

Multicanonical multigrid Monte Carlo method

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To further improve the performance of Monte Carlo simulations of first-order phase transitions we propose to combine the multicanonical approach with multigrid techniques. We report tests of this proposition for the d -dimensional Φ^4 field theory in two different situations. First, we study quantum tunneling for $d = 1$ in the continuum limit, and second, we investigate first-order phase transitions for $d = 2$ in the infinite volume limit. Compared with standard multicanonical simulations we obtain improvement factors of several, and of about one order of magnitude, respectively.

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At first-order phase transitions, standard Monte Carlo simulations in the canonical ensemble exhibit a supercritical slowing down [1]. Here extremely large autocorrelation times are caused by strongly suppressed transitions between coexisting phases which, on finite periodic lattices, can only proceed via mixed phase configurations containing two interfaces. Since the probability P of such configurations is suppressed by a factor $\exp(-2\sigma L^{d-1})$, where σ is the interface tension and L^{d-1} the cross section of the system, the autocorrelation times in the simulation grow exponentially with the size of the system, $\tau \propto \exp(2\sigma L^{d-1})$.

A way to overcome this problem, known as umbrella [2] or multicanonical [3] sampling, is to simulate an auxiliary distribution P' in which the mixed phase configurations have the same weight as the pure phases and canonical expectations are computed by reweighting [4]. Several tests for various models [5] have demonstrated that this method works well in practice and reduces supercritical exponential slowing down to a powerlike behavior with $\tau \propto V^\alpha = L^{d\alpha}$, where $\alpha \approx 1$. While this is clearly an important step forward, the remaining slowing down problem is still severe. In most cases it is even worse than for standard (e.g., Metropolis or heat-bath) Monte Carlo simulations of critical phenomena [6].

For the latter applications several update algorithms have been developed which greatly reduce or even completely eliminate the critical slowing down problem [7]. In addition to overrelaxation and cluster methods, an important class of such algorithms are multigrid techniques [8–10]. Here the general strategy is to perform collective updates on different length scales by visiting various coarsened grids in a systematic, recursively defined way, generally known as the V or W cycle [11].

Because of their conceptual simplicity both the multicanonical reweighting approach and the multigrid update techniques are quite generally applicable. The purpose of this paper is to show that the two approaches can easily be combined and give a much better performance than each component alone. We report tests of this combination for the Φ^4 lattice field theory with a negative mass term in two conceptually different situa-

tions. We first consider the quantum-mechanical tunneling problem in one dimension and study the performance of the new algorithm in the continuum limit. We then discuss field-driven first-order phase transitions in the two-dimensional case and investigate the behavior of the multicanonical multigrid algorithm in the infinite volume limit.

For Potts models an interesting different approach was proposed only recently in Ref. [12]. Here the idea is to combine a multicanonical demon algorithm with cluster update methods in a hybridlike fashion.

The basic idea of the multicanonical approach is to sample the mixed phase configurations with the same statistical weight as the configurations of the pure phases. At a field-driven first-order phase transition this can always be achieved by a suitably chosen reweighting factor $w^{-1}(m) \equiv \exp[-f(m)]$, where $m = \sum_i \Phi_i/V$ is the average field. In a temperature-driven transition, m has simply to be replaced by the average energy. Starting from an initial guess based on experience or on some analytical approximation, a few iterations are usually sufficient to adjust this factor. Once it is fixed, canonical expectation values $\langle \mathcal{O} \rangle_{\text{can}}$ of any observable \mathcal{O} can be computed from the basic reweighting formula

$$\langle \mathcal{O} \rangle_{\text{can}} = \frac{\langle w\mathcal{O} \rangle}{\langle w \rangle}, \quad (1)$$

where $\langle \rangle$ without subscripts denote expectation values in the multicanonical distribution. To update field values with a Metropolis algorithm in the multicanonical approach, we consider as usual local moves $\Phi_i \rightarrow \Phi_i + \Delta\Phi_i$ and compute the energy difference ΔE . The decision of whether such moves are accepted or not, however, is now based on the value of $\Delta E + f(m + \Delta\Phi_i/V) - f(m)$.

The basic idea of multigrid techniques is to perform updates on different length scales. Using the so-called piecewise constant interpolation scheme, this amounts, in the equivalent unigrid viewpoint, to proposing moves for blocks of $1, 2^d, 4^d, \dots, V = L^d = 2^{nd}$ adjacent variables in conjunction, with the sequence of length scales $2^k, k = 0, \dots, n$ chosen in a specific, recursively defined order.

Particular successful sequences are the so-called V cycle with $k = 0, 1, \dots, n-1, n, n-1, \dots, 1, 0$ and the W cycle, whose graphical representation looks like the letter W (for $n = 3$, e.g., this is $0, 1, 2, 3, 2, 3, 2, 1, 2, 3, 2, 3, 2, 1, 0$, and for large n the W looks more and more like a “fractal”). In a canonical simulation the update at level k thus consists in considering a common move $\Delta\Phi$ for all 2^{kd} variables of one block, $\Phi_i \rightarrow \Phi_i + \Delta\Phi$, $i \in \text{block}$.

The modifications for a multicanonical multigrid simulation are quite trivial. Since at level k the proposed move would change the average field by $2^{kd}\Delta\Phi/V$, the decision of acceptance is now simply to be based on the value of $\Delta E + f(m + 2^{kd}\Delta\Phi/V) - f(m)$, with ΔE computed as in the canonical case. For didactic reasons we have emphasized here the conceptually simpler *unigrid* viewpoint. It should be stressed that in the recursive *multigrid* formulation, which can be implemented more efficiently (similar to the fast-Fourier transformation FFT), the multicanonical modification is precisely the same.

We have tested the multicanonical multigrid algorithm for the scalar Φ^4 lattice field theory in $d = 1$ and $d = 2$ dimensions, defined by the partition function

$$Z = \prod_i^{L^d} \left[\int_{-\infty}^{\infty} d\Phi_i/A \right] \exp \left[-\epsilon \sum_{i=1}^{L^d} \left(\frac{1}{2\epsilon^2} (\nabla\Phi_i)^2 - \frac{\mu^2}{2} \Phi_i^2 + g\Phi_i^4 \right) \right], \quad (2)$$

with $A = \sqrt{2\pi\epsilon}$ and $\mu^2, g > 0$. We always impose periodic boundary conditions. For $d = 1$ we keep $L\epsilon = \beta$ fixed. Here the model describes the quantum statistics of a particle tunneling back and forth in a double-well potential in contact with a heat bath at temperature $T = 1/\beta$ [13]. At fixed β the limit $L \rightarrow \infty$ corresponds to the *continuum* limit. For $d \geq 2$ we put $\epsilon = 1$. Here reflection symmetry is spontaneously broken for all $\mu^2 > \mu_c^2(g) > 0$ as $L \rightarrow \infty$, which is now the *infinite volume* limit. Consequently, if a term $h \sum_i \Phi_i$ is added to the energy, the system exhibits a first-order phase transition driven by the field h .

Even though in the one-dimensional case no spontaneous symmetry breaking occurs, the numerical difficulties are quite similar. This is due to the fact that, for small quartic coupling g , tunneling events are strongly suppressed by a factor $\sim \exp(-\text{const}/g)$, which plays a role similar to the factor $\exp(-2\sigma L^{d-1})$ at a first-order phase transition. The important difference is, of course, that the suppression factor stays roughly constant in the continuum limit, while at a first-order phase transition it rapidly decreases in the infinite volume limit. Nevertheless, for small values of g , analogous slowing down problems in canonical simulations of the quantum problem are notorious, and a number of modified Monte Carlo schemes have been proposed in the past; see e.g. Refs. [14, 15]. None of these techniques, however, is general enough to be easily adapted to different potential shapes.

To evaluate the performance of the multicanonical multigrid algorithm, we have recorded the time series for several observables and studied their autocorrelation times. In this paper we shall concentrate on the aver-

age field $m = \sum_i \Phi_i/V$, which reflects most directly the tunneling process.

In previous investigations [5] emphasis was placed on the *exponential* autocorrelation time $\tau_m^{(0)}$ of m , i.e., directly on the multicanonical dynamics. While this nicely illustrated the absence of exponential slowing down, it is not immediately clear how the remaining autocorrelations enter into the error estimates for *canonical* expectation values computed according to (1). To be precise, we are interested in the variance $\Delta^2 = \sigma_{\hat{O}}^2 = \langle \hat{O}^2 \rangle - \langle \hat{O} \rangle^2$ of the (weakly biased) estimator for $\langle \mathcal{O} \rangle_{\text{can}}$, $\hat{O} = \sum_{i=1}^{N_m} w(m_i) \mathcal{O}_i / \sum_{i=1}^{N_m} w(m_i) \equiv \overline{w_i \mathcal{O}_i / w_i}$, if N_m (multicanonical) measurements are performed. To facilitate a direct comparison with canonical simulations, we hence *define* for multicanonical simulations an effective autocorrelation time τ^{eff} by the standard error formula for N_m correlated measurements,

$$\Delta^2 = \sigma_{\text{can}}^2 2\tau^{\text{eff}}/N_m, \quad (3)$$

where $\sigma_{\text{can}}^2 = \langle \mathcal{O}_i^2 \rangle_{\text{can}} - \langle \mathcal{O}_i \rangle_{\text{can}}^2$ is the variance of the canonical distribution of single measurements, which can be computed in a multicanonical simulation by using Eq. (1). The squared error Δ^2 can be estimated either by blocking or better by jack-knife blocking [16] procedures, or by applying standard error propagation to the variance of $\hat{O} = \overline{w_i \mathcal{O}_i / w_i}$, which involves the (multicanonical) variances and covariances of $w_i \mathcal{O}_i$ and w_i , and the three associated autocorrelation times $\tau_{\mathcal{O}, \mathcal{O}} \equiv \tau_{\mathcal{O}}$, $\tau_{w \mathcal{O}; w \mathcal{O}} \equiv \tau_{w \mathcal{O}}$, and $\tau_{w \mathcal{O}; \mathcal{O}} \equiv \tau_{w; \mathcal{O}}$ [17]. By symmetry, for $\mathcal{O} = m$ this simplifies to

$$\Delta^2 = \frac{\langle w_i m_i; w_i m_i \rangle}{\langle w_i \rangle^2} \frac{2\tau_{wm}}{N_m} \equiv \sigma_{\text{muca}}^2 \frac{2\tau_{wm}}{N_m}, \quad (4)$$

where $\langle x; y \rangle \equiv \langle xy \rangle - \langle x \rangle \langle y \rangle$ and $\tau_{x; y} = 1/2 + \sum_k \langle x_0; y_k \rangle / \langle x_0; y_0 \rangle$ is the integrated autocorrelation time of multicanonical measurements. In this way properties of the multicanonical distribution (given by σ_{muca}^2) are disentangled from properties of the update algorithm (given by τ_{wm}). Note that in $\tau^{\text{eff}} = (\sigma_{\text{muca}}^2 / \sigma_{\text{can}}^2) \tau_{wm}$, it is the autocorrelation time of $w(m)m$ that enters and not that of m , as previously investigated.

Let us first discuss our results for the quantum mechanical case in $d = 1$, where we shall confine ourselves to the case $\mu^2 = 1.0$, $g = 0.04$, and $\beta = 10$. This choice of parameters may perhaps be better characterized by the first few energy eigenvalues (obtained by a numerical integration of the associated Schrödinger equation), $E_0 = -0.913371$, $E_1 = -0.892348$, $E_2 = 0.029846$, and $E_3 = 0.37813$, or by the probability ratio $P_{\text{min}}/P_{\text{max}} = P(0)/P_{\text{max}} \approx 1.9 \times 10^{-3}$, where $P(m)$ is the probability distribution of the magnetization (or, in the present interpretation, of the average path). In a canonical simulation it would consequently be about 500 times harder to sample configurations with $m = 0$ than configurations contributing to the peaks of $P(m)$. To set up the multicanonical reweighting factor we started from a variational approximation [18] that works quite well for not too large β values and is known to provide locally a lower bound on $P(m)$ [19]. Alternatively, as the distribution depends only weakly on L , one could also use the distribution

for small L (which is quite easy to generate by standard techniques) as input for the other simulations. Since the m -values vary continuously, we introduced bins of size $\Delta m = 0.02$ to store the weight factor $w(m)$. A single short run was usually sufficient to improve the initial guess such that the multicanonical distribution $P'(m)$ had the desired flat shape, $P'(m) \approx \text{const}$, between the two peaks.

In this way we performed multicanonical Metropolis and multigrid simulations for $L = 4, 8, 16, 32, 64, 128$, and 256 , and using the multigrid update also for $L = 512$. In the multigrid case we investigated both the V cycle (using $n_{\text{pre}} = n_{\text{post}} = 1$ presweeps, respectively, postsweeps [8–11]) and the W cycle (using $n_{\text{pre}} = n_{\text{post}} = 1$ as well as $n_{\text{pre}} = 1, n_{\text{post}} = 0$). In the log-log plot of Fig. 1 we show our results for τ^{eff} of the multicanonical Metropolis and W cycle (without postsweeps) update algorithm, and for comparison also previous results [20] for the canonical counterparts. We see that canonical and multicanonical simulations exhibit qualitatively the same behavior in the continuum limit $L \rightarrow \infty$. For both distributions, the Metropolis update leads to a power-law growth $\tau \propto L^z$ with $z \approx 2$, while for the W cycle update the autocorrelation times stay roughly constant [21]. Here it is the overall scale which is reduced in the multicanonical simulation. For our choice of parameters we obtain an improvement factor of about 60 (30) for the Metropolis (W cycle) update. For smaller g , since this factor is essentially given by the inverse of the suppression factor $\exp(-\text{const}/g)$, we found the multicanonical Metropolis update to be more favorable than the canonical W cycle for reasonably large L . Eventually, however, there will always be a crossover at some L . For $g = 0.04$, if we compare the Metropolis update and the W cycle in the multicanonical simulation we obtain an improvement factor of about 50 000 for $L = 512$.

In the continuum limit the distribution $P(m)$ and the ratio $P_{\text{min}}/P_{\text{max}}$ stay roughly constant. This implies that the multicanonical approach can only give an improvement factor which is independent of L . In this case it is the update algorithm that plays the dominant role asymptotically for large L , while the multicanonical reweighting procedure sets the overall scale. The relative importance of the two approaches is just reversed at first-order phase transitions when the infinite volume limit is

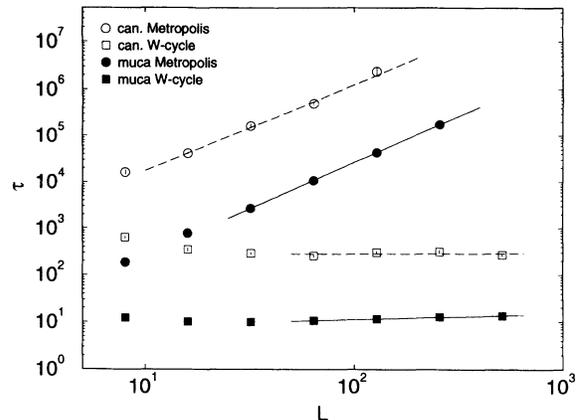


FIG. 1. Effective autocorrelation times τ^{eff} (in units of sweeps, respectively, cycles) for the model (2) in $d = 1$ as a function of lattice size L with $L\epsilon = \beta = 10$, $\mu^2 = 1$, $g = 0.04$ for different Monte Carlo algorithms. The canonical data are taken from Ref. [20].

considered.

As a test case we have studied the model (2) with $\epsilon = 1$. For this model the line of second-order phase transitions separating the broken and unbroken phase in the μ^2 - g plane has recently been determined by Toral and Chakrabarti [22]. Here we concentrate on the first-order phase transition between the two ordered phases at $g = 0.25$ and $\mu^2 = 1.30$, which is sufficiently far away from the critical point at $\mu_c^2 = 1.265(5)$ [22] to display the typical behavior already for quite small lattices. A sensitive measure of the strength of the transition is the interface tension σ_{oo} between the + and - phase, which turns out [17] to be $\sigma_{oo} = 0.034\,43(47)$ (for comparison, about the same value is found for the order-disorder interface tension in the two-dimensional q -state Potts model with $q = 9$, where $\sigma_{od} = 0.033\,55\dots$ [23]). We performed multicanonical simulations using the Metropolis update and the W cycle without postsweeps for lattices of size $V = L^2$ with $L = 8, 16$, and 32 . With the multigrid algorithm, due to the improved performance, we were also able to study lattices of size $L = 64$. Here each time series contains a total of 10^6 measurements taken every n_e th sweep, after discarding $10^4 n_e$ sweeps for thermaliza-

TABLE I. Autocorrelation times (in units of sweeps, respectively, cycles) for the multicanonical simulation using the standard Metropolis (M) or multigrid W cycle (W) update algorithm.

		$L = 8$	$L = 16$	$L = 32$	$L = 64$
$\tau_m^{(0)}$	M	212(12)	668(23)	3120(200)	
	W	11.30(32)	37.2(2.0)	148(11)	746(62)
τ_m	M	204.4(4.0)	690(11)	2984(63)	
	W	10.88(12)	34.69(76)	150.0(4.0)	758(37)
$\tau_{wm}^{(0)}$	M	209(12)	655(31)	2880(190)	
	W	11.34(33)	36.9(2.0)	146(13)	600(120)
τ_{wm}	M	171.1(3.4)	509.8(8.9)	1840(40)	
	W	9.82(11)	27.58(59)	96.6(2.4)	374(23)
τ^{eff}	M	322.7(6.1)	1258(21)	6050(120)	
	W	18.51(20)	67.4(1.3)	321.9(7.6)	1724(86)

tion. The number of sweeps between measurements, n_e , was adjusted in such a way that in each simulation the measurements of wm maximally had an autocorrelation time of 50, i.e., the length of each time series was at least 20 000 τ_{wm} .

A few of our results are collected in Table I, where we give the integrated and exponential autocorrelation times of m and $w(m)m$ as well as τ^{eff} according to Eq. (3) for both update algorithms (in units of sweeps, respectively, cycles). We see that integrated and exponential autocorrelation times for m agree well with each other, showing that the corresponding autocorrelation function can be approximated by a single exponential. For wm we obtain values for $\tau^{(0)}$ that are consistent with those for m within error bars. The integrated autocorrelation times, however, are significantly smaller, implying that the autocorrelation function is composed of many different modes. We also observe that the difference between τ_{wm} and τ^{eff} can be quite appreciable. From $L = 8$ to $L = 64$ the ratio $\tau^{\text{eff}}/\tau_{wm} = \sigma_{\text{muca}}^2/\sigma_{\text{can}}^2$ varies from

about 1.9 to 4.6, reflecting the varying probability distribution shapes with increasing L .

By fitting τ^{eff} to a power law, $\tau^{\text{eff}} \propto V^\alpha$, we obtain for both update algorithms an exponent of $\alpha \approx 1.15$, i.e., in this case it is thus the multigrid update that reduces the overall scale. The autocorrelation times of the W cycle are reduced by a roughly constant factor of about 20 as compared with the Metropolis algorithm. Of course, for a fair comparison we should also take into account that a W cycle requires more elementary operations than a Metropolis sweep [8]. Such a work estimate, however, depends on many details of the implementation, and it is hence difficult to give generally valid figures. With our implementations on a CRAY Y-MP we obtained a *real time* improvement factor of about 10.

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