_1 \leq E \leq E_2 \); and \( W(E) = \beta E + \text{const} \), otherwise. Because \( n_S(E) \) is what we are trying to compute in the first place, we have to use an approximate \( W(E) \) instead – obtained, for example, with finite-size scaling, canonical simulations, or previous multicanonical simulations. The measured \( p_W \) is then reweighted with \( e^{W(E)} \) to produce \( n_S(E) \), from which all quantities of interest can be calculated – also the improved \( W(E) \).

Now we want to apply multicanonical ideas to a system consisting of the original spin system and a system of demons. Heuristically, it is clear that the spin system in eq. (4) can be substituted with any other system, also with this composite system. Denoting the weight function with \( G \), the probability density can be written as a joint distribution in the spin system energy \( E_S \) and the demon energy \( E_D \):

\[
p_G(E_S, E_D) \propto n_S(E_S)n_D(E_D) e^{-G(E_T)},
\]

(5)

where \( n_S(E_S) \) and \( n_D(E_D) \) are the spin system and the demon density of states, respectively, and \( E_T = E_S + E_D \) is the total energy. In the most general case the weight \( G \) is a function of both \( E_S \) and \( E_T \), but when \( E_T \) is fixed, we want \( p_G \) to reduce to the microcanonical distribution \( n_S(E_S)n_D(E_T - E_S) \), implying that \( G \) can only be a function of \( E_T \). When \( E_S \) is fixed, \( p_G \) reduces to the multicanonical distribution for the demons: \( n_D(E_D) e^{-G(E_S + E_D)} \).

Thus the probability distribution (5) is preserved in a generic two-step process of a microcanonical spin update and a multicanonical demon update, provided that both of the update steps separately satisfy detailed balance. Note that if \( G(E) = \beta E \), both the demon and spin system will have canonical distributions.

After the Monte Carlo simulation has produced a sample of the distribution (5), \( n_S \) can be solved from it. Although not strictly necessary, it is advantageous to use the known demon density of states: with \( N_D \) demons with discrete energy states 0, 1, ..., \( n_D(E_D) = \frac{(N_D - 1 + E_D)!}{(N_D - 1)!E_D!} \).

(6)

Because eq. (5) is valid separately for each \( E_D \), \( n_S \) can be expressed as a linear combination

\[
n_S(E_S) \propto \sum_{E_D} A_{E_D;E_S} \frac{p_G(E_S, E_D)}{n_D(E_D) e^{-G(E_T)}}, \quad \sum_{E_D} A_{E_D;E_S} = 1.
\]

(7)
The multipliers $A_{ED;ES}$ should be chosen to minimize the error in $n_S$. For each $E_S$ separately, the uncertainty in the (measured) $p_G$ is given by $\delta p_G = \sqrt{\bar{p}_G/N_{ES}}$, where $\bar{p}_G$ is the probability distribution in the limit of infinite statistics and $N_{ES}$ is the number of measurements with this $E_S$. (This is not true for the full distribution $p_G(E_S, E_D)$ because of the correlations between successive measurements; however, for fixed $E_S$, each measurement of $E_D$ is completely independent, as explained below). Minimizing the resulting error in eq. (7), we finally obtain

$$n_S(E_S) \propto \frac{p_S(E_S)}{\sum_{E_D} p_D(E_D) e^{-G(E_T)}} \cdot p_S(E_S) \equiv \sum_{E_D} p_G(E_S, E_D).$$

Note that the final result depends only on the spin system distribution $p_S(E_S)$, not on the demon energy distribution. The distribution $p_S$ corresponds to the standard multicanonical distribution eq. (4) with the weight $e^{-W(E_S)} = \sum_{E_D} p_D(E_D) e^{-G(E_S+E_D)}$.

Quite generally, if we want to simulate a system with a non-canonical weight function $W(E)$, then by inverting eq. (9) we obtain the corresponding $G(E)$. With the two-step update, the function $G$ will produce exactly the same distribution as $W$ with a direct update.

Instead of aiming at a flat distribution of $E_S$, it is now more natural to try to ‘flatten’ the $E_T$ distribution. Then, the optimal $G(E_T)$ equals to $S_T(E_T)$, the entropy of the total system. In the actual runs described here the initial estimate of $G(E_T)$ was obtained (for the lattices $\leq 64^2$) from short runs with $G(E_T) = \beta E_T$; for the $128^2$ lattice, finite-size scaling was used to scale up the function used in the $64^2$ simulation. The $64^2$ and $128^2$ lattices required one further refinement run to obtain the final weight function; in the end two different weights were used for the $128^2$ lattice. To simplify the calculation, $E_T$ was restricted in the range $E_T^{\min} \leq E_T \leq E_T^{\max}$, where the limits were chosen such that the expectation values of $E_S$, as a function of $E_T$, bracket the peak locations $E_1$ and $E_2$ (fig. 1):

$$\langle E_S(E_T^{\min}) \rangle \leq E_1 < E_2 \leq \langle E_S(E_T^{\max}) \rangle.$$

The functional form of $G(E_T)$ is not crucial, as long as it is accurate enough; here a continuous piecewise linear form was used. The required accuracy increases with the volume of the system – the weight $G(E_T)$ is an extensive quantity (or rather $G(E_T) - \beta c E_T \propto L$), but if $G(E_T)$ is ‘wrong’ by an amount of, say, log 2, the probability $p_G(E_T)$ will be changed by a factor of 2.

The left part of fig. 2 shows the joint distribution from the $64^2$ lattice, using $E_S$ and $E_T$ as independent variables. As can be seen, $E_S$ and $E_T$ follow each other very closely – the length and the width of the ridge behave like $L^2$ and $L$, respectively. The demon energy varies only
very little, meaning that the microcanonical temperature \( \partial S(E)/\partial E \) is almost constant, as it should be in the phase coexistence region. The right part is the same distribution, ‘canonized’ by reweighting it with \( e^{G(E_T) - \beta_c E_T} \), where \( \beta_c \) is the transition temperature for this lattice (table 2).

An interesting variation of the algorithm can be obtained by restricting \( E_T \) to a discrete set of values \( E_0, \ldots, E_N \), sufficiently dense so that the neighboring \( E_S \) distributions have large enough overlaps. This is a microcanonical version of the ‘simulated tempering’ method, presented by Marinari and Parisi.[9]

3 The Update Algorithms

3.1 The Microcanonical Cluster Update

In the simulations reported here one update cycle consists of one microcanonical spin + demon update sweep followed by an energy measurement and a multicanonical demon update. As the microcanonical step I used the Swendsen-Wang variation of the microcanonical cluster algorithm presented recently by M. Creutz [10]. As opposed to the standard procedure, the demons are located on the links of the lattice, instead of being connected to the spins. A link is activated only if the spins have the same value at each end of it and the demon does not carry enough energy to frustrate the link. Clusters are grown over the activated links and each cluster is flipped to a random spin value. Finally, the demon energy is increased or decreased by the amount of the corresponding link energy decrease or increase. On a \( d \)-dimensional lattice, this method requires \( d \times V \) demons.

After each update cycle the demon locations are shuffled. If the shuffling were not performed, one would construct exactly the same clusters during the next update cycle – assuming that the demon refresh, described in the next chapter, is also skipped. The shuffling does not need to be perfect: here it was done with random offsets and step lengths when picking the demons from the demon array. The actual cluster search was performed with the Hoshen-Kopelman cluster-finding algorithm [11].

Note that it is also possible to perform local updates with the same demons; the demons can be left on the links or moved to the spins – in the latter case only half (or \( 1/d \)) of the demons are used during one sweep. The probability distribution \( \tilde{p} \) is unaffected, as long as the total number of demons remains the same.

3.2 The Multicanonical Demon Update

The multicanonical demon refresh is greatly facilitated by the fact that each demon is an independent degree of freedom and the demon density of states is known. The most straight-
Table 1: The tunnelling time and the interface tension from the 2d7s Potts model simulations.

| L   | iterations | \(\tau_L\)     | \(\sigma\)  |
|-----|------------|-----------------|-------------|
| 20  | 2 500 000  | 320(5)         | 0.0189(3)  |
| 32  | 5 000 000  | 821(15)        | 0.0169(2)  |
| 64  | 6 000 000  | 2700(81)       | 0.0147(4)  |
| 128a| 9 000 000  | 10720(520)     | 0.01302(17)|
| 128b| 6 000 000  | 10520(620)     | 0.01306(21)|

A forward way to perform the demon update is to touch each demon with the multicanonical heat bath: the demon \(i\) is assigned a new value with the weight \(\exp[-G(E_T - E_D^{\text{old}} + E_D^{\text{new}})]\). For a continuous demon energy this would be the best method, even though this is a non-vectorizable process with \(\sim N_D\) steps. However, since now the demon energy is discrete, there exists a method which enables a major part of the demon update to be performed in \(\sim \sqrt{N_D}\) (non-vectorizable) steps. First, a new total demon energy \(E_D^{\text{new}}\) is calculated with a global heat-bath update: let \(x\) be a random number from even distribution between 0 and 1; now the new demon energy is the smallest \(E_D^{\text{new}}\) satisfying

\[
x \leq \frac{\sum_{E'^{\text{new}}_D=0}^{E_D^{\text{new}}} n_D(E')e^{-G(E'+E_S)}}{\sum_{E'^{\text{new}}_D=0}^{\infty} n_D(E'^{\text{new}})e^{-G(E'^{\text{new}}+E_S)}},
\]

where \(G(E_T) = \infty\), when \(E_T < E_T^{\text{min}}\) or \(E_T > E_T^{\text{max}}\). This guarantees that the demon energy at fixed \(E_S\) is free from autocorrelations, justifying the use of the multinomial distribution prior to eq. (8). A new demon state with energy \(E_D^{\text{new}}\) can then be constructed from the old one by adding or subtracting energy from randomly selected demons. However, care has to be taken to ensure proper counting of states: energy is added or subtracted unit by unit, and the demon to be changed is chosen according to the respective probabilities

\[
p^i_+ \equiv p^i_{E_D \rightarrow E_D + 1} = \frac{E_D + 1}{N_D + E_D}, \quad p^i_- \equiv p^i_{E_D \rightarrow E_D - 1} = \frac{E_D}{E_D}.
\]

To prove that eq. (12) is correct, it is sufficient to show that starting from the state \(E_D = 0\), \(p_+\) produces with equal probability all the states with the same energy. Let us construct a specific demon state \(\omega\) with an energy \(E_\omega\): by repeatedly applying \(p_+\), the probability of a particular sequence of additions \({i}\) leading to this state becomes

\[
p_{{i}} = \prod \frac{(N_D - 1)!}{(N_D - 1 + E_D)!} (1)^{N_1} (2!)^{N_2} (3!)^{N_3} \cdots , \quad E_\omega = N_1 + 2N_2 + 3N_3 + \cdots \text{,}
\]

where \(\sigma\) is the interface tension.
where $N_e$ is the number of demons with energy $e$. Because the numbers $N_e$ are characteristic of the state $\omega$ and not of the sequence $\{i\}$, all the sequences leading to this state have the same probability. Then the probability $p_\omega$ of producing the state $\omega$ is obtained by multiplying $p_{\{i\}}$ with the number of sequences $N_{\text{seq}}^\omega$ ($= \text{number of permutations}$) leading to this state,

$$N_{\text{seq}}^\omega = \frac{E_\omega!}{(1!)^{N_1} (2!)^{N_2} (3!)^{N_3} \cdots}$$

(15)

giving $p_\omega = 1/n_D(E_\omega)$ [eq. (3)]. This is just what we want – all the states with the same energy are equally probable, and the sum of the probabilities is 1. It is obvious that $p_-$ is the probability of the inverse process. Because the old demon state can be understood as an intermediate step in the energy addition/subtraction sequence, we can start building the new state directly from it.

Remember that during one update cycle only additions or only subtractions are performed. Because the average energy change in one cycle is $\sim \sqrt{V}$, only as many demons need to be updated; the demon shuffling after each cluster update takes care of proper mixing. By careful use of auxiliary arrays, also the integrations in eq. (11) can be performed in $\sim \sqrt{V}$ steps, but this was not fully implemented in the simulations.

An important technical question is how to implement the demon selection according to the probabilities of eq. (12). Two simple methods were tested: first, one can employ an appropriate accept/reject step at a random demon location – this is a true $\alpha \sqrt{N_D}$ method, but the poor acceptance rate (8% for the 2d7s Potts model) makes this rather slow in practice. In the second method one constructs a pointer array $a$, which has an entry for the location of each unit of the demon energy. The array $a$ has $E_D$ elements, of which $E_D^i$ are pointing to the demon $i$. When $E_D \rightarrow E_D + 1$, the demon is chosen as follows: one generates a random integer $i$ in the range $[1, N_D + E_D]$; if $i \leq N_D$, the demon $i$ is selected, and if $i > N_D$, one chooses the demon $a_i$. By construction, this gives just the correct probability $p_{\text{new}}^i$. The demon address is then added to the array $a$, and $E_D$ is increased. The process is repeated until $E_D^\text{new}$ is reached. The subtraction of the energy is performed analogously; only now does one select a random pointer $a_i$, decrease the energy of the demon $a_i$, and set $a_i = 0$. The bottleneck in this method is the initial generation of the pointer array, which requires $\sim N_D$ steps; however, it is a vectorizable process, and since $E_D$ has to be measured anyway, it can be performed with little overhead. In the tests the pointer array method was found to be 5–8 times faster than the accept/reject procedure, so it was chosen for the actual simulations. On the $128^2$ lattice, the whole measurement and demon update cycle used less than 6% of the CPU time, the rest being taken up by the cluster operations, which contain the only non-vectorizable $\propto V$ loop. Using a Cray X-MP, one full cycle took $\sim 3.9 \mu s$ per spin.
4 Results

The performance of the algorithm is best measured by the tunnelling time, which is defined as in ref. [7]: four times the tunnelling time, \(4\tau_L\), is the average number of updates for the system to get from \(E_L^1\) to \(E_L^2\) and back. This definition gives comparable autocorrelation time definition. The times are listed in table \(1\), and shown in fig. 3. The fit to the three largest lattices gives \(\tau_L = 1.49(17) \times L^{1.82(3)}\). This scales better than the standard multicanonical method [7], which has \(\tau_L = 0.082(17) \times L^{2.65(5)}\). In fact, this is even better than the optimal scaling given by the random-walk picture: in the first-order transitions, the energy gap behaves as \(V\), but the width of the system energy distribution with fixed total energy increases only like \(\sqrt{V}\). Assuming an ideal update algorithm, this is also the average change in the system energy during one sweep. The system has to random-walk across the gap in order to tunnel from one phase to another, and this takes \((\text{gap/step})^2 \sim V = L^2\) sweeps. The discrepancy is largely due to the shift of \(E_L^1/V\) and \(E_L^2/V\) (see figs. 1 and 8), which have a finite size dependence \(\sim 1/L\). If we ignore these and calculate \(\tau_L\) from tunnellings between the infinite volume energy density values \(e_1 = 0.4453\ldots, e_2 = 0.7986\ldots\), the tunnelling times of the smaller lattices become shorter and we obtain a scaling law \(\tau_L = 0.66(7) \times L^{1.97(3)}\), which is compatible with the random-walk limit. However, I chose to present the former result in order to enable the comparison with the previous calculation. The quality of the scaling fit is only \(\chi^2 = 6.2/2\) d.o.f., and since the ‘physical’ correlation length is of order \(\sim 30\), it is quite plausible that the true scaling law will be different. The scaling functions are plotted in fig. 3.

In order to compare with the canonical update algorithm, I utilized the results of the 2d7s Potts model simulations by A. Billoire et al. [8]. Their work has high-statistics data from 5 different volumes between \(16^2\) and \(64^2\). I made a finite-size fit to the autocorrelation times with the heuristic function \(\tau_L = aL^\alpha e^{2\sigma L}\), where the interface tension \(\sigma\) had the fixed value 0.01174 (see the next paragraph). The parameter values given by the fit are \(a = 1.01(15)\) and \(\alpha = 2.31(4)\), with \(\chi^2 = 4.2/3\) d.o.f.. (Without the exponential factor, the best power-law fit gives \(\chi^2 = 56/3\) d.o.f.) The function is plotted in fig. 3. The simulations in ref. [8] were performed with the one-hit Metropolis algorithm, which has a notoriously long autocorrelation time; this was balanced by a fast multispin coding. With a heat-bath update the autocorrelation time could be \(\sim 5–8\) times shorter, bringing the low end of the line close to the level of the multicanonical lines. On the \(128^2\) lattice the multicanonical cluster method is \(\sim 3\) times faster than the standard multicanonical, which again is \(\sim 5–40\) times faster than the canonical method.

The interface tension was measured with the Binder method [3], eq. (3). The minima and maxima of the canonical probability distributions were found by fitting a parabola close to
the extrema; the results depend on the fitting range only very weakly, when the range is large enough. All the error analysis was done by jackknifing the data to 50 sets. The measured values of $\sigma$ are shown in fig. 4, together with the measurements of ref. [7]. Using a common FSS fit of the form

$$-\frac{1}{2L} \log p_{\text{min}}^L = \sigma + \frac{c}{L}$$

(16)

to the three largest volumes, we obtain the result $\sigma = 0.01174(19)$ with $c = 0.169(11)$. The result agrees well with ref. [8] ($\sigma = 0.0121(5)$), but is seven standard deviations off from the exact infinite-volume value $\sigma = 0.010396\ldots$, recently calculated by Borgs and Janke [12]. The cited errors are only statistical, and the large difference between the values is obviously caused by the violations of the FSS formula (16). This is supported by the missing ‘flat bottom’ around the $p_{\text{min}}^L$; this flat part corresponds to the variations of the distance between the two interfaces, and the absence of the flat part implies that the interaction between the two interfaces is still non-negligible.

The value of $\sigma$ is at least a factor of 6 smaller than the results of refs. [13, 14, 15], obtained with an unrelated method. In these calculations the interface was stabilized by using different temperatures on the different sides of the lattice, thus enforcing one side into the disordered phase and the other into the ordered one. The interface tension was measured as a function of the temperature difference, and the final answer was obtained by extrapolating the results to the transition temperature. This method has also been applied to $N_\tau = 2$ pure gauge QCD [16, 17], and the results agree with the values obtained with the Binder method [6, 18]. The apparent failure of this method in the case of the 2d7s Potts model is probably due to the too strong pinning effect caused by the temperature difference. In 2d, the amplitude of the interface fluctuations is large, $\sim \sqrt{L/\sigma T}$. These fluctuations are strongly suppressed by the temperature difference, which should then be very small; however, in that case the two-phase configuration would be lost, unless extremely large volumes are used.

Finally, let us compare transition temperature measurements to the exact finite-size expansions [3, 20]. Common definitions for the pseudotransition temperature are the locations

| $L$   | $\beta$(equal height) | $\beta(C_{\text{max}})$ | $\beta(B_{\text{min}})$ | $\beta$(equal weight) |
|-------|------------------------|--------------------------|--------------------------|------------------------|
| 20    | 1.28474(13)            | 1.28443(12)              | 1.28444(13)              | 1.2939(3)              |
| 32    | 1.28976(7)             | 1.28953(7)               | 1.28776(7)               | 1.29379(7)             |
| 64    | 1.29241(4)             | 1.29235(3)               | 1.29194(3)               | 1.29360(4)             |
| 128   | 1.293251(15)           | 1.293234(15)             | 1.293140(15)             | 1.293567(19)           |
| 128b  | 1.293242(19)           | 1.293227(19)             | 1.293133(19)             | 1.293560(19)           |

Table 2: Measured pseudotransition temperatures.
of the maximum of the heat capacity $C = \beta^2 / V \left( \langle E^2 \rangle - \langle E \rangle^2 \right)$ and the minimum of the Binder parameter $V_L = \frac{1}{3} \left( 1 - \frac{\langle E^4 \rangle}{\langle E^2 \rangle^2} \right)$, where $E' = E - 2V$ in order to comply with the definition of energy used in [8, 9]. The differences of the known infinite-volume transition temperature and the measured values are plotted in fig. 5; also shown are the exact lowest order FSS corrections. On the $128^2$ lattices the FSS correction is within the error bars of the measured values, whereas the $64^2$ lattice is still off by $\sim 2\sigma$. Figure 6 shows the behaviour of $V_L$ as a function of $\beta$.

Still another way to find the transition temperature is the 'equal weight' method [19], where $\beta_{w}^L$ is defined as the temperature when the relative probabilistic weights of the ordered and disordered states are $q = 7$ and 1, respectively:

$$q = W_O/W_D = \frac{\sum_{E< E'} p_{\beta_w^L}(E)}{\sum_{E\geq E'} p_{\beta_w^L}(E)},$$

where $E'$ is the energy at the minimum of $p_{\beta}$ at the temperature when the two peaks have equal height. The measurements of $\beta_{c}$ are shown in fig. 7. The FSS corrections in this case are only exponential. An FSS ansatz of the form $\beta_{w}^L = \beta_{w} + a e^{-bL}$ was fitted to the data, with the results $a = 0.0012(12)$, $b = 0.05(3)$, and $\beta_{w} = 1.293562(14)$. The fit gives exactly the correct $\beta_{c}$; however, $\beta_{w}$ is almost completely determined by the $128^2$ data, and the effect of the values of $a$ and $b$ to the value of $\beta_{w}$ is negligible. The various transition temperature measurements are listed in table 2.

The locations of the maxima of the canonical probability distribution $p_{\beta}$ are shown in fig. 8. The FSS fits to the three largest volumes give the infinite-volume result $e_{1,\infty} = 0.4421(24)$ and $e_{2,\infty} = 0.7981(17)$, which agree fairly well with the exact values $0.44539\ldots$ and $0.79867\ldots$. The latent heat is the difference of these two values: $\Delta e = 0.3559(29)$ (exact $0.35327\ldots$).

Even though the difference between the heat capacity of the disordered phase ($C_D$) and of the ordered phase ($C_O$) is exactly known, the actual pure phase values are not. An estimate can be obtained by employing the FSS relation of refs. [20, 7]:

$$C_O = C_{L,\text{max}} - V(\Delta s/2)^2 + 0.0038\ldots + O(V^{-1}),$$

where $\Delta s = \beta_{c}\Delta E/V$ is the entropy difference between the two phases. The result is shown in fig. 9; the FSS fit yields an estimate of $C_O = 44.4 \pm 2.2$. Because of the subtraction of two terms of order $V$, the errors grow rapidly when the volume is increased. Again, this result is consistent with that of ref. [8] $47.5 \pm 2.5$.

5 Conclusions

I have presented a new hybrid-like algorithm, which combines a microcanonical spin system update with demons, and a multicanonical demon update. Like the direct multicanonical
method, this algorithm does not suffer from the exponential slowing down in the first-order phase transitions. In the 2d7s Potts model simulations, the tunnelling time was found to increase like $\tau_L \sim L^{1.82(3)}$ with lattices up to $L^2 = 128^2$. Where appropriate, the measurements were compared with the analytical finite-size scaling formulas by Borgs et al. [6]; within the statistical errors, the $128^2$ lattice was found to be in complete agreement with the order $1/V$ FSS predictions. Also, all results are fully compatible with those of ref. [7]. However, the common FSS ansatz for the interface tension, $\sigma_L = \sigma_\infty + c/L$, fails to produce the correct infinite-volume value. This is probably due to the interactions between two interfaces, which are ignored by the FSS ansatz. Clearly, a better FSS function is needed.

The main advantage of the multicanonical demon algorithm is that it offers various possibilities in choosing the algorithm. In addition to simply using either local or cluster updates, one can also adjust the number of the demons and the number of the microcanonical updates before each multicanonical step. For example, if one has a very fast local microcanonical algorithm, it might be preferable to interleave many microcanonical updates for each demon refresh, and to use a large number of demons ($N_D > V$) in order to allow large fluctuations in the system energy during the microcanonical phase – the demon refresh can still be performed in $N_D \times \text{fast} + \sqrt{N_D} \times \text{slow}$ operations. The method can also be generalized to magnetic transitions by using demons carrying magnetization; in this case the cluster algorithm cannot be used.

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References

[1] B. A. Berg and T. Neuhaus, Phys. Lett. B267 (1991) 249 and Phys. Rev. Lett. 68 (1992) 9.

[2] M. Creutz, Phys. Rev. Lett. 50 (1983) 1411.

[3] K. Binder, Phys. Rev. A25 (1982) 1699.

[4] R. B. Potts, Proc. Cambridge Philos. Soc. 48 (1952) 106.

[5] F. Y. Wu, Rev. Mod. Phys. 54 (1982) 235.
[6] C. Borgs and R. Kotecký, J. Stat. Phys. 61 (1990) 79; C. Borgs, R. Kotecký and S. Miracle-Solé, J. Stat. Phys. 62 (1991) 529.

[7] W. Janke, B. A. Berg and M. Katoot, Florida State Univ. preprint FSU-SCRI-92-40.

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

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

[10] M. Creutz, Phys. Rev. Lett. 69 (1992) 1002.

[11] J. Hoshen and R. Kopelman, Phys. Rev. B14 (1976) 3438.

[12] C. Borgs and W. Janke, Berlin preprint FUB-HEP 13/92.

[13] J. Potvin and C. Rebbi, Phys. Rev. Lett. 62 (1989) 3062.

[14] K. Kajantie, L. Kärkäinen and K. Rummukainen, Phys. Lett. B223 (1989) 213.

[15] K. Rummukainen, Z. Phys. C49 (1991) 467.

[16] K. Kajantie, L. Kärkäinen and K. Rummukainen, Nucl. Phys. B333 (1990) 100; B357 (1991) 693.

[17] S. Huang, J. Potvin, C. Rebbi and S. Sanielevici, Phys. Rev. D42 (1990) 2864; errata D43 (1991) 2056.

[18] B. Grossmann, M. L. Laursen, T. Trappenberg and U.-J. Wiese, Jülich preprint HLRZ-92-31.

[19] C. Borgs and W. Janke, Phys. Rev. Lett. 68 (1992) 1783.

[20] J. Lee and J. M. Kosterlitz, Phys. Rev. B43 (1991) 3265.
Figure captions

Fig. 1. The canonical probability distributions $p_{\beta_c}(E)$ obtained from the multicanonical distributions with eq. (8).

Fig. 2. The multicanonical joint probability distribution $p_G(E_S, E_T)$, measured from the $64^2$ 7s Potts model simulation (left) and the canonical distribution corresponding to $\beta = 1.29241$ (right). The canonical distribution is obtained from the multicanonical one by reweighting it with $e^{G(E_T) - \beta E_T}$.

Fig. 3. The tunnelling time as a function of the lattice size $L$ on a log-log scale with scaling laws. Solid line (a): this work, $\tau_L \propto L^{1.82}$; dash-dotted line (b): multicanonical simulation by Janke et al. [7], $L^{2.65}$; dashed line (c): canonical simulation by Billoire et al. [8], $L^{2.3} e^{2\sigma L}$.

Fig. 4. The interface tension as a function of the lattice size. The black circles correspond to this work, and white squares to measurements by Janke et al. [7]. The line is a fit to 3 largest volumes, and the white circle is the infinite volume extrapolation. The arrow is the exact infinite volume result [12].

Fig. 5. The difference between the infinite volume transition temperature $\beta_c^\infty$ and the measured transition temperature $\beta_L^c$, plotted on a log-log scale. The black circles are the measured locations of the maxima of the heat capacity ($C_{max}$) and the white circles the locations of the minima of the Binder parameter ($V_{L,\text{min}}$). The solid line and the dashed line are the exact order $1/V$ expansions. For clarity, the data of the second $128^2$ lattice has been shifted slightly to the right.

Fig. 6. The Binder parameter $V_L$. The dashed line shows the exactly known infinite volume limit.

Fig. 7. The transition temperature determined by the equal weight method, and the FSS fit to the data. The dashed line is the exact infinite-volume $\beta_c$.

Fig. 8. The locations of the maxima of the canonical probability distribution $p_{\beta}^L$, together with the linear fit to three largest volumes.

Fig. 9. The maximum of the heat capacity with the leading finite size correction subtracted.