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Suppressing critical slowing down in two-dimensional Ising model simulations by the multigrid Monte Carlo method

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Abstract. Statistically independent equilibrium configurations of interacting systems can easily be generated with little computing effort by multigrid coarse-to-fine transforms. The very slow long-wavelength motions close to critical points are thereby accelerated by many orders of magnitude. This is demonstrated with a novel updating algorithm from small to large two-dimensional Ising systems specifying effective interactions according to renormalisation group considerations, corrected for non-linearities and saturation effects.

To ensure ergodicity in computer simulations of equilibrium properties, many independent configurations equally distributed over the entire phase space are needed. The critical slowing down close to second-order phase transitions (see e.g. Hohenberg and Halperin 1977 and Ma 1976) inflates the slowest relaxation scale many orders of magnitude relative to those of the system's fast evolution. To avoid systematic artefacts due to correlated configurations located in a small phase subspace, extremely long simulation runs with very high computing costs are needed, even with current supercomputers. To minimise this waste of computer time, new algorithms have been invented based on physical principles to prevent critical slowing down. One presented by Swendsen and Wang (1987) uses mappings from the Ising and Potts models to percolation according to Kasteleyn and Fortuin (1969) and to Fortuin and Kasteleyn (1972). With this procedure the critical slowing-down exponent for the two-dimensional Ising model is reduced from 2.125 to 0.35, thus improving computing performance by a factor of 1000–10 000.

To further improve such an algorithm by suppressing the residual slowing-down exponent (0.75 for the three-dimensional Ising model), Kandel *et al* 1988, 1989) combined the Swendsen and Wang (1987) formalism with the multigrid method. Dividing the Ising Hamiltonian into one acting in a restricted space governing the largest part of the thermodynamics and the remainder, they were able to combine percolation and multigrid theory to eliminate completely critical slowing down. Another way was proposed by Decker (1988). He introduced a multigrid Monte Carlo algorithm for the lattice gauge problem, then tested and optimised it using renormalisation group considerations.

In this communication the implementation of the block-spin formalism, the basic idea of Wilson's renormalisation-group theory (Wilson 1975) is discussed for the multigrid Monte Carlo algorithm. Special care has to be taken to handle correctly the effects of

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saturation, non-linearity and neglected interaction terms in the decimation procedure for effective interactions large compared to the critical one. Furthermore, in allowing the spins that were frozen in the block at an earlier stage to melt, the interaction energy of the spins which formed the block has to be determined such that the free energy satisfies renormalisation-group requirements.

Critical slowing down is due to slow motions with long wavelengths (Kawasaki 1968). The multigrid method, (see e.g. Briggs 1987), was first introduced for accelerating the solution of linear equations with large sparse matrices. The basic idea of this method is to transform large systems into small ones with fast short-wavelength motions. Upon increasing the system size, short-wavelength amplitudes are transformed into long-wavelength amplitudes and the time scale is extended. This scaling can best be understood within the context of the renormalisation-group formalism of Wilson (1975) which specifies how effective spin interactions have to be recalculated during the transformation process.

A picture proposed by Domb (1976) elucidates these phenomena. Close to a critical point, two kinds of clusters appear: correlated clusters, containing the physics of the phase transition and critical slowing down, characterised by Fisher's droplet model (Fisher 1967), and so-called ramified clusters. Domb *et al* (1975) and Müller-Krumbhaar and Stoll (1976) verified this view with computer simulations, interpreting ramified clusters as uncorrelated but connected percolation clusters. This phenomenon of at least two different timescales is also readily apparent in the motion picture by Schneider and Stoll (1974), where percolation clusters appear and disappear very quickly, together with slowly evolving compact clusters.

The multigrid Monte Carlo method used here follows Decker's procedure (Decker 1988). Due to spin-number duplication at each multigrid step it is convenient that the system contains $N = 2^M$ spins where M is an integer. The spin arrangements prior to and after each step correspond to those in Wilson's fundamental review (Wilson 1975). His renormalisation scheme for the first- and second-nearest neighbour interactions

$$K_k = \rho^2(2K_{k-1}^2 + L_{k-1}) \tag{1}$$

and

$$L_k = \rho^2 K_{k-1}^2 \tag{2}$$

has the following fixed point:

$$K^* = (2\rho^2 + \rho^4)^{-1} \qquad L^* = \rho^2(2\rho^2 + \rho^4)^{-2}. \tag{3}$$

For the correction factor ρ he used the value $2^{1/16}$.

The meaning of this fixed point is that all points on a certain line at the (K, L)-plane map to its end point (K^*, L^*) upon iterating formulae (1) and (2) many times. Such a coordinate pair is ($K = K_c'$ and $L = 0$); in renormalisation-group theory K_c' is the critical interaction, but in an approximate implementation K_c' is smaller than Onsager's exact K_c (see Yang 1952), e.g.

$$K_c' = 0.7990\, K_c = 0.3995 \ln(\sqrt{2} + 1) \tag{4}$$

in Wilson's case (Wilson 1975).

The following considerations are by no means exact but are based on heuristic considerations. Not too close to the critical coupling K_c and for $K > K_c$, to correct non-linearity and saturation effects and to avoid too large interaction changes in the first renormalisation step, only nearest-neighbour interactions are considered in contrast to

Wilson (1975). In formulae (1)–(3), K_k and L_k are used as parameters to calculate the effective nearest-neighbour interactions. To correct the critical interaction shift (4), K_0 and L_0 are given the values

$$K_0 = KK^*/K_c \qquad L_0 = KL^*/K_c \tag{5}$$

and K_1' is calculated accordingly:

$$K_1' = K_1 K_c/K^*. \tag{6}$$

A measure of non-linearities for $K > K_c$ and not too close to K_c is the deviation between the eighth power of the order parameter calculated from Yang's exact formula (Yang 1952)

$$(m(K))^8 = 1 - 16/(e^{2K} - e^{-2K})^4 \tag{7}$$

and the linear approximant

$$(m_a(K))^8 = 8\sqrt{2}(K - K_c). \tag{8}$$

The interaction K_1 is therefore calculated using formulae (6)–(8)

$$K_1 = K + [(m(K_1'))^8 - (m(K))^8]/8\sqrt{2}. \tag{9}$$

For K-values close to K_c, K_1 is close to K_1', just like in Wilson (1975), but only with one interaction parameter. In the next iterations K is replaced by K_1 and the steps between (1) and (2) and between (6) and (9) are repeated again.

A further problem occurs when the new finer lattices are inserted between the old sites. The probability $p(s_i = +1)$ for new configurations $\{s_i\}$ calculated only on the basis of the old spin distributions $\{s_j\}$ and the spin–spin interaction K leads to too small an entropy, and equilibrium cannot be reached within a few Monte Carlo cycles. The probability $p(s_i = +1)$ for having a positive spin s_i is usually assumed to be

$$p(s_i = +1) = \prod_j W_j(s_i = -1 \to s_i = +1) \Big/ \left(1 + \prod_j W_j(s_i = -1 \to s_i = +1)\right) \tag{10}$$

where $W_j(s_i = -1 \to s_i = +1)$ in the Metropolis *et al* (1953) transition probability for flipping a negative spin $s_i = -1$ into a positive one $s_i = +1$, satisfying the detailed balance conditions

$$W_j(s_i = -1 \to s_i = +1) = e^{2Ks_j}. \tag{11}$$

To bring the entropy closer to its final value and thereby to save computer time between updating steps, $W_j(s_i = -1 \to s_i = +1)$ is replaced by

$$W_{m,j}(s_i = -1 \to s_i = +1) = e^{2Ks_j}(1 + q_0/2 - E_0/N)^{-s_j/4} \tag{12}$$

with

$$E_0 = \tfrac{1}{2} \sum_{l=1}^{N} \sum_{\delta=1}^{q_0} s_l s_{l+\delta}. \tag{13}$$

δ runs over the nearest neighbours on the old lattice with N spins and $q_0 = 4$ is the number of such neighbours. Afterwards a Monte Carlo procedure similar to that of Metropolis *et al* (1953) with the usual $W_j(s_i = -1 \to s_i = +1)$ in (10) is used to relax the spins $\{s_j\}$ of the old smaller lattice before those of the new inserted lattice $\{s_i\}$. In this

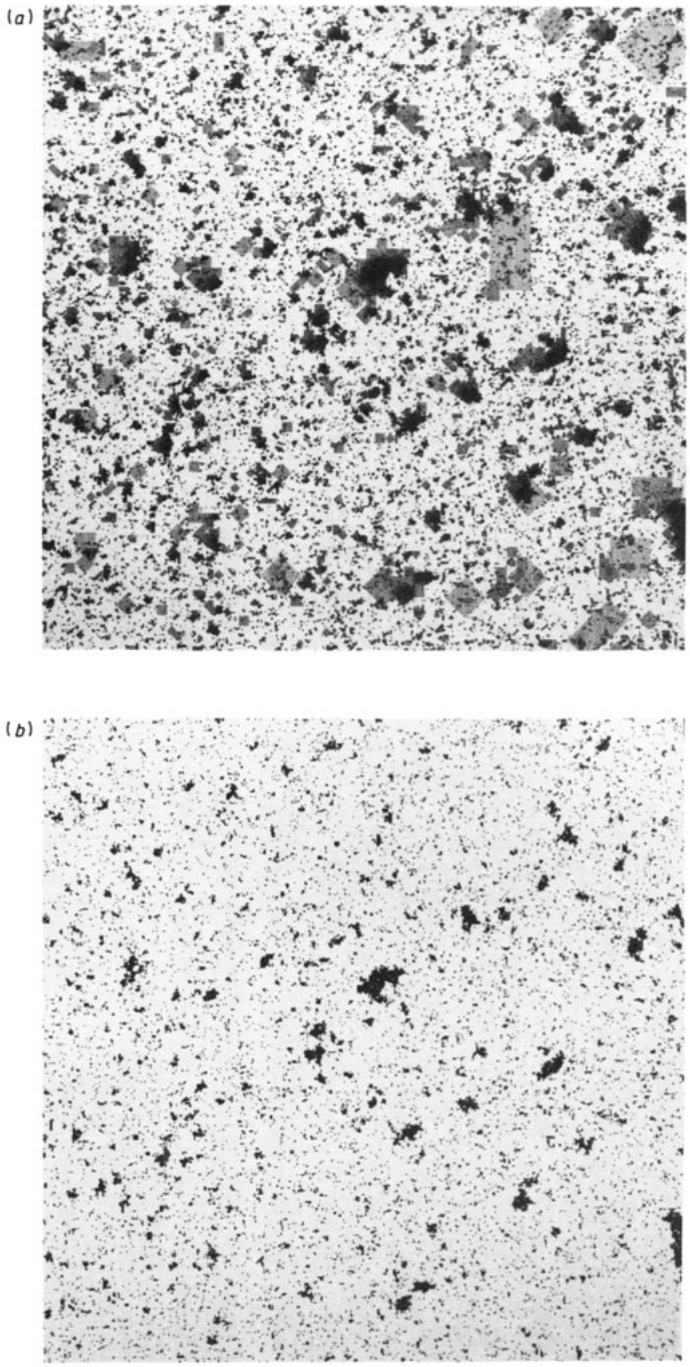

Figure 1. Plot for $K > K_c (K_c/K = 0.96)$ of 'frozen' block-spins being disensembled during the updating process (*a*) and 512 × 512 single spins in the final system (*b*). In (*a*) the size of the 'frozen' block-spins is the picture area divided by their number $N = 2^M$. In an early stage with small M and N the large negative block-spins are light grey, whereas for large M and N the negative block-spins are dark grey and in the final state the negative spins are black. To visualise the evolution the large light-grey block-spins appear transparent. In (*b*) the negative spins of the largest system are black.

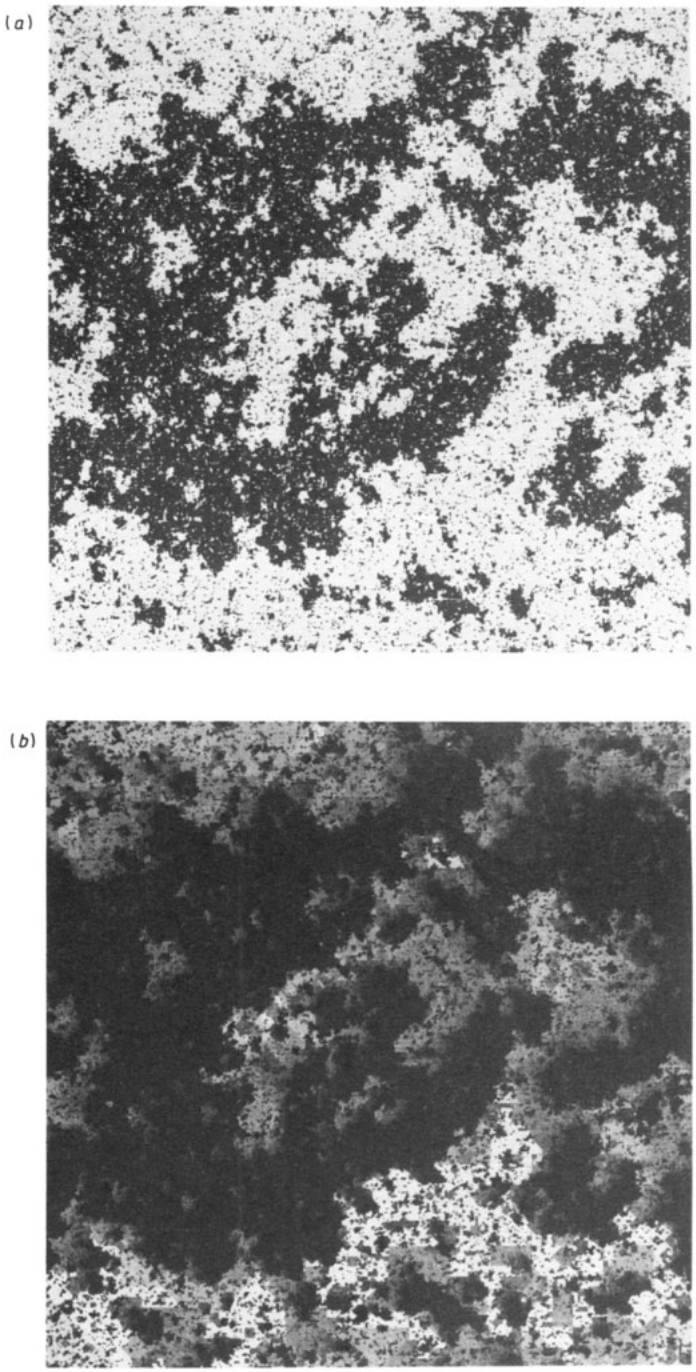

Figure 2. The same as in figure 1, but for $K = K_c$.

heuristic procedure, using the energy E_0 of the old smaller lattice in (13), the entropy remains nearly constant during updating and only a few Monte Carlo steps per spin are needed for relaxation.

Another more fundamental procedure for the renormalisation steps was proposed and tested for smaller systems (32×32) spins by Hahn and Streit (1988), but their considerations apply only to $K < K_c$.

To guarantee Markoffian chains for these processes, the lattice is subdivided into four sublattices (four are needed to also include next-nearest neighbour interactions). The transition probabilities W_j in (11) are calculated, and afterwards all sublattice spins are flipped according to these probabilities. However, for very weak interactions or high temperatures, the sublattice spins flip at nearly every step, and equilibrium can only be reached after very long simulation runs. To obtain fast thermalisation under such conditions spin configurations are calculated according to (10) and (11). This implies that these sublattice configurations reach the largest entropy in the field of the remaining sublattices at each step.

The results obtained with this updating algorithm have the following properties: for interactions K significantly larger than K_c, the computed order parameter $m(K)$, interaction energy $E(K)$ and energy fluctuation $(\Delta E)^2$ are close to Yang's exact results (Yang 1952), but the order parameter fluctuations $(\Delta m)^2$ are several orders of magnitude larger than those calculated from the isothermal susceptibility formula of Essam and Fisher (1963). Moreover, these unexpected fluctuations deviate only towards smaller-order parameter values. This artefact can be reduced a great deal, however, by using more than four Monte Carlo steps instead of one per spin between two updatings, so that local equilibrium is approximately established. For K close to K_c deviations are then small. As is apparent from table 1, the order parameter $m(K)$ is still too large and the interaction energy $E(K)$ too strong. The specific heat c_v and the susceptibility χ have the correct order of magnitude as theoretical values, but show deviations there too. These deviations are not size dependent and indicate the limitations of coarse-to-fine grid multilevel updating only. The statistical errors for m and E are smaller than the last digit. For c_v and χ, these errors exceed the fluctuations of independent samples (3 and 10%) for $K > K_c$, and are again an indication that coarse-to-fine transform only is not sufficient. Furthermore, the number of five Monte Carlo steps between two updatings seems to be too small.

Figures 1 and 2 show the system evolution starting from 16 positive spins following a multigrid expansion for $K > K_c$ and $K = K_c$, respectively. Comparing the square-like ensembles of 'frozen' negative block-spins in (*a*) and the 'molten' negative spins of the final system in (*b*), it is readily apparent that for $K > K_c$ (with only one Monte Carlo step per spin between updatings) the clusters nearly retain their rescaled size and position in later stages. This may explain the above-mentioned strong order-parameter fluctuations. For $K = K_c$, however, the clusters 'diffuse' through the system with updating.

In conclusion, by ensuring local equilibrium in ever-larger subsystems, the multigrid Monte Carlo method is found to have a very promising potential to suppress critical slowing down. This is demonstrated for the two-dimensional Ising model. Compared to the method of Kandel *et al* (1988, 1989), where transformation to percolation is needed to 'freeze' the spins into block-spins, the application of renormalisation transformations with the full Hamiltonian offers a more direct alternative. Nevertheless, the problems of neglected interaction terms, non-linearities and saturation effects require further theoretical efforts. With further improvements (e.g. according to the suggestions of Hahn and Streit (1988) extended to $K > K_c$), and to include fine-to-coarse block-spin

Table 1. Monte Carlo simulation results of a two-dimensional Ising system containing 1024 × 1024 spins averaged over 1000 independent configurations. (The values marked with * are results of systems with 4096 × 4096 spins and 100 configurations.) The initial 16 block-spins are positive. For the theoretical values of the order parameter m_T, the energy E_T and the specific heat c_{vT} the formulation by Yang (1952) is used. For χ_T and $K > K_c$ the expression by Essam and Fischer (1963) and for $K < K_c$ those by Sykes *et al* (1972) are taken into account.

$T/T_c = K_c/K$	m	m/m_T	E/K	E/E_T	χ/χ_T	c_v/c_{vT}
0.80	0.953	0.999	−1.851	0.999	0.82	1.01
0.90	0.894	0.998	−1.713	1.000	1.40	1.04
0.95	0.834	1.004	−1.609	1.004	1.54	1.02
0.98	0.765	1.025	−1.524	1.009	1.24	0.97
0.99	0.719	1.046	−1.486	1.011	0.75	0.88
—	0.718	1.047	−1.486	1.011	0.96	1.01*
0.995	0.677	1.075	−1.462	1.011	0.50	0.88
—	0.676	1.074	−1.462	1.011	1.27	0.96*
0.999	0.592	1.148	−1.435	1.009	0.20	0.84
—	0.590	1.145	−1.435	1.009	0.23	0.82*
1.00	—	—	−1.421	1.005	—	—
—	—	—	−1.421	1.004	—	—*
1.01	—	—	−1.345	0.990	0.25	0.96
—	—	—	−1.344	0.990	0.21	0.75*
1.02	—	—	−1.301	0.988	0.34	0.95
—	—	—	−1.301	0.987	0.36	0.81*
1.05	—	—	−1.207	0.986	0.52	0.85
1.10	—	—	−1.097	0.989	0.63	0.89
1.20	—	—	−0.944	0.993	0.74	0.95

transforms as well, this method will provide a key to solve a variety of problems in computational physics otherwise untreatable even with present and planned generations of supercomputers. The absence of exact solutions for more complex models will make the estimation of correction terms more difficult; non-linearities and saturation effects will have to be determined simultaneously at the fine-to-coarse grid transform.

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