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# Hybrid Multicanonical Cluster Algorithm for Efficient Simulations of Long-Range Spin Models

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An efficient, flat histogram Monte Carlo algorithm is proposed that simulates long-range spin models in the multicanonical ensemble with very low dynamic exponents and drastically reduced computational effort. The method combines a random-walk in energy space with cluster updates, where bond weights depend continuously on the lattice energy. Application to  $q$ -state Potts chains with power-law decaying interactions is considered. Lattice sizes as high as  $2^{16}$  spins, unattainable with conventional flat histogram algorithms, are investigated. Numerical results demonstrate the remarkable performance of the method over a wide spectrum of model parameters.

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## I. INTRODUCTION

Amidst powerful methods dedicated to the study of long-range spin models, Monte Carlo (MC) methods have now gained a prominent role [1, 2, 3, 4]. Whether they rely on single-spin or cluster updates, *canonical* MC simulations of long-range models still pose the same limitations as do numerical studies of their short-range counterparts: (i) the computation of free energies is cumbersome, rendering e.g., a precise determination of the order of the transition intractable; (ii) for models exhibiting complicated energy landscapes or first-order phase transitions, the dynamics of the Markovian chain often sticks to local free energy minima, making it necessary to carry out simulations over exceedingly long times [5]. Efficient algorithms that work out these limitations are flat histogram algorithms, which operate in the multicanonical ensemble [5, 6, 7, 8], and engender a random-walk in energy space. The Markovian chain is thus weighed by a *multicanonical* weight  $w(E) \sim 1/n(E)$ , where  $n(E)$  is an estimate of the density of states. In the last decade, several efficient schemes have been devised that compute  $n(E)$  in the course of the simulation itself, e.g., Wang-Landau's algorithm [6] or the transition matrix method [8].

Local-update implementations of these algorithms were shown to reduce tunneling times from an exponential- to a power-law of the lattice size  $\tau_e \sim L^z$  [7], yet with dynamic exponents  $z$  being still substantially higher than the ideal value  $z \sim D$  expected from a random-walk argument. For long-range spin models, the need to compute the lattice energy anew at every MC sweep brings about an additional hurdle, since of order  $L^{2D}$  operations are involved. This yields a total CPU load per independent measurement scaling as  $L^{2D+z}$ , and limits studies to modest lattice sizes [4], where strong finite-size effects constitute a serious hindrance.

Conversely, cluster algorithms [1, 9] are known to drastically reduce dynamic exponents, owing to their ability to

minimize correlations by updating spins in a collective way. Because such algorithms hinge on particular symmetries of the model, and the multicanonical weight  $w(E)$  does not keep track of them, embedding collective updates in a multicanonical algorithm is not straightforward. The purpose of the present work is to develop a hybrid method which successfully tackles this challenge in an efficient and versatile way. In the case of long-range interactions, the method also drastically reduces the simulational effort through an optimized computation of the lattice energy.

## II. ALGORITHM

Our method is primarily based on the observation that, in local-update multicanonical algorithms, it is the microcanonical temperature which governs the dynamics of the Markovian chain [4]. Indeed, a single spin is flipped, and the move is accepted with the acceptance rate  $W = \min[1, n(E)/n(E+\epsilon)]$ , where  $E$  and  $\epsilon$  denote the initial energy and the energy variation respectively. Carrying out a series expansion in  $\epsilon$  yields  $W \sim \min[1, \exp(-\beta(E)\epsilon)]$ , where  $\beta(E) = d \ln n(E)/dE$  is an estimate of the inverse microcanonical temperature; hence a multicanonical dynamics is *locally* equivalent to a canonical dynamics at inverse temperature  $\beta(E)$ . We therefore propose to build clusters of spins by placing bonds between spins with the same probability as given by a canonical cluster algorithm operating at  $\beta(E)$ . To be specific, we consider a ferromagnetic long-range Potts model whose Hamiltonian reads  $E = -\sum_{i<j} J(|i-j|)\delta_{\sigma_i, \sigma_j}$ . The  $\sigma_i$  variables take on integer values between 1 and  $q$ , and  $J(|i-j|) > 0$ . We write the multicanonical weight as  $w(E) = \phi(E) \exp[-\beta(E)E]$  and, taking guidance from Swendsen-Wang's algorithm [9], expand the Boltzmann-like exponential term as a trace over the bonds of a random-bond cluster. This yields

$$w(E) = \phi(E) \sum_{[b]} \prod_{i<j} p_{|i-j|}(E) \delta_{\sigma_i, \sigma_j} \delta_{b_{ij}, 1} + \delta_{b_{ij}, 0},$$

where the trace is over all lattice bonds, a bond is active (inactive) whenever  $b_{ij} = 1$  (0), and  $p_{|i-j|}(E) = \exp[\beta(E)J(|i-j|)] - 1$  is interpreted as the statistical weight of a bond linking spins  $i$  and  $j$ . As opposed to Swendsen-Wang's algorithm,

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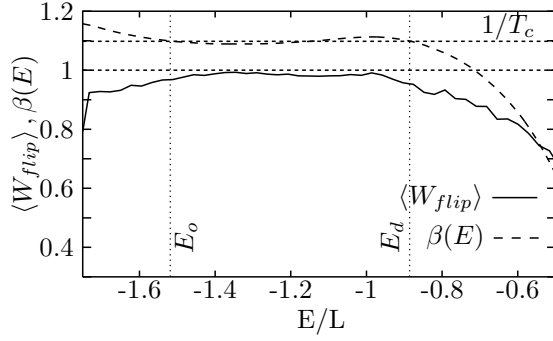


FIG. 1: Inverse microcanonical temperature  $\beta(E)$  and mean acceptance rate  $\langle W_{flip} \rangle$  as a function of the energy per spin, for the long-range Potts chain with  $q = 6$ ,  $\sigma = 0.7$ , and  $L = 1024$  spins.  $E_o$  and  $E_d$  denote the energy of the histogram peaks corresponding to the ordered and disordered phase, respectively. The finite size transition temperature  $T_c$  and the 100% line are shown for convenience.

bond weights thus vary continuously with the lattice energy. A simple way of constructing clusters may then consider each pair of spins in turn for bond activation, and activate a bond with a probability  $1 - \exp[-\beta(E)J(|i - j|)]$ . For interactions decaying with the interparticle distance, however, a large number of bonds have a negligible activation probability; a more efficient approach [1] consists, for each spin, in drawing at random the index of the next spin to be *provisionally* added to it using a cumulative probability, and then to place a bond if both spins match. This method was shown to reduce the number of operations per cluster construction from  $L^{2D}$  to roughly  $L^D$ . Finally, each cluster is assigned a random spin value, and the new configuration at energy  $E + \epsilon$  is accepted with the following acceptance rate,

$$W_{flip} = \min \left( 1, \frac{\phi(E + \epsilon)}{\phi(E)} \prod_{l>0} \left[ \frac{p_l(E + \epsilon)}{p_l(E)} \right]^{B(l)} \right), \quad (1)$$

where  $B(l)$  refers to the number of active bonds of length  $l$ . The computation of the lattice energy is obviously a crucial part of the update procedure, yet its complexity scales as  $O(L^{2D})$ . This can be efficiently cut down to  $O(L^D \ln L^D)$  by relying on an FFT implementation of the convolution theorem [10]. Noteworthy enough, such a reduction is of benefit only because a whole lattice update is carried out at a time.

### III. NUMERICAL RESULTS

In order to investigate the efficiency of our algorithm, we have conducted simulations on  $q$ -state Potts chains with  $q = 3, 6$  and  $12$ , and power-law decaying interactions, i.e.,  $1/|i - j|^{1+\sigma}$ . The density of states  $n(E)$  was estimated using Wang-Landau's method [6], and the microcanonical temperature  $\beta(E)$  was periodically updated from it using a spline interpolation. It also proved advantageous to rely on a transition matrix scheme [8, 11] to bootstrap the computation of  $\beta(E)$  during the very first iterations of Wang-Landau's algorithm. We briefly discuss some of our estimates of transition

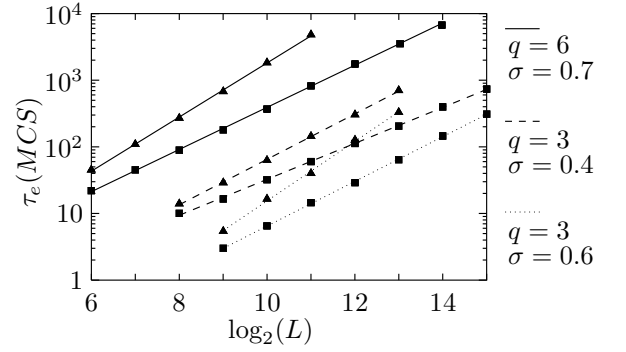


FIG. 2: Tunneling times for the long-range Potts chain. Triangles and squares refer to the local-update and to our algorithm, respectively.

temperatures, which we computed in two distinct ways:  $T_{eqh}$ , corresponding to peaks of the reweighted histogram having equal height; and  $T_W$ , defined from the intersections of the ratio  $W_o/W_d$  at successive lattice sizes, where  $W_o$  and  $W_d$  denote the histogram weights of the ordered and disordered phases respectively [12]. Infinite-size temperatures were determined from a fit to  $T(L) = T(\infty) + a/L^b$ . For  $q = 3$  and  $\sigma = 0.5$ , for instance, we found  $T_{eqh} = 1.6877(2)$  and  $T_W = 1.68744(2)$ , with a perfect fit from  $L = 2^9$  to  $L = 2^{16}$ . These estimates are far more precise than the value of  $1.686(4)$  obtained recently with a local-update approach [4]. For the sake of completeness, we performed simulations of the two-dimensional nearest-neighbor Potts model for sizes up to  $256 \times 256$  and  $q = 7$  and  $10$ , and obtained transition temperatures matching the exact results with a five-digits precision [11].

How fast does our algorithm explore the configuration space? A relevant indicator here is the mean acceptance rate, since by construction the acceptance rate in Eq. 1 is not equal to unity. Interestingly, a series expansion shows that  $1 - \langle W_{flip} \rangle$  is proportional to  $|\beta'(E)\epsilon|$ . As sketched in Fig. 1,  $\beta(E)$  varies smoothly between the energy peaks of the disordered and the ordered phase, and  $W_{flip}$  remains well above 90% inside this energy range, incidentally the energy range of primary interest where analysis of first order transitions is concerned. Other values of  $q$  and  $\sigma$  corresponding to the first-order regime yielded an acceptance rate which never fell below 80%. Let alone the benefit of the cluster dynamics itself, which we consider below, this already represents an improvement of a factor 3 over a single-spin-update implementation [4]. In terms of correlations between successive configurations, a convenient indicator is the so-called *tunneling time* [13, 14] defined as one quarter of the number of MC steps needed to travel from one histogram peak to the other, and back. Shown in Fig. 2 are fits to the power law  $\tau_e \sim L^z$ , giving  $z = 0.89(1)$  and  $z = 1.11(1)$  for  $q = 3$ ,  $\sigma = 0.4$  and  $\sigma = 0.6$ , and  $z = 1.05(1)$  for  $q = 6$ ,  $\sigma = 0.7$ . This represents a strong reduction with respect to the local-update implementation where we obtained, respectively,  $z = 1.13(2)$ ,  $z = 1.48(2)$  and  $z = 1.35(3)$ ; moreover, prefactors clearly favor our method even at small lattice

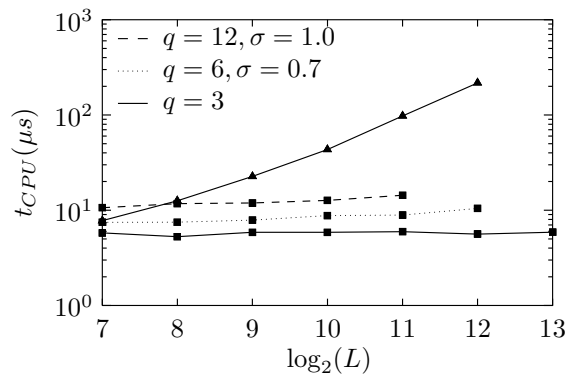


FIG. 3: CPU time per MC step and per spin for the long-range Potts chain. Triangles indicate typical CPU times for the local-update algorithm, irrespective of  $q$  and  $\sigma$ . Filled squares refer to our algorithm, where for  $q = 3$  estimates were obtained by averaging over  $\sigma = 0.4, 0.5$  and  $0.6$ .

sizes. For the nearest-neighbor model, we found  $z = 1.82(2)$  for  $q = 7$  and  $z = 2.23(1)$  for  $q = 10$ . These exponents are comparable with those obtained with the multibond approach [14]. Our exponents lie thus systematically closer to — and in some cases even below — the ideal value  $z \sim D$  expected from a random-walk argument than those obtained with a local-update algorithm.

Restraining the rest of the discussion to the long-range case exclusively, we now consider the gain in CPU time introduced by the FFT accelerated computation of the energy. Figure 3 shows averages of the CPU (user) time per MC step and per

spin as measured over a series of one-hour long simulations on various Intel-based CPU architectures. Clearly, the FFT acceleration cuts down the CPU load from a linear to a roughly constant one, with however small fluctuations owing to CPU caches differing in size. For higher  $q$ , a slight overhead can be witnessed; this is accounted for by the correspondingly higher number of FFT's to be computed, for the use of the convolution theorem for  $q > 3$  requires first mapping the Potts Hamiltonian to an  $O(q - 1)$  vector model, and then carrying out an FFT for each vector component separately. The local-update implementation is outperformed already at sizes of several hundreds spins; chains containing up to  $2^{16}$  spins were simulated in a few days, whereas challenging such huge sizes with local updates would have demanded several months of intensive computation.

In conclusion, we have developed a new Monte Carlo method which combines in an efficient and straightforward way the benefits of flat histogram algorithms with the fast-decorrelating capabilities of cluster updates. We have shown that this method proves remarkably powerful when applied to long-range spin models, where the algorithm complexity reduces to that of a short-range model having the same number of spins. Our formulation is nonetheless versatile, and the method can be applied to any spin model for which a random-bond representation can be devised, and to a variety of density of states estimation schemes.

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