Replica Monte Carlo Simulation of Spin-Glasses

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A new Monte Carlo method is presented for simulations of systems with quenched random interactions. The approach greatly reduces the long correlation times characteristic of standard methods, allowing the investigation of lower temperatures with less computer time than previously necessary.

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Over the past decade, there have been continuing controversies about the properties of systems with quenched random interactions, such as spin-glasses[1-5] and random-field models.[6-8] Extensive work has been carried out to answer some of the questions by Monte Carlo simulations. While these efforts have been partially successful, they have been greatly hampered by the extremely long relaxation times that are characteristic of systems with frustrated interactions. Similar difficulties are also found in some engineering applications involving optimization subject to conflicting constraints.[9] In this paper, we present a new approach to Monte Carlo computer simulations, which provides rapid relaxation times, making possible the study of equilibrium properties with relatively modest amounts of computer time.

In constructing a Markov process for Monte Carlo simulations, two conditions should be met: A sequence of transitions with nonzero probability must connect any two configurations, and the condition of detailed balance must be satisfied. The standard Monte Carlo algorithm satisfies both conditions, ensuring that equilibrium will be achieved eventually (although not necessarily within budget limitations).

By retaining standard Monte Carlo methods as part of the new simulation, we satisfy the first condition and provide a fast process for relaxation of local fluctuations. Additional processes satisfying detailed balance are then introduced to reduce relaxation times for large fluctuations. This strategy has been shown to be effective when the form of the important large-scale fluctuations is known.[10] The method described below provides for the automatic recognition of important fluctuations in a spin-glass.

To illustrate our method, we will discuss its application to the Ising spin-glass,

$$H=\sum_{\langle i,j\rangle} B_{ij}Ks_is_j, \tag{1}$$

where s_i takes on the values ± 1 and the factor $-1/k_BT$ has been absorbed into the coupling constant K. The $B_{i,j}$ are dimensionless variables, which describe the quenched, random interactions.

Instead of simulating different temperatures sequentially, we treat several independent "replicas" of this system at different values of K simultaneously. By including a replica index, n, we can describe the entire set of replicas with a single Hamiltonian, modifying Eq. (1) to become

$$H_R=\sum_n\sum_{\langle i,j\rangle} B_{ij}K^{(n)}s_i^{(n)}s_j^{(n)}. \tag{2}$$

Information is transferred by the "mixing" of two neighboring replicas, by use of new variables, $t_i^{(n)}$, defined at each site:

$$s_i^{(n+1)}=t_i^{(n)}s_i^{(n)}. \tag{3}$$

The pair of replicas can now be represented by the variables $\{s^{(n)}\}$ and $\{t^{(n)}\}$ and the part of the Hamiltonian describing this pair of replicas becomes

$$H_{\text{pair}}=\sum_{\langle i,j\rangle} B_{i,j}[K^{(n)}+K^{(n+1)}t_i^{(n)}t_j^{(n)}]s_i^{(n)}s_j^{(n)}. \tag{4}$$

Changing $s_i^{(n)}$ while holding $t_i^{(n)}$ fixed is equivalent to changing both $s_i^{(n)}$ and $s_i^{(n+1)}$. The effective interaction between $s_i^{(n)}$ and $s_j^{(n)}$ now depends on the sign of the product $t_i^{(n)}t_j^{(n)}$. If the product is -1, the effective coupling is proportional to $K^{(n)}-K^{(n+1)}$, which can be small if the temperature difference between replicas is small, even at low temperatures. If there is no frustration, the percolation representation[11] can now be used to simulate $\{s^{(n)}\}$, with $\{t^{(n)}\}$ held fixed. However, if the Hamiltonian contains frustration, this is only efficient for replicas that are *extremely* close in temperature.

Equation (4) was simulated with a "cluster Monte Carlo" technique, identifying clusters[12] with a "template" of sites for which the nearest neighbors have the same value of $t_i^{(n)}$. A cluster Monte Carlo step allows all spins in a cluster to be reversed. In terms of the original spin variables, this corresponds to reversal of all values of $s_i^{(n)}$ and $s_i^{(n+1)}$ in the cluster simultaneously.

The idea behind this procedure is that if the product $t_i^{(n)}t_j^{(n)}$ is positive, the original spins in each replica have the same relative alignment and are more likely to be part of a favorable local configuration than if they are aligned differently in each replica. This is the key feature that allows our method to identify important

clusters of spins. New configurations are generated in high-temperature replicas, and energetically favorable configurations are transferred to lower temperatures through replica mixing.

To implement this procedure, each cluster c is initially assigned a value $r_c = +1$, and a cluster Hamiltonian is constructed:

$$H_{\rm cl} = \sum_{\langle b,c \rangle} k_{b,c} r_b r_c. \tag{5}$$

The new effective coupling constants $k_{b,c}$ are found from Eq. (4), by addition of contributions along the boundaries between the clusters. They tend to be small in comparison with $K^{(n)}$, both because they are proportional to $K^{(n)} - K^{(n+1)}$, and because of cancellations between frustrated and satisfied interactions.

After performance of a standard Monte Carlo simulation with the cluster Hamiltonian, Eq. (5), the new values of $s_i^{(n)}$ (for fixed $t_i^{(n)}$) are found by multiplication of the old values by r_c for the appropriate cluster. The new values of $s_i^{(n+1)}$ are then found from Eq. (3).

The complete simulation procedure consists of a sweep of all replicas with standard Monte Carlo procedures, followed by application of replica Monte Carlo techniques to all pairs of replicas at neighboring temperatures. One full sweep involves a total of three updates for each replica (except the replicas at the highest and lowest temperatures), since each replica is mixed with both neighboring replicas.

The gain in efficiency requires the use of both replica mixing and cluster Monte Carlo computation. With just replica mixing and standard Monte Carlo procedure, many bonds are double strength and the simulation is very inefficient. Without replica mixing, all couplings remain strong and we cannot identify useful clusters.

For our calculations, two complete sets of replicas were used. Each set had the same distribution of temperatures, and all replicas were subject to the same quenched random bonds $\{B_{i,j}\}$. The spins $\{s_i\}$ in each replica in each set were initialized with different random numbers.

The use of two sets of replicas provides a direct consistency check and allows a convenient calculation of the overlap between two independent replicas at the same temperature.[13] For each temperature, we compute

$$q^{(n)} = N^{-1} \sum_i s_i^{(n,1)} s_i^{(n,2)}, \tag{6}$$

where the extra indices 1 and 2 refer to the two independent sets of replicas, and $N = L^d$ is the total number of sites. There is clearly a close connection between the variables $\{t^{(n)}\}$, introduced in Eq. (3), and the Parisi order parameter.[13]

To illustrate the rapid relaxation achieved by the new method, we simulated the two-dimensional Ising spin-glass, with $B_{i,j}$ taking on the values ± 1 with equal probability. Two sets of up to 32 replicas were simulated, with lattice sizes ranging from 4×4 up to 128×128. The longest runs for the largest lattices were 1.8×10^4 sweeps, which far exceeded the longest correlation times.

Figure 1 shows the correlation time τ as a function of the dimensionless inverse temperature K, with the results of a standard simulation (for some of the higher temperatures) shown for comparison. τ was obtained from the integral of the time-dependent correlation function associated with the absolute value of $q^{(n)}$:

$$f(t_1) = \frac{\langle |q(t_0)q(t_0+t_1)| \rangle - \langle |q| \rangle^2}{\langle |q|^2 \rangle - \langle |q| \rangle^2}. \tag{7}$$

Published correlation times for standard Monte Carlo methods[14-16] are even higher than those shown because of the use of different correlation functions, which were inappropriate for comparison since they vanish for the new algorithm.

The data shown are from runs on a 32×32 lattice. Estimates of correlation times for larger and smaller lattices showed no significant size dependence, within statistical errors.

In comparing these correlation times with those of standard Monte Carlo determinations, the question of whether simulation of 32 replicas reduces the efficiency by a factor of 32 arises. The answer depends on what is needed. If data are required at only a single tempera-

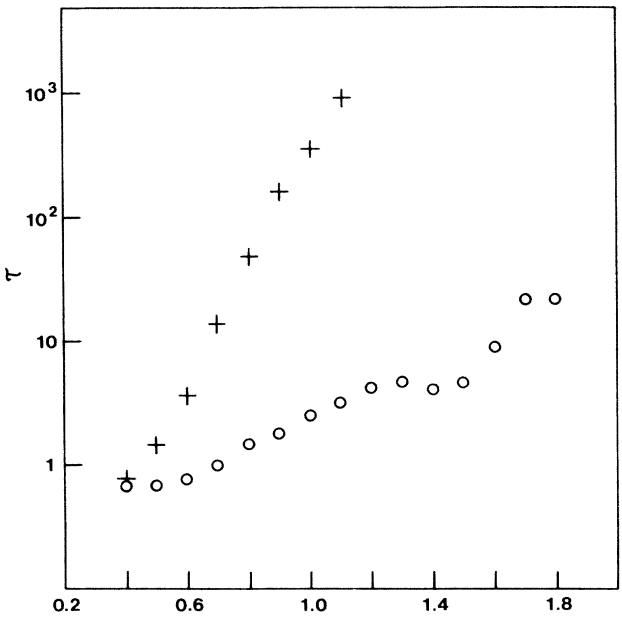

FIG. 1. Semilogarithmic plot of the correlation time as a function of K for the two-dimensional Ising spin-glass $\{B_{i,j} = \pm 1\}$ on a 32×32 lattice, with 4.2×10^5 sweeps. The correlation times for replica Monte Carlo computation are indicated by circles, with the results of a standard Monte Carlo simulation (1.6×10^5 sweeps) indicated by crosses for comparison.

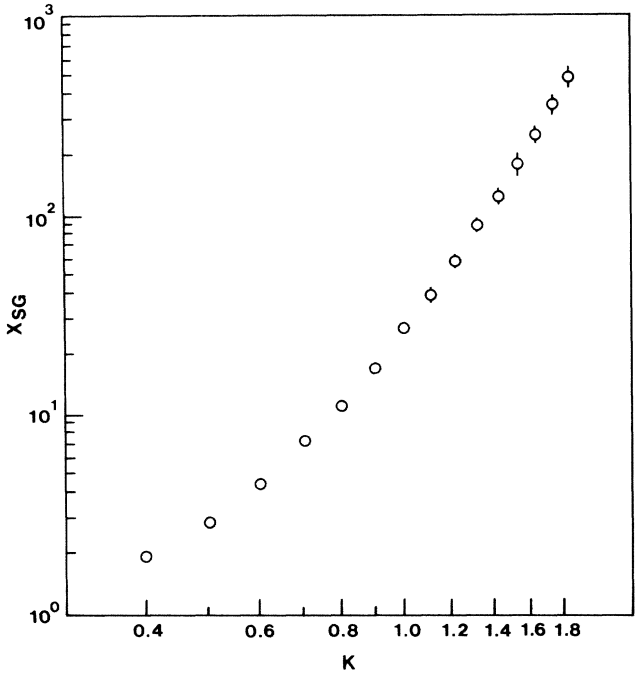

FIG. 2. Log-log plot of the spin-glass susceptibility as a function of the dimensionless inverse temperature K for the two-dimensional Ising spin-glass $\{B_{i,j}=\pm 1\}$ on a 128×128 lattice, with use of several bond distributions with up to 1.8×10^4 sweeps.

ture, this feature might be undesirable. On the other hand, for most current work thermodynamic behavior is of interest over a range of temperatures, so that this is not a drawback.

Our current program, which was written for clarity and ease of modification during development, requires about a factor of 7 more CPU time per site than a similar standard Monte Carlo simulation. Including the time for calculation of correlation functions reduces the factor. We expect future versions of the program to be even more efficient.

Figure 2 shows the spin-glass susceptibility $\chi_{SG}=N\langle q^2\rangle$ as a function of K from an average over five independent random bond configurations on a 128×128 lattice. Note that the largest coupling (lowest temperature) for which McMillan[14] obtained reliable data was $K=1.16$. Data are consistent with the hypothesis that the transition temperture vanishes,[2] with the spin-glass susceptibility diverging roughly as $T^{-5.3}$, which is a larger exponent than found in previous work.[15,16] However, it is equally compatible with a transition in the neighborhood of $K=3.6$. More work is necessary to clarify the situation.

The application of these simulation methods to other models is straightforward. A magnetic field, either uniform or random, presents no problems. Longer-ranged interactions can also be introduced, although it might prove useful to modify the definition of the template to control the average size of clusters. One possibility would be to demand that neighboring spins have the same relative orientation in other pairs of replicas to be in the same template cluster. Any combination of the variables that remain fixed during one Monte Carlo step is allowed. Models with different spin symmetry, such as the XY model, etc., can be treated with an appropriate generalization of Eq. (3). Since one of our main purposes in the present work was to test the method, we kept the two sets of replicas completely independent. However, for optimal efficiency in future work, information can be exchanged between the two sets by the mixing of replicas at the same temperature with a modification of Eq. (4).

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Note added.—Since we submitted this paper a Letter by Singh and Chakravarty[17] has appeared, confirming the value of $\gamma=5.3$, by use of high-temperature series expansions.

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