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Multibondic cluster algorithm for finite-size scaling studies of critical phenomena

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Abstract

For finite-size scaling studies of second-order phase transitions the critical energy range of interest is usually larger than the energy range covered by a canonical Monte Carlo simulation close to the critical temperature. The desired extended energy range can be covered, in principle, by performing a Wang–Landau recursion for the density of states followed by a multicanonical simulation with fixed weights. But in the conventional approach one loses the advantage due to cluster algorithms. We show that a cluster version of the Wang–Landau recursion together with a subsequent multibondic simulation improves for 2D and 3D Ising models the efficacy of the conventional approach by power laws in the lattice size. By using finite-size scaling theory for suitably adapting the extended energy range to the system size, in our simulations real gains in CPU time reach two orders of magnitude.

Keywords: Critical phenomena; Multibondic simulations; Wang–Landau recursion

1. Introduction

In numerical studies of statistical physics systems in the Gibbs canonical equilibrium ensemble, a single Markov chain Monte Carlo (MCMC) simulation [1] at a given temperature combined with standard reweighting techniques [2] can, theoretically, cover the full temperature range. In practice, however, due to finite run lengths, the reliable temperature interval is severely limited by the insufficient statistics in the tails of the simulated energy density. In principle this situation can be improved by patching canonical simulations from several temperatures together, relying on a multi-histogram approach. Besides that dealing with many simulations is tedious, weaknesses of these approaches are that the histograms fluctuate independently and that their patching has to be done in regions where the statistics is reduced due to the decline of the number of histogram entries. It has turned out that in realistic applications more stable estimates can be obtained by constructing a "generalized ensemble" [3–6], which allows to cover the entire region of interest in a dynamical way [7,8].

While the power of generalized ensembles is well documented for first-order phase transitions and complex systems such as spin glasses and peptides (small proteins) [9], this is not the case for second-order phase transitions where one ideally wants to cover the full scaling region in which many physical observables diverge with increasing lattice size. The usefulness of generalized ensembles for this purpose was previously discussed in Ref. [10], but the specific implementation lost the crucial advantage which cluster algorithms [11,12] provide. Here we discuss such a generalization to cluster algorithms [13], starting from the multibondic (MUBO) [14] cluster version of the multicanonical (MUCA) [4] ensemble.

This framework is generally valid for models allowing for cluster algorithms. After a careful study of the scaling properties which is crucial for our approach, we illustrate the performance of the algorithm for 2D and 3D Ising models which capture typical behaviors.

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2. Scaling at second-order phase transitions

Close to the transition temperature T_c of a second-order phase transition many observables exhibit singularities which can be parametrized for an infinite system as

$$S(T) \sim |t|^{-\sigma}, \tag{1}$$

where $t = T/T_c - 1 = \beta_c/\beta - 1$ is the reduced temperature and σ is the critical exponent of S. By comparing the size L of a finite system with the correlation length $\xi \sim |t|^{-\nu}$, finite-size scaling (FSS) theory implies at T_c [15]

$$S_L(T_c) \sim L^{\sigma/\nu}, \tag{2}$$

or more generally in the scaling region $t \to 0$

$$S_L(T) \sim |t|^{-\sigma} f(L/\xi), \tag{3}$$

where f is a scaling function. As $S_L(T_c)$ is finite, $f(L/\xi)$ has to eliminate the singularity of $|t|^{-\sigma}$, implying $f(L|t|^{\nu}) \sim (L|t|^{\nu})^{\sigma/\nu}$ for $t \to 0$ and, therefore, Eq. (2).

The specific heat per site is given via the fluctuation–dissipation theorem by $C_L = \beta^2 L^D (\Delta e)^2$, where $\Delta e = \sqrt{\langle (e - \langle e \rangle)^2 \rangle}$ with $e = E/L^D$ denoting the energy density. A Taylor expansion around T_c gives

$$\langle e \rangle(T) = \langle e \rangle(T_c) + C_L(T_c)(T - T_c) + \cdots. \tag{4}$$

Requiring that $|\langle e \rangle(T) - \langle e \rangle(T_c)| < \Delta e(T_c)$, implies for the *canonical* reweighting range

$$|T - T_c|/T_c < \frac{1}{\sqrt{L^D C_L(T_c)}}. \tag{5}$$

Since at a second-order phase transition $C_L(T_c) \sim L^{\alpha/\nu}$ this takes the scaling form

$$|T - T_c|/T_c < L^{-(D+\alpha/\nu)/2} = L^{-1/\nu}, \tag{6}$$

where for the last equality hyperscaling was assumed to be valid.

The *desired* reweighting range, on the other hand, should cover the maxima $S_L^{\max} = S_L(T_L^{\max}) \sim L^{\sigma/\nu}$ of all divergent observables measured. Reweighting has to cover a reasonable range about the maximum, say in the interval $[T_L^{r-}, T_L^{r+}]$ defined by the two solutions of

$$S_L\big(T_L^{r\pm}\big) = r S_L^{\max}, \quad 0 < r < 1. \tag{7}$$

Usually one considers more than one observable. In this case the desired reweighting interval is given by the smallest T_L^{r-} and the largest T_L^{r+}.

In general the desired interval is not symmetric around T_c. To simplify the notation we use in the following $T_L^r = T_c + \max\{T_c - T_L^{r-}, T_L^{r+} - T_c\}$ and assume

$$\Delta T_L^r = \big|T_L^r - T_c\big| = a^r L^{-\kappa}, \tag{8}$$

where a^r and $\kappa > 0$ are constants (κ independent of r and a^r becomes large for r small). For sufficiently large L we suppose that ($A = \text{const}$)

$$S_L\big(T_L^r\big) = S^{\text{reg}} + A\big(\Delta T_L^r\big)^{-\sigma} \tag{9}$$

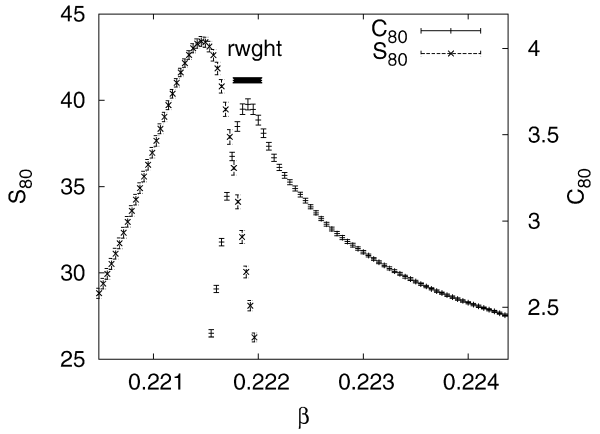

Fig. 1. Canonical (indicated by "rwght") versus desired (entire β axis) reweighting range on an 80^3 lattice.

holds, where $S^{\text{reg}} = S^{\text{reg}}(T)$ is a regular background term. Combining $S_L^{\max} \sim L^{\sigma/\nu}$ with (8) and (9) we find $L^{\sigma/\nu} \sim L^{\sigma\kappa}$ and conclude

$$\kappa = 1/\nu, \tag{10}$$

i.e., the desired range (8) scales with the same exponent as the canonical range (6). However, the proportionality factor a^r in (8) can be much larger than the one encountered for the canonical range. With the modest value $r = 2/3$ this point is made in Fig. 1 for the 3D Ising model on an 80^3 lattice, where the expectation values of the specific heat $C_L(\beta)$ and first structure factor $S_L(\beta)$ (whose maximum scales $\sim L^{\gamma/\nu}$ [16]) are shown. The desired reweighting range is more than 17 times larger than the canonical reweighting range from a simulation at $T_L^{\max}$ of the specific heat (in realistic applications one does not know T_c a priori and $T_L^{\max}$ of a suitable observable is a good substitute).

Some special care is necessary when the observable S exhibits a logarithmic singularity. Then the $t \to 0$ multiplicative cancellation (3) of the singularity is no longer possible, but becomes additive,

$$S_L(T) = S^{\text{reg}} - A \ln|t| + f(L/\xi), \tag{11}$$

such that

$$f(L/\xi) = \frac{A}{\nu} \ln\big(|t|^{\nu} L\big) = A \ln|t| + \frac{A}{\nu} \ln L, \tag{12}$$

$$S_L^{\max} = S_{\max}^{\text{reg}} + \frac{A_m}{\nu} \ln L. \tag{13}$$

Since

$$\begin{aligned} \frac{r A_m}{\nu} \ln L \sim r S_L^{\max} &= S_L\big(T_L^r\big) \\ &= r S_{\max}^{\text{reg}} - A_m \ln\big|t_L^r\big| \sim A_m \kappa \ln L \end{aligned} \tag{14}$$

one finds in this case that the exponent κ in Eq. (8) is no longer independent of r, but

$$\kappa = r/\nu. \tag{15}$$

While the canonical reweighting range scales still $\sim L^{-1/\nu}$, the desired reweighting range becomes $\sim L^{-r/\nu}$, so that the ratio

"desired/canonical" diverges $\sim L^{(1-r)/\nu}$. With $S = C$ the 2D Ising model provides an example.

This shows that typically more than one canonical simulation will be needed to cover the relevant part of the scaling region of a second-order phase transition. Employing the static multi-histogram approach [17] is one possibility to cope with this problem. More stable estimates, however, are obtained by constructing a generalized ensemble, which allows a random walker to cover the entire region of interest in a single simulation.

3. Multibondic cluster updating and Wang–Landau recursion

Generalized ensemble simulations require two steps: (i) Obtain a working estimate of the weight factors. (ii) Perform a MCMC simulation with fixed weights. For step (ii) we follow the extension to cluster algorithms [14,18] of MUCA simulations [4], focusing on the MUBO version [14]. With "working estimate" of step (i) we mean that the weights of the generalized ensemble are sufficiently accurate that the energy range in question is sampled in step (ii). Several efficient general purpose recursions for the weight determination were reported in a number of papers [19], see also Refs. [7,8,18]. Here we adapt the Wang and Landau (WL) approach [6] which differs fundamentally from the earlier approaches by iterating the weight at energy E *multiplicatively* with a factor $f_{\rm WL} > 1$ rather than additively. At a first glance the WL approach is counter-intuitive, because the correct iteration of the weight factor close to the desired fixed point is obviously proportional to the inverse number of histogram entries, $1/H(E)$, and not to $(1/f_{\rm WL})^{H(E)}$. However, what matters is a rapid approach to a working estimate. The advantage of the WL over the other recursions is that it moves right away rapidly through the targeted energy range. When this range is sufficiently covered, the iteration factor is refined by $f_{\rm WL} \to \sqrt{f_{\rm WL}}$, so that it approaches 1 rapidly.

We consider q-state Potts models with energy

$$E = -2\sum_{\langle ij\rangle} \delta_{s_i s_j}, \tag{16}$$

where the sum is over all nearest-neighbor pairs of a D-dimensional cubic lattice of L^D Potts spins, which take the values $s_i = 1, \ldots, q$, in a normalization where the special case $q = 2$ matches with the energy and β conventions of the standard Ising model.

The Fortuin–Kasteleyn (FK) representation [20] of the Potts model reads

$$\mathcal{Z}_{\rm FK} = \sum_{\{s_i\}} \sum_{\{b_{ij}\}} Z\big(\{s_i\}, \{b_{ij}\}\big) \tag{17}$$

with Boltzmann weight

$$Z\big(\{s_i\}, \{b_{ij}\}\big) = \prod_{\langle ij\rangle} [a\delta_{s_i s_j}\delta_{b_{ij}1} + \delta_{b_{ij}0}], \tag{18}$$

where $a = e^{2\beta} - 1$. The bond variables b_{ij} (simply called bonds in the following) take the values $b_{ij} = 0$ and 1, interpreted as "broken" and "active" or "set" bonds, respectively. By summing over the $\{b_{ij}\}$-configurations, one recovers the canonical Potts Boltzmann factor:

$$Z\big(\{s_i\}\big) = \prod_{\langle ij\rangle} [a\delta_{s_i s_j} + 1] = \prod_{\langle ij\rangle} e^{2\beta\delta_{s_i s_j}} \tag{19}$$

since $(e^{2\beta} - 1)x + 1 = e^{2\beta x}$ holds for $x = \delta_{s_i s_j} = 0, 1$.

The Swendsen–Wang cluster update [11] starts from the FK weight (18) and generates on links with $\delta_{s_i s_j} = 1$ new bonds $b'_{ij} = 1$ with probability $p_1 = a/(a+1) = 1 - e^{-2\beta}$ and bonds $b'_{ij} = 0$ with probability $p_0 = e^{-2\beta}$. On $\delta_{s_i s_j} = 0$ links one always sets $b'_{ij} = 0$. A cluster is defined as a set of spins connected by active bonds and in the subsequent spin update one assigns randomly a new value $s' = 1, \ldots, q$ to an entire cluster of spins.

With $B = \sum_{\langle ij\rangle} b_{ij}$ denoting the number of active bonds, the MUBO partition function [14] is defined by

$$\mathcal{Z}_{\rm MUBO} = \sum_{\{s_i\}} \sum_{\{b_{ij}\}} Z\big(\{s_i\}, \{b_{ij}\}\big) W(B), \tag{20}$$

where a bond weight factor $W(B)$ has been introduced which modifies the cluster update procedure as follows. If $s_i \neq s_j$ a bond is never set, B does not change, and $W(B)$ is irrelevant. For $s_i = s_j$ there are two possibilities: The initial bond is not set, $b_{ij} = 0$. Then $B' = B$ for $b'_{ij} = 0$ and $B' = B + 1$ for $b'_{ij} = 1$. The updating probabilities are ($a = e^{2\beta} - 1$)

$$P_1(0 \to 0) = \frac{W(B)}{W(B) + aW(B+1)} \tag{21}$$

and $P_1(0 \to 1) = 1 - P_1(0 \to 0)$. If the initial bond is set, $b_{ij} = 1$, then $B' = B - 1$ for $b'_{ij} = 0$ and $B' = B$ for $b'_{ij} = 1$. The updating probability $P_2(1 \to 0)$ hence equals $P_1(0 \to 0)$ with $B \to B - 1$. Once the configuration is partitioned into clusters, the update of the spin degrees of freedom proceeds as in the canonical cluster algorithm by assigning with uniform probability a spin in the range $1, \ldots, q$ to each cluster.

In this cluster formulation the WL recursion generalizes to [13,21]

$$\ln W(B) \to \ln W(B) - a_{\rm WL}, \qquad a_{\rm WL} = \ln(f_{\rm WL}), \tag{22}$$

whenever a configuration with B bonds is visited. All recursions are started with $a_{\rm WL} = 1$ and we iterate $a_{\rm WL} \to a_{\rm WL}/2$ according to the following criteria: (i) The Markov chain just cycled from B_L^{r-} to B_L^{r+} and back. Here B_L^{r-} and B_L^{r+} are bond values corresponding to T_L^{r-} and T_L^{r+}, respectively, determined by short canonical simulations. (ii) The bond histogram $h(B)$, measured since the last iteration, fulfilled a flatness criterion $h_{\rm min}/h_{\rm max} > cut$, where cut was equal to 1/3 in most of our runs.

We freeze the weights after a last iteration is performed with the desired minimum value $a_{\rm WL}^{\rm min}$.

4. Numerical results

After the weight recursions and a short equilibration run, we performed MUBO simulations with the run length tuned

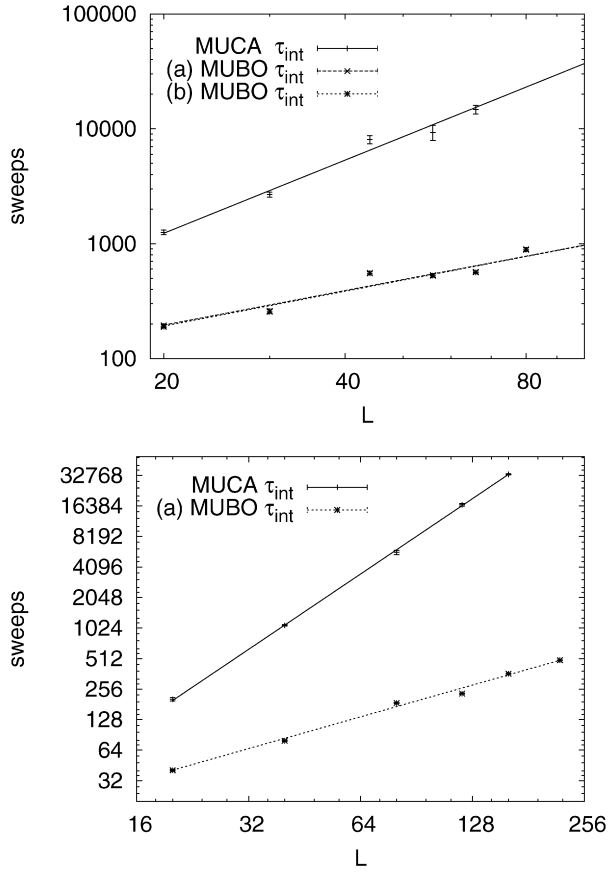

Fig. 2. Integrated autocorrelation times $\tau_{\rm int}(L)$ vs. lattice size L for the 3D (top) and 2D (bottom) Ising model. Error bars are computed with the Jackknife method.

to cover approximately 1000 cycling events. In all simulations, the recursions never took more than 3% of the statistics used for production runs. Similarly, also the initial canonical simulations used to determine B_L^{r-} and B_L^{r+} took less than 3% (provided they are started with an appropriate initial configuration).

The resulting integrated autocorrelation times $\tau_{\rm int}$ are compared in Fig. 2 with those of a MUCA simulation of similar statistics. From the MUBO time series we calculated $\tau_{\rm int}$ for (a) energies and (b) bonds, which is slightly higher for the energies, but indistinguishable on the scale of the figure. For MUCA the estimates are from energies. Up to a constant factor practically identical results are obtained from cycling times. In our code one MUCA sweep was about three times faster than one MUBO sweep.

The critical slowing down is described by $\tau_{\rm int} \sim L^z$. For the dynamical critical exponent we find $z = 2.22(11)$ for MUCA and $z = 1.05(5)$ for MUBO. So the performance gain is a bit better than linear with the lattice size L. The data in Fig. 2 scatter more than one might have expected about the fits because our T_L^{r-} and T_L^{r+} values are based on MCMC estimates, which are by themselves noisy. The exponent for MUBO cluster updating is significantly higher than the one estimated from canonical simulations at T_c, $z = 0.50(3)$, with the Swendsen–Wang algorithm [22]. The reason is that the efficiency of the cluster algorithm deteriorates off the critical point, even when one is still in the scaling region. This is particularly pronounced in the long tail of the specific heat for $T < T_L^{\max}$. Therefore, our exponent $z \approx 1$ should reflect the true slowing down in realistic applications better than the small literature value at T_c.

The lower part of Fig. 2 shows $\tau_{\rm int}$ from simulations of the 2D Ising model for which we adjusted our simulation parameter to cover the full width at half-maximum of the specific heat. This corresponds to $r = 1/2$ in Eq. (15). The dynamical critical exponent takes then the values $z = 2.50(4)$ for MUCA and $z = 1.04(2)$ for MUBO. The MUCA value reflects that the number of canonical simulations needed to cover the desired energy range grows now $\sim L^{1/2}$, while the canonical critical value is slightly above two [7,23].

5. Summary and conclusions

At second-order phase transitions, the energy range explored by canonical MCMC simulations is often too small to allow accurate reweighting analyses around the peak of a given quantity. Generalized ensembles such as those generated with the multicanonical or Wang–Landau methods can provide specifically tailored broader ranges but suffer in their conventional formulations from large autocorrelation times due to the use of local update algorithms. We first recall that much more efficient nonlocal cluster algorithms can be employed in the multibondic formulation and then propose a generalization of this method to weight recursions of Wang–Landau type. When the desired broad reweighting range is adjusted to the lattice size L according to finite-size scaling theory, we obtain for the Ising model with this cluster approach a gain in efficiency by power laws in L ($\simeq L^{1.45}$ in 2D and $\simeq L^{1.15}$ in 3D) compared to the conventional Wang–Landau multicanonical approach with local updates.

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