Microcanonical Approach to the Simulation of First-Order Phase Transitions

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A simple microcanonical strategy for the simulation of first-order phase transitions is proposed. At variance with flat-histogram methods, there is no iterative parameters optimization nor long waits for tunneling between the ordered and the disordered phases. We test the method in the standard benchmark: the Q-states Potts model ($Q = 10$ in two dimensions and $Q = 4$ in $D = 3$). We develop a cluster algorithm for this model, obtaining accurate results for systems with more than 10^6 spins.

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First-order phase transitions [1] are hard to study by means of Monte Carlo simulation [2], specially for large system linear size L (or space dimension D). The intrinsic problem is that, at a first-order phase transition, two (or more) phases coexist. The simulated system tunnels between pure phases by building an interface of size L. The free-energy cost of such a mixed configuration is ΣL^{D-1} (Σ: surface tension), the interface is built with probability $\exp[-\Sigma L^{D-1}]$ and the natural time scale for the simulation grows with L as $\exp[\Sigma L^{D-1}]$. This disaster is called *exponential* critical slowing down (ECSD).

No cure is known for ECSD in canonical simulations (cluster methods [3,4] do not help, yet see [5]). In the multicanonical ensemble [6] the probability for the energy density is constant, at least in the energy gap $e^o < e < e^d$ (e^o and e^d: energy densities of the coexisting low-temperature ordered phase and high-temperature disordered phase). In these flat-histogram methods [6–9], the canonical probability minimum in the energy gap ($\propto \exp[-\Sigma L^{D-1}]$) is filled by means of an iterative parameter optimization. A random walk is performed in the gap, that still suffers ECSD [10]. For the standard benchmark (the $Q = 10, D = 2$ Potts model [11]), the barrier of 10^4 spins was reached in 1992 [6]. The largest simulated system (to our knowledge) had 4×10^4 spins [7].

ECSD in flat-histogram simulations is probably understood [10]: on its way from e^d to e^o, the system undergoes several (four in $D = 2$) "transitions." First comes the condensation transition [10,12], at a distance of order $L^{-D/(D+1)}$ from e^d, where a macroscopic droplet of the ordered phase is nucleated. Decreasing e, the droplet grows to the point that, for periodic boundary conditions, it reduces its surface energy by becoming a strip [13]; see Fig. 1 (in $D = 3$, the droplet becomes a cylinder, then a slab [14]). At lower e the strip becomes a droplet of *disordered* phase. Finally, at the condensation transition close to e^o, we encounter the homogeneous ordered phase.

Here we present a method to simulate first order transitions without iterative parameter optimization nor energy random walk. We extend the configuration space as in hybrid Monte Carlo calculations [15]: to our N variables, σ_i (named spins here, but they could be atomic positions) we add N real momenta, p_i. The *microcanonical* ensemble for the $\{\sigma_i, p_i\}$ offers two advantages. First, microcanonical simulations [16] are feasible at any value of e within the gap. Second, we obtain fluctuation dissipation relations [Eqs. (5)–(7)] where the (inverse) temperature $\hat{\beta}$, a function of e and the spins, plays a role dual to that of e in the canonical ensemble. The e dependence of the mean value $\langle\hat{\beta}\rangle_e$, interpolated from a grid as it is almost constant over the gap, characterizes the transition. We test the method in the Q-states Potts model, for which we develop a cluster algorithm. We handle systems with 10^6 spins for $Q = 10$ in $D = 2$ and for $Q = 4$ in $D = 3$ [17].

Let U be the spin Hamiltonian. Our total energy is

$$\mathcal{E} = \sum_{i=1}^{N} \frac{p_i^2}{2} + U, \qquad (e \equiv \mathcal{E}/N, u \equiv U/N). \tag{1}$$

In the canonical ensemble, the $\{p_i\}$ are a trivial Gaussian bath decoupled from the spins. Note that, at inverse temperature β, one has $\langle e\rangle_\beta = \langle u\rangle_\beta + 1/(2\beta)$.

Microcanonically, the entropy density $s(e, N)$ is given by ($\sum_{\{\sigma_i\}}$: summation over spin configurations)

$$\exp[Ns(e, N)] = \int_{-\infty}^{\infty} \prod_{i=1}^{N} dp_i \sum_{\{\sigma_i\}} \delta(Ne - \mathcal{E}), \tag{2}$$

or, integrating out the $\{p_i\}$ using Dirac's delta function,

$$\exp[Ns(e, N)] = \frac{(2\pi N)^{N/2}}{N\Gamma(N/2)} \sum_{\{\sigma_i\}} \omega(e, u, N), \tag{3}$$

[$\omega(e, u, N) \equiv (e - u)^{(N-2)/2}\theta(e - u)$]. The step function, $\theta(e - u)$, enforces $e > u$. The microcanonical average at fixed e of any function of e and the spins, $O(e, \{\sigma_i\})$, is

$$\langle O\rangle_e \equiv \sum_{\{\sigma_i\}} O(e, \{\sigma_i\})\omega(e, u, N) \Big/ \sum_{\{\sigma_i\}} \omega(e, u, N). \tag{4}$$

The Metropolis simulation of Eq. (4), is straightforward.

Calculating ds/de from Eq. (3) we learn that [18]

$$\frac{ds(e,N)}{de} = \langle \hat{\beta}(e;\{\sigma_i\})\rangle_e, \qquad \hat{\beta}(e;\{\sigma_i\}) \equiv \frac{N-2}{2N(e-u)}. \tag{5}$$

Fluctuation dissipation follows by derivating Eq. (4):

$$\frac{d\langle O\rangle_e}{de} = \left\langle \frac{\partial O}{\partial e} \right\rangle_e + N[\langle O\hat{\beta}\rangle_e - \langle O\rangle_e\langle\hat{\beta}\rangle_e]. \tag{6}$$

As in the canonical case [19], an integral version of (6) allows to extrapolate $\langle O\rangle_{e'}$ from simulations at $e \geq e'$:

$$\langle O\rangle_{e'} = \frac{\langle O(e';\{\sigma_i\})\omega(e',u,N)/\omega(e,u,N)\rangle_e}{\langle \omega(e',u,N)/\omega(e,u,N)\rangle_e}. \tag{7}$$

For $e < e'$, configurations with $e < u < e'$, suppressed by a factor $(e'-u)^{N/2-1}$, are ignored in (7). Since we are limited in practice to $|e-e'| \leq \sqrt{\langle u^2\rangle_e - \langle u\rangle_e^2}/|d\langle u\rangle_e/de| \sim N^{-1/2}$, the restriction $e \geq e'$ can be dropped, as it is numerically negligible.

Let $I(e_1, e_2, \beta)$ be the e integral of $(\langle\hat{\beta}\rangle_e - \beta)$ from e_1 to e_2. The canonical probability density for e, $P_\beta^{(L)}(e) \propto \exp[N(s(e,N) - \beta e)]$, follows from

$$\log P_\beta^{(L)}(e_2) - \log P_\beta^{(L)}(e_1) = NI(e_1, e_2, \beta). \tag{8}$$

In the thermodynamically stable region (i.e., $d\langle\hat{\beta}\rangle_e/de < 0$), there is a single root of $\langle\hat{\beta}\rangle_e = \beta$, at the maximum of $P_\beta^{(L)}$. But (see Fig. 2) in the energy gap $\langle\hat{\beta}\rangle_e$ has a maximum and a minimum (L-dependent spinodals [1]), and there are several roots of $\langle\hat{\beta}\rangle_e = \beta$. The rightmost (leftmost) root is $e_L^d(\beta)$ ($e_L^o(\beta)$), a local maximum of $P_\beta^{(L)}$ corresponding to the disordered (ordered) phase. We define $e_L^*(\beta)$ as the *second rightmost* root of $\langle\hat{\beta}\rangle_e = \beta$.

At the finite-system (inverse) critical temperature, β_c^L, one has [20] $P_{\beta_c^L}^{(L)}(e_L^d(\beta_c^L)) = P_{\beta_c^L}^{(L)}(e_L^o(\beta_c^L))$, which is equivalent, Eq. (8) and Ref. [21], to Maxwell's construction:

$$0 = I(e_L^o(\beta_c^L), e_L^d(\beta_c^L), \beta_c^L), \tag{9}$$

(for large N, $\beta_c^\infty - \beta_c^L \propto 1/N$ [22]). Actually, at fixed e in the gap, also $\langle\hat{\beta}\rangle_e$ tends to β_c^∞ for large N. In the strip phase it converges faster than β_c^L; see Table I.

In a cubic box the surface tension is estimated as [25]

$$\Sigma^L = NI(e_L^*(\beta_c^L), e_L^d(\beta_c^L), \beta_c^L)/(2L^{D-1}). \tag{10}$$

$L \to \infty$ extrapolations $\Sigma^\infty - \Sigma^L \propto 1/L$ [26] are popular.

As for the specific heat, for $N \to \infty$ the inverse function of the canonical $\langle e\rangle_\beta$ is the microcanonical $\langle\hat{\beta}\rangle_e$:

$$\frac{d\langle u\rangle_\beta}{d\beta} \approx \left[\frac{1}{2\langle\hat{\beta}\rangle_e^2} + \frac{1}{d\langle\hat{\beta}\rangle_e/de}\right]_{e=\langle e\rangle_\beta} \equiv C_L(e). \tag{11}$$

For large N, $e_L^d(\beta_c^L)$, $e_L^o(\beta_c^L)$, $C_L(e_L^d(\beta_c^L))$, $C_L(e_L^d(\beta_c^L))$ tend to e^d, e^o, or the specific heat of the coexisting phases (we lack analytical hints about convergence rates).

We now specialize to the Potts model [11]. The spins $\sigma_i = 0, 1, \ldots, Q-1$, live in the $N = L^D$ nodes of a (hyper)cubic lattice of side L with periodic boundary conditions, and interaction $U = -\sum_{\langle ij\rangle}\delta_{\sigma_i,\sigma_j}$ (summation restricted to lattice nearest neighbors).

For the cluster method, we write our weight as $\tilde{\omega}(e,u,\kappa,N)\exp[-\kappa Nu]$ [see (4)], with κ a tunable parameter and $\tilde{\omega}(e,u,\kappa,N) = \omega(e,u,N)\exp[\kappa Nu]$. We express $\exp[-\kappa Nu]$ using bond variables [27] (adjacent spins connected by an *occupied* bond belong to the same *cluster* [2,28]). The conditional probability of bonds *given the* $\{\sigma_i\}$ is "adjacent spins are in the same cluster only if equal and, in that case, with probability $1-\exp[-\kappa]$." That of $\{\sigma_i\}$ *given the clusters* is "all spins in a cluster are equal, the weight of a given assignment being $\tilde{\omega}(e,u,\kappa,N)$." We accept a single-cluster [4] flip with Metropolis probability $p(e,\kappa) = \min\{1, \tilde{\omega}(e,u^{\text{final}},\kappa,N)/\tilde{\omega}(e,u^{\text{initial}},\kappa,N)\}$. Equations (5)–(7) tell that $\kappa = \langle\hat{\beta}\rangle_e$ maximizes $p(e,\kappa)$ (a short Metropolis run provides a first κ estimate). We obtain $\langle p(e,\kappa)\rangle_e > 0.99$ for $e \leq e^d$, and still $\langle p(e,\kappa)\rangle_{e=e^o} > 0.78$.

We simulated the ($Q = 10$, $D = 2$) Potts model [23], for $L = 32, 64, 128, 256, 512$, and 1024, sampling $\langle\hat{\beta}\rangle_e$ at 30 points evenly distributed in $-1.416\,66 \leq e \leq -0.45$. For $L = 512$, we made 15 extra simulations to resolve the

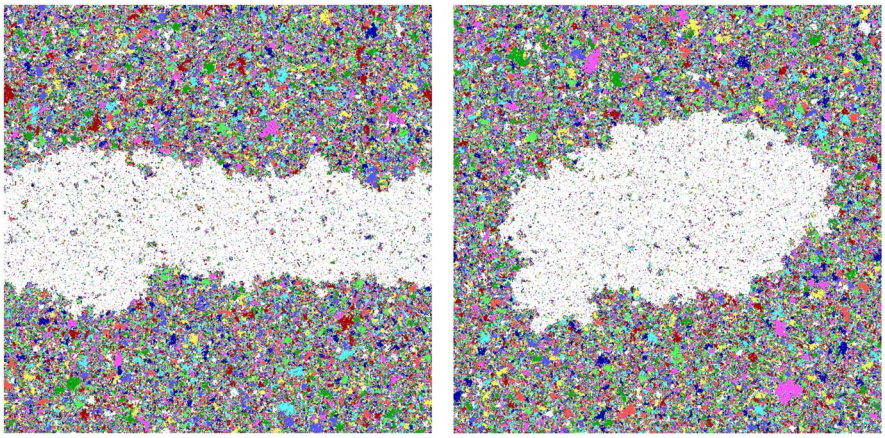

FIG. 1 (color online). $L = 1024$ equilibrium configurations for the ferromagnetic $Q = 10$, $D = 2$ Potts model with periodic boundary conditions, at the two sides of the droplet-strip transition, namely, $e = -0.809$ (left) and $e = -0.8$ (right). For details see text and Fig. 2.

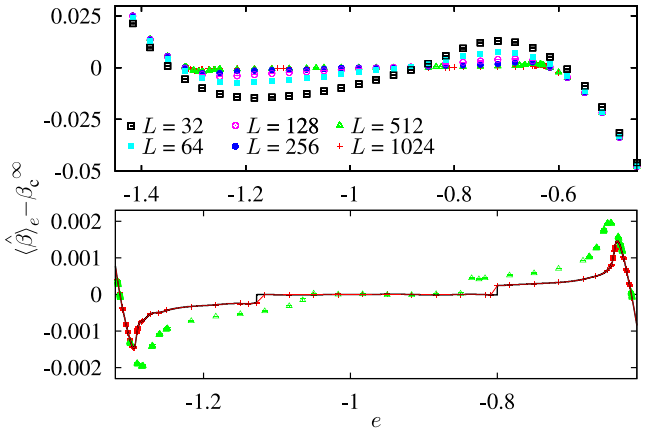

FIG. 2 (color online). Excess of $\langle\hat{\beta}\rangle_e$ over $\beta_c^{L=\infty}$ vs e, for the $Q = 10, D = 2$ Potts model and several system sizes. Bottom: magnification for $L \geq 512$. The flat central region is the strip phase (the strip width varies at fixed surface free energy). Lines (shown for $L = 1024$) are the two interpolations used for $L \geq 512$. We connect three independent cubic splines, in the strip phase and in its sides, either by a linear function or by a steplike $1/100$ power. Differences among the two interpolations are used to estimate the error induced by the uncertainty in the location of the strip-droplet transitions.

narrow spinodal peaks (26 extra points for $L = 1024$). For each e, we performed 2×10^6 elementary Monte Carlo steps (EMCS) [29], dropping the first 10% for thermalization [30]. A similar computation was carried out for the $(Q = 4, D = 3)$ Potts model (for details see Table I and [31]).

Our $\langle\hat{\beta}\rangle_e$ in $D = 2$ is shown in Fig. 2. Data reweighting (7) were used only to reconstruct the narrow spinodal peaks. To find the roots of $\langle\hat{\beta}\rangle_e = \beta$, or to calculate the integrals in Eqs. (9) and (10), we interpolated $\langle\hat{\beta}\rangle_e$ using a cubic spline [32]. For $L \geq 512$ the strip-droplet transitions produce two "jumps" in $\langle\hat{\beta}\rangle_e$, causing oscillations in the interpolation (Gibbs phenomenon), cured by either of two interpolation schemes; see Fig. 2.

We obtain β_c^L, Σ^L, $e_L^o(\beta_c^L)$, $e_L^d(\beta_c^L)$, $C_L(e_L^o(\beta_c^L))$, and $C_L(e_L^d(\beta_c^L))$ from the interpolation of $\langle\hat{\beta}\rangle_e$ and of $d\langle\hat{\beta}\rangle_e/de$; see (6). The jackknife method [28] was used to estimate statistical errors (the ith block is obtained interpolating the ith jackknife blocks for $\langle\hat{\beta}\rangle_e$). There are also interpolation and integration errors. Fortunately, errors of order ϵ in $e_L^o(\beta_c^L)$ or $e_L^d(\beta_c^L)$ yield errors of order ϵ^2 in β_c^L: the main error in β_c^L is the quadrature error for $\langle\hat{\beta}\rangle_e$ divided by the latent heat. On the other hand, $e_L^*(\beta_c^L)$ is near to the droplet-strip transition, and an error on it does have an impact on Σ_L.

In Table I are our results for $(D = 2, Q = 10)$ and the known large L limits. A fit for c in $\beta_c^\infty - \beta_c^L = c/L^D$ [22] is unacceptable for $L \geq 32$ (χ^D/d.o.f. $= 14.32/4$), but good for $L \geq 64$ (χ^D/d.o.f. $= 1.77/3$): our accuracy allows to detect subleading corrections. A fit $e_L^o(\beta_c^L) - e^o = b_1/L^D$ works only for $L \geq 256$ (χ^2/d.o.f. $= 1.90/2$; for $e_L^d(\beta_c^L)$ we get χ^2/d.o.f. $= 1.41/2$). However, $\beta^{\text{strip},L}$ (see caption of Table I) is compatible with β_c^∞ for $L \geq 256$. Then, the simplest strategy to get β_c^∞ and the latent heat is (1) for L large enough to display a strip phase, locate it with short runs, (2) get $\beta^{\text{strip},L}$ accurately, and (3) find the leftmost (rightmost) root for $\langle\hat{\beta}\rangle_e = \beta^{\text{strip},L}$.

As for Σ^L, the inequality $\Sigma^\infty \leq 0.047\,350\,5$ [24] (equality under the hypothesis of complete wetting) was violated by $1/L$ extrapolations performed with $L \leq 100$ [6]. The data for $L \leq 256$ in Table I extrapolate above $0.047\,350\,5$ but drop below for $L \geq 512$. Indeed, the consistency of our results for β_c^L implies that the integration error for $\langle\hat{\beta}\rangle_e$ is (at most) 2×10^{-6} for $L = 1024$. Hence, the integration error for Σ_L is at most 10^{-3}. Adding it to the difference between the linear and the steplike interpolation, Fig. 2, we

TABLE I. Size dependent estimates of quantities characterizing the first-order transition [Σ^L, from (10)], for the $Q = 10, D = 2$ Potts model (top) and $Q = 4, D = 3$ (bottom). Errors are jackknife's. Also shown is $\beta^{\text{strip},L}$: $\langle\hat{\beta}\rangle_{e=-0.95}$ $(D = 2)$ or $\langle\hat{\beta}\rangle_{e=-0.764\,443}$ $(D = 3)$. Superscript $A(B)$: results obtained with the linear (steplike) interpolation scheme; see Fig. 2.

L^D	β_c^L	Σ^L	$-e_L^o(\beta_c^L)$	$-e_L^d(\beta_c^L)$	$-C_L(e_L^o(\beta_c^L))$	$-C_L(e_L^d(\beta_c^L))$	$\beta^{\text{strip},L}$
32^2	1.423 082 (17)	0.051 74(9)	1.331 8(2)	0.573 6(3)	5.13(13)	3.99(7)	1.420 28(7)
64^2	1.425 287 (9)	0.050 24(1 1)	1.322 0(2)	0.599 9(2)	6.44(17)	5.78(19)	1.424 79(4)
128^2	1.425 859 (7)	0.049 225 (14)	1.316 76(1 6)	0.611 64(1 6)	7.4(3)	7.8(3)	1.425 92(2)
256^2	1.426 021 (5)	0.048 8(2)	1.314 78(8)	0.615 78(8)	8.0(3)	8.7(4)	1.426 06(2)
$512^{2(A)}$	1.426 051 (4)	0.047 3(3)	1.313 92(6)	0.617 10(4)	8.6(4)	9.1(4)	1.426 048 (12)
$512^{2(B)}$	1.426 048 (4)	0.046 7(4)	1.313 90(6)	0.617 08(5)	8.6(4)	9.1(4)	1.426 048 (12)
$1024^{2(A)}$	1.426 059 9(19)	0.043 0(3)	1.313 75(3)	0.617 48(3)	9.7(5)	8.7(4)	1.426 066 (9)
$1024^{2(B)}$	1.426 060 0(18)	0.042 4(2)	1.313 75(3)	0.617 48(3)	9.7(5)	8.7(4)	1.426 066 (9)
∞^2	1.426 062 4 ... [23]	$\Sigma^\infty \leq 0.047\,35$ [24]	1.313 636 ... [23]	0.617 58 ... [23]	...	...	1.426 062 4 ... [23]
8^3	0.627 394 (7)	0.005 591 (10)	1.155 3(7)	0.514 12(1 2)	23.0(5)	3.856 (16)	0.626 25(4)
16^3	0.628 440 (3)	0.007 596 (6)	1.118 9(4)	0.518 18(5)	30.1(8)	3.620 (13)	0.626 687 (15)
32^3	0.628 595 7(10)	0.009 824 (6)	1.107 51(1 5)	0.522 066 (16)	34.2(9)	4.019 (17)	0.627 889 (6)
64^3	0.628 613 3(7)	0.011 557 (6)	1.105 42(8)	0.522 831 (8)	33.2(9)	4.11(2)	0.628 621 (3)
$128^{3(A)}$	0.628 623 7(5)	0.011 778 (7)	1.105 48(3)	0.522 93(2)	35.4(9)	4.25(17)	0.628 6206 (10)
$128^{3(B)}$	0.628 623 9(5)	0.01 1674 (9)	1.105 49(2)	0.522 93(2)	35.4(9)	4.25(17)	0.628 620 6(10)

obtain $\Sigma^{L=1024} = 0.043(2)$, which is slightly below 0.047 350 5.

As for $(Q = 4, D = 3)$, see Table I, $\beta^{\mathrm{strip},L}$ has converged (within accuracy) for $L \geq 64$. Hence, our preferred estimate is $\beta_c^\infty = 0.628\,620\,6(10)$, that may be compared with Janke and Kapler's $\beta_c^\infty = 0.628\,63(2)$ [17]. Accordingly, we find $e^o(\beta^{\mathrm{strip},L}) = -1.105\,37(4)$, $e^d(\beta^{\mathrm{strip},L}) = -0.522\,91(2)$, $C_L(e^o(\beta^{\mathrm{strip},L})) = 35.4(9)$, and $C_L(e^d(\beta^{\mathrm{strip},L})) = 4.24(18)$. The reader will note that $\beta_c^{L=128}$ is far too high (for instance, from the χ^2/d.o.f. of the extrapolation $\beta_c^L = \beta_c^\infty + cL^{-D}$). Therefore, the integration error is $\sim 4 \times 10^{-6}$ (larger than the statistical one), which provides a bound for the error in the surface tension: $\Sigma^{L=128} = 0.011\,8(4)$. This is compatible with $\Sigma^{L=64}$, and provides a reasonable Σ^∞.

We propose a microcanonical strategy for the Monte Carlo simulation of first-order phase transitions. The method is demonstrated in the standard benchmarks: the $Q = 10, D = 2$ Potts model (where we compare with exact results) and the $Q = 4, D = 3$ Potts model. For both, we obtain accurate results in systems with more than 10^6 spins. Envisaged applications include first-order transitions with quenched disorder [17,33], colloid crystallization [34], peptide aggregation [35] and the condensation transition [12].

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[29] Our EMCS was $\max\{10, N/(\langle \mathcal{N}\rangle_e \langle p(e,\kappa)\rangle_e)\}$ cluster flip attempts. $\mathcal{N}$ is the number of spins in the traced cluster ($\langle \mathcal{N}\rangle_{e^d}$ is N independent, but $\langle \mathcal{N}\rangle_{e^o} \propto N$). Every EMCS we flip on average at least N spins.
[30] The largest (in EMCS) *exponential* autocorrelation times, for $\hat{\beta}$ and the squared magnetization, arise at the droplet-strip transition: $\{\tau_{\hat{\beta}}, \tau_{M^2}/100\} = \{85(8), 26.7(7)\}^{L=256}$, $\{174(7), 136(3)\}^{L=512}$, and $\{176(6), 411(8)\}^{L=1024}$.
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[32] Not the so-called natural spline. We fixed the derivative at the first (last) e value, from a 3 points parabolic fit.
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