Physica A 170 (1991) 278–281
North-Holland

CLUSTER MONTE CARLO ALGORITHMS FOR RANDOM ISING MODELS

Vl.S. DOTSENKO[a], W. SELKE[b] and A.L. TALAPOV[a]

[a]*Landau Institute for Theoretical Physics, Academy of the Sciences of the USSR, Moscow, USSR*

[b]*IFF des Forschungszentrums Jülich, W-5170 Jülich 1, Germany*

Received 8 August 1990

Variations of the Swendsen–Wang and Wolff cluster flip algorithms are proposed to perform Monte Carlo simulations of Ising models with random bonds and random fields, including systems with frustration. The new methods are tested by applying them to small lattices and comparing the results with exact data.

To obtain Monte Carlo data of high accuracy in cases of critical slowing down, Swendsen and Wang [1] (S–W) proposed and applied a novel cluster flip algorithm for studying nearest neighbour Ising and Potts models. In that method new configurations are generated by connecting neighbour sites in clusters of equal spins, $\sigma_i = \sigma_j$, with a probability $1 - e^{-2K}$, where K is the coupling strength $(=J/k_B T)$. Thereby subclusters are formed which then will be reversed with probability $\frac{1}{2}$. The algorithm has been shown to be ergodic and to fulfill detailed balance. The method has been applied to various cases, in particular, to antiferromagnetic Potts models, Ising models in homogeneous fields and random-bond ferromagnetic Ising models as well as to models with continuous spins, see the review by Wang and Swendsen [2].

The S–W cluster flip algorithm has been modified by Wolff [3] in the form of a single cluster (1C) method. The essential idea is to choose randomly a site, i, and to consider only the cluster around that site. Using the same probabilities as before, other sites of the cluster will possibly be connected to site i, thereby forming one subcluster, which will be reversed with probability one. The algorithm turned out to be extremely efficient [3, 2].

So far, the main disadvantage of the cluster flip approach, as compared to the conventional single spin flip Metropolis algorithm, seems to be its restricted range of applicability. Of course, in studying kinetic properties by Monte Carlo techniques, the single spin flip method provides a more realistic type of

dynamics (Glauber kinetics). But even in the case of studying equilibrium properties, the applicability of the cluster flip algorithm to complicated models is hampered simply by the fact that it is not always straightforward to construct subclusters and to assign to them probabilities for their reversals correctly. In particular, the intriguing problems of spin models with competition or frustration, say, either due to random local magnetic fields or random bonds of different signs, have been studied in the past extensively by using the standard Metropolis algorithm, see, e.g., ref. [4] for spin glasses.

In this note we propose rules for constructing and reversing clusters in models of these types. For convenience, we shall concentrate on two-dimensional nearest-neighbouring Ising models described by Hamiltonians of the form

$$\mathcal{H}/k_{\mathrm{B}}T = -\sum_{i,j} K_{ij}\sigma_i\sigma_j - \sum_i h_i\sigma_i\,, \qquad \sigma_i = \pm 1\,, \tag{1}$$

where the exchange constant $K_{ij} = \pm K$ couples neighbour sites, i and j, and the local field, $h_i = \pm h$, can vary from site to site. The Hamiltonian (1) includes one of the standard models for spin glasses, the $\pm J$ model, and the random field Ising model.

Let us first consider the case of random fields. To take into account a homogeneous field, $h_i = h$, in the S–W algorithm, various schemes have been suggested, as reviewed in ref. [2]. In particular, one may construct the subclusters as before (neglecting the magnetic field) and flip them then with a probability proportional to $\mathrm{e}^{\pm hn}$, where n is the number of spins in the subcluster.

We propose a similar procedure in the 1C case for random local fields in (1), $h_i = \pm h$. The subcluster, built in the usual manner (disregarding the magnetic field term in the Hamiltonian), around a site, i, chosen at random will be flipped with the probability, p_{s},

$$p_{\mathrm{s}} = \frac{\mathrm{e}^{\pm h\Delta n}}{\mathrm{e}^{h\Delta n} + \mathrm{e}^{-h\Delta n}}\,, \tag{2}$$

where Δn denotes the difference in the numbers of sites in the subcluster around the site i which experience "up" or "down" fields. Generalizations to situations with local fields of different strengths follow by replacing in the reversal probability the term $h\Delta n$ by $\Sigma_j h_j$, where the sum runs over the subcluster, to satisfy detailed balance.

To test our algorithm for local random fields we compared its results on the energy for various distributions of fields in (1), $K_{ij} = K > 0$, and at various temperatures for lattices of (4×4) spins, subject to full periodic boundary

conditions, with exact data. The exact data are readily obtained by evaluating numerically the partition sums over all 2^{16} possible spin configurations. Indeed, in all cases the comparisons support clearly the correctness of our algorithm.

For the case of random bonds with different signs, we propose the following 1C procedure: As before, a site, i, is picked at random. It will now be flipped immediately. The neighbours of the chosen center site are reversed with the same probability, p, as in the S–W algorithm, i.e.

$$p = \begin{cases} 1 - \exp(-K_{ij}\delta_{\sigma_i,\sigma_j}) & \text{for } K_{ij} = K > 0\,, \\ 1 - \exp(K_{ij}\delta_{\sigma_i,-\sigma_j}) & \text{for } K_{ij} = -K \ll 0\,. \end{cases} \tag{3}$$

Further possible sites of spin reversals are then the neighbours of those sites whose spins have been flipped, and the process continues until no new site is visited, completing one cluster step. However, due to the frustration because of couplings of different signs, one may, by the rule (3), reverse the same spin several (and even, possibly, infinitely many) times. This difficulty can be circumvented by requiring that each spin can be flipped at most once during one cluster step. Alternatively, one may choose neighbours of flipped spins in such a way that each site is visited at most once.

Again, we tested the algorithm for random bonds by comparing its results on the energy for various distributions of bonds in (1), setting $h_i = 0$, and at various low and high temperatures with exact data for lattices of sizes (4×4). Within the accuracy of the calculations, we observed agreement in all cases, suggesting the correctness of the procedure, fulfilling detailed balance.

Summarizing, we have proposed cluster flip algorithms to simulate Ising models with random bonds and random fields. The crucial open question is, whether these methods are more efficient than the standard one-spin-flip approach. Actually, after completion of our study we received information about very recent work in which cluster flip algorithms have been applied to the $\pm J$ model [5–7]. The results on systems of large sizes confirm the feasibility of the approach, but they suggest that the cluster method is less economical in computer time than the conventional one. The efficiency of cluster flips for random field Ising models remains to be seen.

Acknowledgement

W.S. thanks the Landau Institute for Theoretical Physics for its very kind hospitality during his visit in Chernogolovka, where this study was completed. He also thanks J.-S. Wang for a useful discussion and D. Stauffer for a critical reading of the manuscript and for pointing out refs. [6, 7].

References

[1] R.H. Swendsen and J.-S. Wang, Phys. Rev. Lett. 58 (1987) 86.
[2] J.-S. Wang and R.H. Swendsen, Physica A 167 (1990) 565.
[3] U. Wolff, Phys. Rev. Lett. 62 (1989) 361.
[4] K. Binder and A.P. Young, Rev. Mod. Phys. 58 (1986) 801.
[5] H. Paulsen, diploma thesis, University of Kiel (1990).
[6] T.S. Ray, private communication.
[7] A. Coniglio, NATO ASI, H.E. Stanley and N. Ostrowsky, eds., Cargese (1990).