Collective Monte Carlo Updating for Spin Systems

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(Received 13 October 1988)

A Monte Carlo algorithm is presented that updates large clusters of spins simultaneously in systems at and near criticality. We demonstrate its efficiency in the two-dimensional O(n) σ models for $n=1$ (Ising) and $n=2$ (x-y) at their critical temperatures, and for $n=3$ (Heisenberg) with correlation lengths around 10 and 20. On lattices up to 128^2 no sign of critical slowing down is visible with autocorrelation times of 1–2 steps per spin for estimators of long-range quantities.

PACS numbers: 05.50.+q, 11.15.Ha

Recently Swendsen and Wang (SW)[1] have put forward a novel Monte Carlo algorithm for Potts spin models using ideas from percolation theory.[2] Whole clusters of spins are thus enabled to move in one step, and consequently critical slowing down is greatly improved. The information residing in the clusters can also be used to construct reduced variance estimators[3] for physical observables. The combination of both advantages was quite useful in recent studies of the physics of the four-dimensional φ^4 theory in the Ising limit.[4] In Ref. 16, the sign of a variable length φ^4 field in two dimensions has been updated by SW, leading to the expected acceleration. The SW method has been developed further in two directions: In Ref. 5 it is claimed that critical slowing down in the two-dimensional Ising model is eliminated completely by a synthesis of SW with multigrid ideas. Other research[6-8] was motivated by the desire to simulate models other than Potts systems, and, in particular, ones with continuous fields such as the x-y model. There the results on slowing down have been essentially negative so far; improved estimators could be exploited in Ref. 6 for the O(3) σ model albeit only for a variant action. In this Letter we present another percolation-inspired algorithm that allows the simulation of spin models with standard actions. It is tested numerically in the two-dimensional Ising and x-y models at criticality. Preliminary tests are also performed for the O(3) model.

The algorithm.—For simplicity, we only consider O(n) σ models on a cubic lattice Λ of $|\Lambda|$ sites with periodic boundary conditions,

$$Z=\prod_{x\in\Lambda}\int_{S_{n-1}} d\sigma_x \exp\left\{\beta\sum_{\langle xy\rangle}\sigma_x\cdot\sigma_y\right\}, \tag{1}$$

where σ_x are unit vectors in $\mathbb{R}^n$, β is the inverse coupling temperature, and the sum runs over all nearest-neighbor pairs. An important concept for the new algorithm is the generalization of the spin-flip operation $\sigma_x\to-\sigma_x$ in the Ising model. For $n\geq 2$ and any $\mathbf{r}\in S_{n-1}$ we define it as the reflection with respect to the hyperplane orthogonal to $\mathbf{r}$

$$R(\mathbf{r})\sigma_x=\sigma_x-2(\sigma_x\cdot\mathbf{r})\mathbf{r}. \tag{2}$$

Clearly this is an idempotent operation[9]

$$R(\mathbf{r})^2=1, \tag{3}$$

and the action in (1) is invariant under global R transformations

$$[R(\mathbf{r})\sigma_x]\cdot[R(\mathbf{r})\sigma_y]=\sigma_x\cdot\sigma_y. \tag{4}$$

An elementary cluster update step now consists of the following sequence of operations:

(a) Choose a random reflection $\mathbf{r}\in S_{n-1}$ and a random lattice site $x\in\Lambda$ as the first point of a cluster $c\in\Lambda$ to be built. (b) Flip $\sigma_x\to R(\mathbf{r})\sigma_x$ and mark x. (c) Visit all links connecting $x\in c$ to its nearest neighbors y. The bond $\langle xy\rangle$ is activated with probability

$$\begin{aligned}P(\sigma_x,\sigma_y)&=1-\exp(\min\{0,\beta\sigma_x\cdot[1-R(\mathbf{r})]\sigma_y\})\\&=1-\exp\{\min[0,2\beta(\mathbf{r}\cdot\sigma_x)(\mathbf{r}\cdot\sigma_y)]\},\end{aligned} \tag{5}$$

and, if this happens, σ_y is flipped, and y is marked and adjoined to c. (d) Continue iteratively in the same way for all bonds leading to unmarked neighbors of newly adjoined sites until the process stops. Ergodicity of processes (a) to (d) is guaranteed by the fact that there is always a nonvanishing probability that c consists of only one site, and that there is always a reflection connecting any two spins. Then each configuration may be reached in principle by at most $|\Lambda|$ update steps. Detailed balance is also easily seen to be fulfilled. We consider two configurations $\{\sigma_x\}$ and $\{\sigma'_x\}$ that differ by a flip $R(\mathbf{r})$ on a cluster c. The transition probabilities W obey

$$\frac{W(\{\sigma_x\}\to\{\sigma'_x\})}{W(\{\sigma'_x\}\to\{\sigma_x\})}=\prod_{\langle xy\rangle\in\partial c}\frac{1-P(R(\mathbf{r})\sigma_x,\sigma_y)}{1-P(R(\mathbf{r})\sigma'_x,\sigma'_y)}=\exp\left\{\beta\sum_{\langle xy\rangle\in\partial c}\sigma_x\cdot[R(\mathbf{r})-1]\sigma_y\right\}=\exp\left\{\beta\sum_{\langle xy\rangle}(\sigma'_x\cdot\sigma'_y-\sigma_x\cdot\sigma_y)\right\}, \tag{6}$$

where the surface ∂c of c consists of all links $\langle xy\rangle$ with $x\in c$ and $y\notin c$. All probabilities for activating bonds *within* c are the same starting from $\{\sigma_x\}$ or $\{\sigma'_x\}$ because of (3) and (4). To grow a specific cluster c, its surface bonds must *not*

be activated, and these probabilities supply the noncanceling factors in (6). Note that $R(\mathbf{r})$ appears in the left argument of $P(\ldots,\ldots)$ because σ_x has already been flipped when $\langle xy\rangle \in \partial c$ is probed. The desired action-energy difference in the exponent finally arises in a way similar to the Metropolis algorithm.

The adequacy of discrete flips for continuous spins may seem surprising at first sight. Intuitively, it works for the following reason: If we choose $\mathbf{r}$ and start a cluster in a region where spins are nearly orthogonal to $\mathbf{r}$, then (2) is effectively a small deformation. Bond probabilities (5) typically lead to small clusters in this case. If $\mathbf{r}$ is (anti)parallel to the local spin direction, the cluster tends to grow until it reaches an energetically acceptable surface.

For the Ising case ($n=1$), the bond activation probabilities that we use are the same as in the SW process [$1-\exp(-2\beta)$ if the original spins are parallel and 0 otherwise]. The connection between both algorithms becomes clearer by consideration of a less efficient but equivalent implementation of the new algorithm.[10] It consists of our first activating all bonds of the lattice with the appropriate probabilities and decomposing all sites into clusters. These are the SW clusters c_{SW}. Then we pick a random site x, flip the cluster connected to x, and ignore the remaining ones. The one cluster that we flip is reached from any of its sites, and consequently the probability of our choosing a particular SW cluster is given by the fraction $|c_{\mathrm{SW}}|/|\Lambda|$ of sites it occupies. The mean size of flipped clusters is

$$\langle |c| \rangle = \left\langle \frac{1}{|\Lambda|} \sum_{c_{\mathrm{SW}}} |c_{\mathrm{SW}}|^2 \right\rangle , \tag{7}$$

which for $n=1$ is the improved estimator[6] for the magnetic susceptibility χ. We thus expect (and find)

$$\chi = \frac{1}{|\Lambda|} \left\langle \left(\sum_{x\in\Lambda} \sigma_x \right)^2 \right\rangle = \langle |c| \rangle \tag{8}$$

to hold. The average size of SW clusters in the critical Ising model, on the other hand, is seen to be constant from data in Ref. 6 since their number grows proportional to L^2. We conclude that with our variation of the SW algorithm for $n=1$, we invest a relatively higher fraction of the central processing unit time into large clusters. This should bring about an even better decorrelation behavior. To quote values for dynamical exponents is beyond the scope of the present paper. Here we rather concentrate on the applicability for $n>1$.

Numerical results.— In Table I a subset of our numerical results is listed. The first two columns distinguish the three different $O(n)$ nonlinear σ models that were simulated on L^2 lattices. The exactly known critical $\beta_c = \log(1+\sqrt{2})/2$ was chosen for the Ising model. For the x-y model the value $\beta=1.12$ is expected to be very close to the Kosterlitz-Thouless point[11,12] or possibly somewhat beyond in the critical spin-wave phase.[13] The lower values $\beta=1.04$ and 1.07 were simulated to check if a possible finite-size shift of the transition region leads to rising autocorrelation times there. For $\beta=1.5$, 1.6, and $n=3$ we expect (and confirm) a spatial correlation length around 10 and 20.[14] The numbers of generated clusters c follow together with their average size. To diagnose the algorithm we quote the magnetic susceptibility χ and the autocorrelation time τ_χ manifested in the estimates for this observable. It is derived as follows: Measurements of physical observables are separated by a fixed number of m cluster update steps (in the quoted results, $m=1$ for $n=1,2$ and $m=10$ for $n=3$). In equilibrium the connected autocorrelation function in time is

TABLE I. Results for the magnetic susceptibilities χ and autocorrelation times τ_χ (in units comparable to sweeps) for simulations of $O(n)$ σ models on L^2 lattices. In each run a total of c update steps have been performed involving clusters of an average of $\langle |c| \rangle$ spins. The effective autocorrelation time τ_χ^{eff} is directly relevant for error estimation.

n	L	β	$c\times 10^{-6}$	$\langle \lvert c \rvert \rangle L^{-2}$	χL^{-2}	τ_χ	τ_χ^{eff}
1	32	0.4406...	0.50	0.4602(7)	0.4598(7)	2.3(3)	1.4
1	64	0.4406...	0.25	0.3858(11)	0.3852(10)	2.3(3)	1.9
1	128	0.4406...	0.20	0.3225(11)	0.3229(10)	2.7(5)	1.8
2	32	1.12	0.62	0.3582(5)	0.4420(2)	3.6(7)	1.4(2)
2	64	1.12	0.26	0.3043(6)	0.3754(3)	2.4(6)	1.3(2)
2	128	1.12	0.20	0.2582(7)	0.3190(3)	2.1(6)	1.2(2)
2	32	1.07	0.26	0.3247(7)	0.3985(4)		1.5(3)
2	64	1.07	0.13	0.2629(9)	0.3245(5)		1.1(2)
2	128	1.07	0.10	0.2114(9)	0.2608(5)		1.2(2)
2	128	1.04	0.26	0.1638(5)	0.2032(5)		1.4(2)
				$\langle \lvert c \rvert \rangle$	χ		
3	128	1.5	1.54	132.0(4)	174.4(0.9)		0.25(4)
3	128	1.6	2.00	334.5(7)	444.9(1.4)	1.0(6)	0.40(6)

measured from successive estimates for χ (and other quantities). An autocorrelation time $\bar{\tau}_\chi$ is determined from its exponential falloff in time separation. All entries in the table are based on our seeing constant stable logarithmic ratios for successive values of the correlation function at least in a window from $\bar{\tau}_\chi$ to $3\bar{\tau}_\chi$. Unless the statistics is increased enormously, noise then takes over. The errors on $\bar{\tau}_\chi$ are estimated subjectively from its fluctuations in the stability window, and from some repeated experiments. The measured correlation is also summed and a tail, approximated as an exponential (using $\bar{\tau}_\chi$), added to incorporate autocorrelations into error estimates. Finally, τ_χ is related to $\bar{\tau}_\chi$ as

$$\tau_\chi = \bar{\tau}_\chi m\langle |c| \rangle L^{-2}. \tag{9}$$

This is a reasonable quantity to compare to the sweeps that are common and natural in local algorithms: $\tau_\chi = 1$ means that on the average one has to "touch" (here, reflect) each spin once to suppress correlations by a factor of $1/e$. Needless to say the values of τ_χ signal an enormously enhanced efficiency for the simulation of spin models. We also estimated errors from the fluctuations of blocks of 1000 measurements each. The two results always agreed within 10%. The effective autocorrelation time is defined as

$$\bar{\tau}^{\text{eff}} = \tfrac{1}{2}(\epsilon_{\text{block}}/\epsilon_{\text{naive}})^2. \tag{10}$$

Here ϵ_{block} and ϵ_{naive} are the representative errors, and an exactly simply exponential autocorrelation with scale $\bar{\tau}^{\text{eff}}$ would produce the same errors. Where errors for τ^{eff} are quoted, they were estimated by a further division of the data into subsamples. For extreme short-range quantities like the nearest-neighbor correlation and $n = 2,3$, we saw somewhat longer correlation times up to $\tau^{\text{eff}} \simeq 4$ but flat in L. These observables, however, are physically less interesting, and one could always intersperse local update steps if the *short*-wavelength modes evolve too slowly. In Fig. 1 we see the size distribution of clusters for 128^2 runs. While both critical models look similar, the finite physical correlation length in O(3) is clearly visible as a sharp cutoff.

Some reference runs with a local random site updating heat-bath algorithm for $Z(16) \simeq O(2)$ at $\beta = 1.12$ yielded $\tau_\chi \simeq 20(4)$ at $L = 16^2$ and indicated the expected growth $\propto L^2$. Cluster runs were also made for Z(16) (with reflections suitably restricted) and produced results indistinguishable from O(2). The difference in speed is only small for the new algorithm, and there is consequently no need for the discrete spin approximation. The equality (8) of χ and $\langle |c| \rangle$ is clearly borne out by the data for $n = 1$. For $n = 2,3$ the ratios $\langle |c| \rangle / \chi$ are also very nearly β-independent constants in the range that we investigate. The only remarks on the physics of the models we wish to make here is that the growth of χ at criticality is compatible with the expected scaling behavior

$$\chi \propto L^{2-\eta}, \tag{11}$$

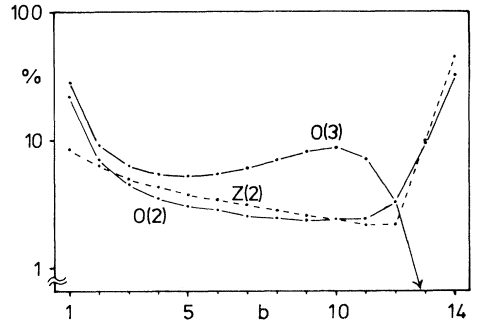

FIG. 1. Distribution of the number of spins updated collectively in $L = 128$ simulations at $\beta = 0.44\ldots$, 1.12, and 1.6 for $n = 1$, 2, and 3, respectively. Bin b comprises clusters of size $2^{b-1} \le c < 2^b - 1$.

and $\eta = 0.25$ in the Ising model. For the x-y case at $\beta = 1.12$ our results give $\eta = 0.235(1)$. We conclude by mentioning that now an accurate and detailed study of the Kosterlitz-Thouless picture and asymptotic freedom scaling behavior for the $n = 2$ and $n \ge 3$ σ models, respectively, which have both recently been challenged,[15] should be feasible.[17] The new algorithm should also be useful in the simulation of four-dimensional O(4) models to study Higgs physics and triviality. The generalization to spin-glasses or neural networks, where β is bond dependent, seems straightforward. Attempts for extensions to lattice gauge theory are under way.

All numerical calculations were carried out on the Cray-XMP/18 at Kiel University. I wish to thank Alan Sokal for exchange, Istvan Montvay for discussions, and the DESY theory group for their hospitality.

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[9]Note that for the x-y model written with U(1) spins (phases), this is an antilinear operation.

[10]This connection with SW clusters can also be employed to prove (6).

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