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Simulations without Critical Slowing Down

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We have developed a novel simulation method that combines a multigrid technique with a stochastic blocking procedure. Our algorithm eliminates critical slowing down completely, as demonstrated by simulations of the two-dimensional Ising model at criticality.

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Considerable effort has been devoted in recent years to simulations of various problems, that range from calculating hadron masses,[1] through equilibrium phase transitions,[2] to a variety of nonequilibrium, complex time-dependent phenomena.[2,3] Of the many problems that hinder large-scale simulations we address that of *critical slowing down* (CSD). This phenomenon gives rise to a divergent relaxation time τ as the critical point is approached.[4] Thus, the times needed to equilibrate the system and to generate statistically independent configurations (at equilibrium) become exceedingly large. At criticality, τ grows as

$$\tau \sim L^z, \tag{1}$$

with the linear size L of the system. Here τ is measured in units that scale with the total number of sites (i.e., L^d), and z is the dynamic critical exponent.

In this Letter we present a method that overcomes this difficulty. While a number of recently reported simulation techniques[5,6] have partially eliminated CSD, this is the first simulation that evades CSD completely for a nontrivial model. We illustrate the method by simulating the $d=2$ Ising model at the critical temperature of the infinite lattice. The equilibration time for the energy is found to be constant, $\tau \approx 3.0$, for lattices of linear sizes $8 \leq L \leq 128$ (see Fig. 1). The method used is a combination of a *multigrid* method[8-10] with a *stochastic blocking* (coarsening) technique.[6,11,12] General features of our method (applicable to discrete or continuous-state

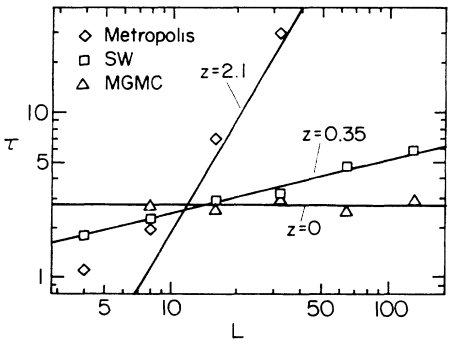

FIG. 1. Relaxation time τ vs (linear) system size L. Three methods are compared: Metropolis algorithm (Ref. 7), Swendsen and Wang's method (Ref. 6) (SW), and the multigrid Monte Carlo technique (MGMC).

Hamiltonians, and a wide class of coarse-to-fine interpolations) were first presented recently.[8]

The structure of this Letter is as follows: First, we provide an elaborate description of our algorithm and show that it satisfies detailed balance. Details of the simulations mentioned above are given next. Finally, we explain why our procedure does eliminate CSD completely, whereas the Swendsen-Wang method[6] (SW), which uses stochastic blocking without incorporating multigrid ideas, does not.

Description of the algorithm.—In our coarsening procedure, simulation of the full Hamiltonian is replaced by simulation of a stochastically generated, simplified Hamiltonian, over a restricted space with fewer degrees of freedom. Write $\mathcal{H}=\mathcal{H}_0+V$, where factors of $1/k_BT$ have been absorbed into $\mathcal{H}$ and where $\mathcal{H}_0$ is somehow easier to simulate than the original $\mathcal{H}$. Assume that the system is in some state Q. We "kill" the interaction V either by "deleting" it with probability $p_d=C_V\times\exp[V(Q)]$ or by "freezing" it with probability $p_f=1-p_d$. If the interaction is frozen, only states Q' with $V(Q')=V(Q)$ are considered in the ensuing simulation. If the interaction is deleted, no such restriction is placed on the states. In either case, the thermodynamics is subsequently governed only by the simplified Hamiltonian $\mathcal{H}_0$. One must choose C_V so that $p_d,p_f\in[0,1]$. The largest choice of C_V produces the best statistics.

In practice, $\mathcal{H}_0$ is still nontrivial to simulate (without CSD) and so additional terms of the Hamiltonian must be killed. After killing all the interactions in $\mathcal{H}$, one arrives at a system which is completely decoupled—and so is trivial to simulate—but is subject to an arbitrary set of restrictions on its states.

For the two-dimensional ferromagnetic Ising model $\mathcal{H}=-\sum_{\langle ij\rangle}K_{ij}s_is_j$, we kill the interactions $K_{ij}s_is_j$ one at a time. The optimal probability for deletion, then, is $p_d=\exp[-K_{ij}(1+s_is_j)]$. Interactions between antiparallel spins will always be deleted; only parallel spins can be frozen together. We may kill the interactions, generate a new configuration for the decoupled system, and then return to the full Hamiltonian to continue the simulation. This is the procedure followed by SW; it still suffers from CSD, although with a considerably reduced dynamical exponent.

To eliminate CSD completely, we combine this stochastic blocking procedure with multigrid ideas. As an example, consider Fig. 2(a). Choose the boxed sites as our coarse lattice, which has $(L/b)^2$ spins; here the length rescaling factor is $b=2$. We coarsen by considering all pairs of coupled sites i,j. If *both* i and j have already been frozen to coarse spins, we move on to the next pair; otherwise kill $K_{ij}s_is_j$. Figure 2(a) is a possible coarsening. Single (double) lines between sites indicate living (frozen) bonds; deleted bonds are not marked. Each cluster of fine spins connected by frozen bonds constitutes an irregular, stochastically generated block. A

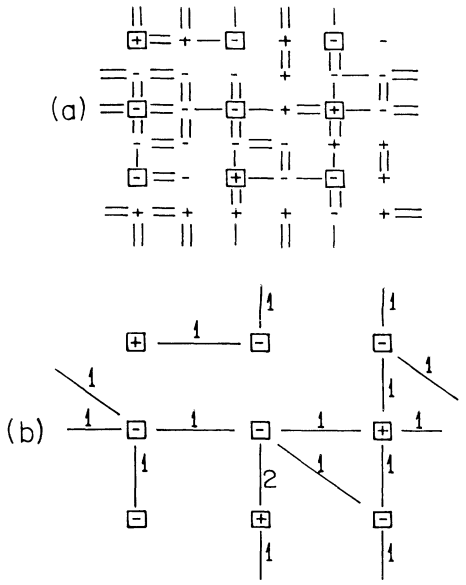

FIG. 2. Coarsening of a fine-spin configuration. Boxed spins constitute the coarse lattice. (a) Outcome of a possible coarsening. Single (double) lines denote living (frozen) bonds; deleted bonds are not marked. (b) Coarse lattice. Numerals near bonds denote the number of fine couplings added together to form the associated coarse bond.

block is either frozen to (and viewed as) a single coarse spin or it is completely decoupled.

Finally, the coarse Hamiltonian is constructed: The coupling between coarse spins s_i and s_j is the sum of the living couplings that connect fine spins associated with coarse spins s_i and s_j. This is illustrated in Fig. 2(b): Numerals on the lines between sites indicate the number of fine couplings that contribute to the coarse bond. The new Hamiltonian is inhomogeneous, and may contain long-range interactions.

In addition to coarsening the system, we need "uncoarsening" and Metropolis procedures as well. To "uncoarsen" the system, decoupled blocks are set to some arbitrary value of spin, all fine-lattice spins take the value of the block spin to which they were frozen, and the fine-lattice couplings are restored. Metropolis updates may be performed at any length scale by use of a standard Metropolis algorithm[13] on the block spins at that scale, with the corresponding Hamiltonian.

Our dynamic procedure "cycles" through all length scales, starting from the finest. At each intermediate length scale, the system is coarsened γ times before it is uncoarsened (see Fig. 3). At the coarsest level all blocks are decoupled, and each time this level is reached, it is immediately uncoarsened. The cycle ends when the finest level is reached. A few Metropolis sweeps are performed at each level. These sweeps, however, are not essential to elimination of CSD. The SW procedure[6]

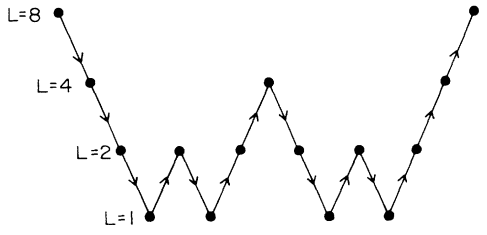

FIG. 3. An example of a cycle on an 8×8 lattice, with length rescaling factor $b=2$ and $\gamma=2$.

corresponds to $\gamma=1$ with $b=L$, going directly from the finest to the coarsest level and back, without Metropolis sweeps at the finest level.

Proof of detailed balance.—Clearly, our procedure is strongly ergodic since there is always a nonzero probability that no restriction will be placed on the simulation, allowing nonzero transition probabilities between all states. Consider a transition generated by coarsenings and a Metropolis step, which satisfies detailed balance with respect to the coarse Hamiltonian. It can be viewed as taking place between the two corresponding fine-spin states, and we want to show that detailed balance with respect to the fine-spin Hamiltonian is satisfied. Once proven, this implies that the transitions satisfy detailed balance with respect to the *finest* Hamiltonian.

Start from some level in state Q with a Hamiltonian $\mathcal{H}$, and "kill" an interaction V to get the coarse Hamiltonian $\mathcal{H}_0=\mathcal{H}-V$. Then a transition from Q to another state Q', with $V(Q)\neq V(Q')$, can take place only if V has been deleted:

$$T(Q\rightarrow Q')=C_V e^{V(Q)}T_0(Q\rightarrow Q'), \tag{2}$$

where T_0 are transition probabilities with $\mathcal{H}_0$. Hence,

$$\frac{T(Q\rightarrow Q')}{T(Q'\rightarrow Q)}=\frac{e^{V(Q)}e^{-\mathcal{H}_0(Q')}}{e^{V(Q')}e^{-\mathcal{H}_0(Q)}}=\frac{e^{-\mathcal{H}(Q')}}{e^{-\mathcal{H}(Q)}}. \tag{3}$$

Alternatively, if $V(Q)=V(Q')$, the interaction V may either be deleted for frozen:

$$\begin{aligned}T(Q\rightarrow Q')&=C_V e^{V(Q)}T_0(Q\rightarrow Q')+(1-C_V e^{V(Q)})T_0^f(Q\rightarrow Q')\\&=[C_V e^{V(Q)}T_0(Q'\rightarrow Q)+(1-C_V e^{V(Q)})T_0^f(Q'\rightarrow Q)]e^{-\mathcal{H}_0(Q')}/e^{-\mathcal{H}_0(Q)},\end{aligned} \tag{4}$$

where T_0^f are transition probabilities with the reduced Hamiltonian over the restricted space. Remembering that $V(Q')=V(Q)$ yields

$$T(Q\rightarrow Q')=T(Q'\rightarrow Q)e^{-\mathcal{H}(Q')}/e^{-\mathcal{H}(Q)}, \tag{5}$$

completing the proof of detailed balance.

Details of simulations.—We simulated the $d=2$ Ising model on square lattices of linear size $8\leq L\leq 128$ with periodic boundary conditions. A cycle of $\gamma=2$ with rescaling factor $b=2$ was used. At each level, one Monte Carlo sweep was performed. Starting from a fully magnetized state we measured the decay of the energy to its equilibrium value,[14] averaged over an ensemble of up to 100 systems. From such data we extracted the relaxation times $[\tau(L)]$, and found $\tau\approx 3.0$ *for all lattice sizes.* Figure 1 is a log-log plot of $\tau(L)$ measured with three different algorithms: standard Metropolis procedure[7] ($z\approx 2.1$), the SW algorithm[6] ($z\approx 0.35$), and our method ($z=0$).

Why does it work?—To eliminate CSD, one must allow flips of large domains with high acceptance ratios. Had our coarsening procedure created lattices with higher connectivity or stronger bonds than those of the fine lattices, the acceptance ratios for the large-scale moves would have become prohibitively small. The production of lower connectivities or weaker couplings would have generated decoupled blocks at short length scales, and large-scale flips would not have been possible. Hence, since our algorithm does produce $z=0$, we expected and indeed confirmed that our coarsening procedure yields similar distributions of bonds and connectivities in lattices at different length scales.

The SW algorithm[6] does not eliminate CSD completely. The reason for this is that coarsening introduces spin-spin correlations on an average length scale of b (the rescaling factor of the coarsening transformation) by freezing spins on that scale. Equilibration of the coarse lattice has no effect on these correlations. One has to repeat the process of coarsening, equilibration, and uncoarsening several times, in order to decorrelate and equilibrate the fine lattice. Note, however, that in each such step equilibration involves further coarsening, for which the same considerations hold. Hence a nested sequence of coarsening-equilibration-uncoarsening steps is needed. Denote by $\tau_0(b)$ the number of coarsening-equilibration-uncoarsening steps needed to eliminate correlations on length scale b. If we assume scale invariance at criticality, i.e., that $\tau_0(b)$ is the same for all levels in the hierarchy,[15] the equilibration process described above is precisely the cycle shown in Fig. 3, with $\gamma=\tau_0$. Therefore, if such a cycle is used, the configuration of the fine lattice becomes independent of the initial configuration after τ_0 cycles. To estimate τ_0, recall that the SW procedure is one coarsening step with $b=L$, yielding $\tau_0(L)\sim L^{z_{\rm sw}}$. Combining scale invariance with the SW result, we get $\tau_0(b)\approx b^{z_{\rm sw}}$. From the same reasoning it follows that, if one uses a cycle with $\gamma<\tau_0$, the number of cycles needed to decorrelate diverges as $L^{z_{\rm sw}-\log_b\gamma}$. Hence, in order to equilibrate in a finite number of cycles, γ must satisfy the inequality $\gamma\geq b^{z_{\rm sw}}$. Since the time needed to complete a cycle (measured in

steps per site) diverges (as $L \to \infty$) if $\gamma > b^d$, CSD is eliminated completely only if $b^{z_{sw}} \leq \gamma < b^d$. For the Ising model, this condition translates to $b^{0.35} \leq \gamma < b^2$ for $d=2$, and $b^{0.75} \leq \gamma < b^3$ for $d=3$. For the three-state Potts model in two dimensions we must satisfy $b^{0.6} \leq \gamma < b^2$. For values of b and γ that do not satisfy these bounds, we expect CSD. In particular, for the three-state Potts model in $d=2$, with $\gamma=2$ and $b=4$, we expect to get $\tau \sim L^{z_{sw} - \log_b \gamma} \approx L^{0.1}$.

A more complete account of this work as well as detailed tests of the scaling arguments given above will be reported elsewhere.[16] We are also working on optimal coarsening procedures that reduce statistical fluctuations and are starting simulations on the 2D XY model.

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