

Replica Monte Carlo Simulation (Revisited)

Jian-Sheng WANG⁽¹⁾ and Robert H. SWENDSEN⁽²⁾

⁽¹⁾*Department of Computational Science, National University of Singapore,
Singapore 117543, Republic of Singapore*

⁽²⁾*Department of Physics, Carnegie Mellon University, Pittsburgh, PA 15213, USA*

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In 1986, Swendsen and Wang proposed a replica Monte Carlo algorithm for spin glasses [Phys. Rev. Lett. **57** (1986) 2607]. Two important ingredients are present, (1) the use of a collection of systems (replicas) at different of temperatures, but with the same random couplings, (2) defining and flipping clusters. Exchange of information between the systems is facilitated by fixing the τ spin ($\tau = \sigma^1 \sigma^2$) and flipping the two neighboring systems simultaneously. In this talk, we discuss this algorithm and its relationship to replica exchange (also known as parallel tempering) and Houdayer's cluster algorithm for spin glasses. We review some of the early results obtained using this algorithm. We also present new results for the correlation times of replica Monte Carlo dynamics in two and three dimensions and compare them with replica exchange.

§1. Introduction

The spin glass problem has been studied extensively over the past 30 years.^{1)–3)} Monte Carlo simulation has been one of the main tools. However, spin glass models are among the most difficult to simulate, due to their extremely slow dynamics at low temperatures. Unlike the ferromagnetic models,⁴⁾ cluster algorithms for spin glasses have only limited success.

In 1986, a cluster algorithm by the name “replica Monte Carlo” was proposed for spin glasses.⁵⁾ Although several other algorithms were later developed,^{6)–9)} replica Monte Carlo remains one of the best algorithm for spin glasses. Replica Monte Carlo works very well in two dimensions, reducing the correlation time enormously comparing to single spin flips. In one dimension, it is similar to the Swendsen-Wang cluster algorithm with a constant correlation time independent of system size. In three and higher dimensions, it still provides a great improvement over single spin flips, although improvement is not as dramatic. As we will show here, replica Monte Carlo becomes essentially equivalent to “replica exchange” or “parallel tempering” of Hukushima and Nemoto⁸⁾ in three or higher dimensions.

§2. Replica Monte Carlo

Replica Monte Carlo actually contains two ideas, (1) the simultaneous simulation of a collection of systems at different temperatures, (2) cluster moves defined through the τ spin, where $\tau = \sigma^1 \sigma^2$ is the overlap of the systems at nearby temperatures. The first idea was later used in parallel tempering and also in a similar proposal by Geyer.¹⁰⁾

The reason for simulating an array of systems with the same random couplings at different temperature T_i is that configurations can be rapidly equilibrated at high temperatures and the information can be quickly transferred to low temperatures. Exchanges are carried out pairwise for systems at neighboring temperatures. Consider two replica configurations σ^1 and σ^2 . The joint distribution of the two spin configurations σ^1 and σ^2 is a product of the two independent Boltzmann distributions at temperature T_1 and T_2 , respectively. The combined system has the “Hamiltonian”

$$H_{\text{pair}}(\sigma^1, \sigma^2) = - \sum_{\langle i, j \rangle} (\beta^1 J_{ij} \sigma_i^1 \sigma_j^1 + \beta^2 J_{ij} \sigma_i^2 \sigma_j^2), \quad (2.1)$$

where $\beta^1 = 1/(kT_1)$ and $\beta^2 = 1/(kT_2)$, with a probability distribution proportional to $\exp(-H_{\text{pair}}(\sigma^1, \sigma^2))$. Clearly, any Monte Carlo moves that keep the above distribution invariant are valid. Specifically, we can design Monte Carlo moves that satisfy detailed balance with respect to the joint distribution. There are many possible such choices.

In our original replica Monte Carlo implementation,^{5), 11), 12)} we proposed cluster moves. The clusters are defined by connected region of the same τ -spin, $\tau_i = \sigma_i^1 \sigma_i^2$. Two nearest neighbor sites i and j are considered connected and in the same cluster if $\tau_i = \tau_j$. To keep the definition of the τ -cluster invariant with respect to the move, we must simultaneously flip both systems. More precisely, we rewrite the pair Hamiltonian in the form

$$H_{\text{pair}}(\sigma^1; \tau) = - \sum_{\langle i, j \rangle} (\beta^1 + \beta^2 \tau_i \tau_j) J_{ij} \sigma_i^1 \sigma_j^1. \quad (2.2)$$

Since τ -spins are fixed, the system is a new spin glass with interaction strength proportional to $\beta^1 + \beta^2$ inside a τ -cluster and decreased to $\beta^1 - \beta^2$ between the τ -clusters. In particular, if $\beta^1 = \beta^2$ these τ clusters are free to flip without costing any energy. In such a case, the τ clusters also have a good physical meaning – they correspond to the Edwards-Anderson order parameter for spin glass. The interactions between the clusters are governed by the above Hamiltonian and can be rewritten as an effective Hamiltonian between clusters. Let $\eta_a = 1$ be the initial spin value for all cluster a indicating non-flipping, and $\eta_a = -1$ indicating a flip of the cluster, the effective interaction Hamiltonian between clusters is

$$H_{\text{cls}}(\eta) = - \sum_{a, b} k_{a, b} \eta_a \eta_b, \quad (2.3)$$

where the effective coupling is from the sum of the couplings along the boundary between cluster a and b ,

$$k_{a, b} = (\beta^1 - \beta^2) \sum_{\langle i \in a, j \in b \rangle} J_{ij} \sigma_i^1 \sigma_j^1. \quad (2.4)$$

Note that the σ above should take the value before the cluster flips. We can now simulate the above cluster model with any valid Monte Carlo algorithm, e.g., Metropolis

single spin flip, or even Swendsen-Wang cluster flip. After the cluster update to variables η_a , the original spins are changed according to $\sigma_i^1 \leftarrow \eta_a \sigma_i^1$ and $\sigma_i^2 \leftarrow \eta_a \sigma_i^2$ for $i \in a$. The replica cluster moves must be supplemented by a normal Metropolis simulation of σ^1 and σ^2 to break the conservation of τ . The Metropolis step makes the algorithm ergodic.

In our earlier implementation, we made a sequential sweep of all the clusters with a heat-bath rate. It is interesting to note that the replica exchange (parallel tempering) is equivalent to a trial move where all the $\tau = -1$ clusters are flipped, or a move where all $\tau = +1$ clusters are flipped, followed by a global sign flip. Since the τ spins are constant with respect to the replica Monte Carlo moves, any move based on values of τ satisfies detailed balance and is thus valid. Iba gave further discussion for the relation between replica Monte Carlo and other extended ensemble methods.¹³⁾ Another connection is with the cluster algorithm of Houdayer.⁷⁾ In Houdayer's implementation,¹⁴⁾ a site is picked at random, the associated τ -cluster with that site is formed and flipped with probability 1 for systems with same temperature. This is similar to the Wolff variation¹⁵⁾ of the Swendsen-Wang algorithm. For systems between different temperatures, replica exchange was used.

Another improvement that was suggested in 1986, but not implemented,¹¹⁾ is to introduce a Swendsen-Wang step within the τ clusters. In such case, each bond has interaction strength $(\beta^1 + \beta^2)J_{ij}\sigma_i^1\sigma_j^1$. The presence of a bond is set with probability $P = 1 - \exp(-2(\beta^1 + \beta^2)|J_{ij}|)$ if the interaction is satisfied, i.e., $J_{ij}\sigma_i^1\sigma_j^1 > 0$. The bond is absent otherwise. We do not apply this step between the τ clusters. This further breaks up the τ clusters. One technical advantage of having this step is that ergodicity can be maintained without evoking a single-spin-flip sweep. Although it is a great help at high temperatures, at interesting temperatures for spin glass phase transitions, $\beta \approx 1$, the value of $P \approx 0.98$ is too large. The dynamics is nearly the same as the original version.

As it is obvious, most of the CPU time is devoted to the computation of the effective coupling, $k_{a,b}$. This can be done efficiently at about $O(N)$ where N is the number of spins of the system. This is because that the number of possible interactions is bounded by Nd where d is the dimension of the system. We can pre-allocate sufficient memory based on cluster size and the total number of clusters. In a new implementation of the algorithm, on a 1GHz Itanium 2, each replica Monte Carlo sweep (MCS) per spin takes 1.06 μsec (on a 128×128 lattice). This should be compared with a straightforward Metropolis algorithm, which runs at 0.29 μsec per MCS per spin. Little size dependence is seen on the speed.

§3. Some Early Results

The replica Monte Carlo was used to compute two-dimensional spin-glass susceptibility⁵⁾ and low-temperature heat capacity¹¹⁾ for the $\pm J$ spin glass model, where the coupling J_{ij} takes $+J$ or $-J$ with equal probability. The spin-glass susceptibility was analyzed in the form of power-law divergence $\chi \sim T^{-\gamma}$, assuming $T_c = 0$. The exponent $\gamma \approx 5.1$ was found. Recent work⁷⁾ seems to support

$\chi \sim \exp(2(2 - \eta)\beta J)$ instead, where η is the critical exponent associated with correlation function, $g(r) \sim r^{-\eta}$.

The low-temperature heat capacity is more interesting. We found¹¹⁾ that $c \sim \beta^2 \exp(-2\beta J)$ from our simulations and argued that the elementary excitations in $\pm J$ Ising spin glass are kink/antikink pairs. This result was disputed,¹⁶⁾ but recent more extensive calculations with exact algorithms for partition function¹⁷⁾ supported our result.

We also used the replica Monte Carlo algorithm with a renormalization group analysis.¹⁸⁾ The results show an early confirmation of the absence of a phase transition at finite temperature in two dimensions, and clear evidence of a finite-temperature spin-glass phase transitions in three and four dimensions.

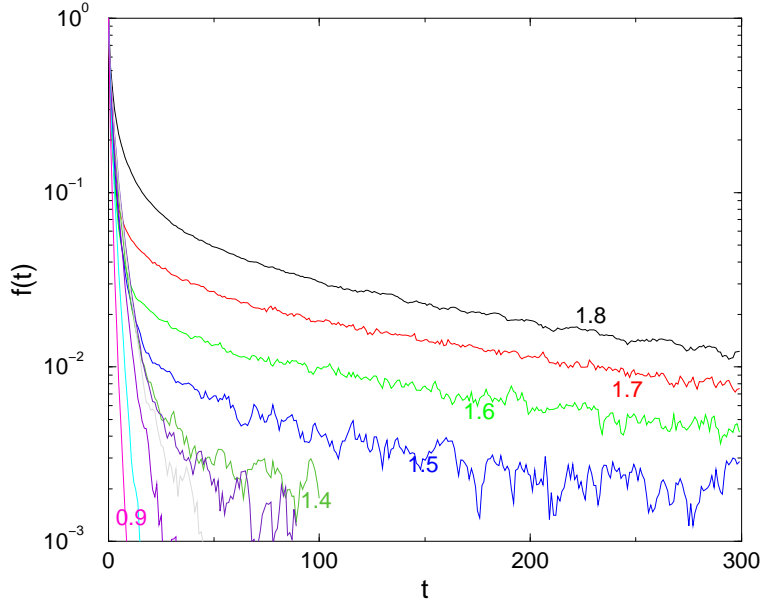


Fig. 1. Time correlation function for the order parameter q on a 128×128 $\pm J$ Ising spin glass system, using replica Monte Carlo with βJ distributed from 0.1 to 1.8 in steps of 0.1 (only 0.9 to 1.8 are plotted).

§4. Relaxation Times and Comparison

In order to compute the spin-glass order parameter and susceptibility, two sets of replica are used. In each sweep, we do one single-spin-flip sweep for the two sets, and replica Monte Carlo between nearby temperatures for both sets, and replica Monte Carlo at same temperature between the sets. Swendsen-Wang clusters are generated within a τ -cluster. The Edwards-Anderson order parameter appears to contain the slowest relaxation mode (the energy correlations decay faster). Thus we

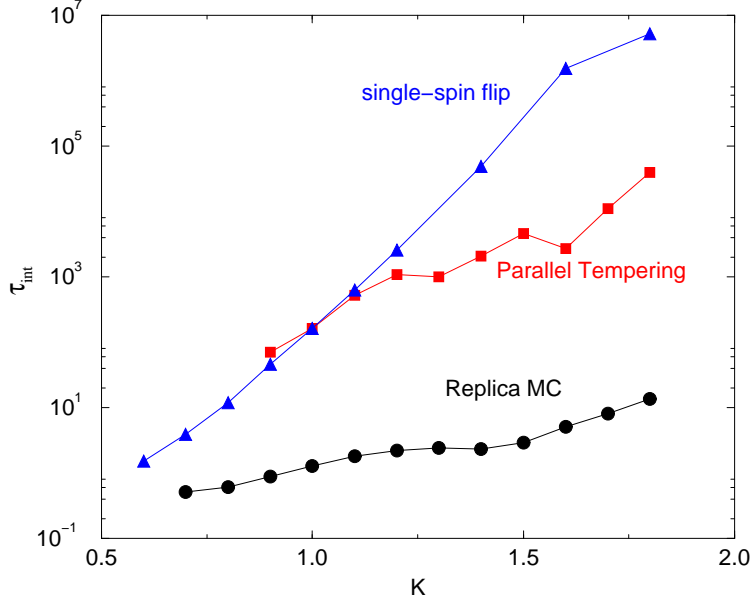


Fig. 2. Comparison of integrated correlation time on a 128×128 lattice for single-spin-flip (triangles), parallel tempering (squares), and replica Monte Carlo (circles). The $K = \beta J$ value is distributed from 0.1 to 1.8 in spacing of 0.1. Typically, 10^6 MCS are used.

compute (for a single realization of random coupling)

$$f(t) = \frac{\langle q(t)q(0) \rangle - \langle q(0) \rangle^2}{\langle q(0)^2 \rangle - \langle q(0) \rangle^2}, \quad (4.1)$$

where $q = (1/N)|\sum_i \tau_i|$, τ_i is the overlap spin at the same temperature.

In figure 1, we present correlation functions at some typical temperatures. The function has an initial fast decay followed by a slow relaxation at long time. This causes a factor of 10 difference between the integrated correlation time, defined by

$$\tau_{\text{int}} = \int_0^\infty f(t) dt, \quad (4.2)$$

and exponential correlation time, $f(t) \approx A \exp(-t/\tau)$, $t \rightarrow \infty$. The initial fast decay reflects the quick swap of configurations between neighboring temperatures. However, they can be swapped back again, leading to a longer exponential correlation times. In any case, the integrated correlation time is relevant to the error in sample average. In figure 2, we present τ_{int} for one single random sample of 128×128 . In contrast to single-spin-flip and parallel tempering, remarkably small correlation times are observed for the replica Monte Carlo algorithm.

In figure 3, we compare several algorithms at 32×32 . Comparing to the results in fig. 2, we found that size effect is small. The curve labelled Houdayer is from

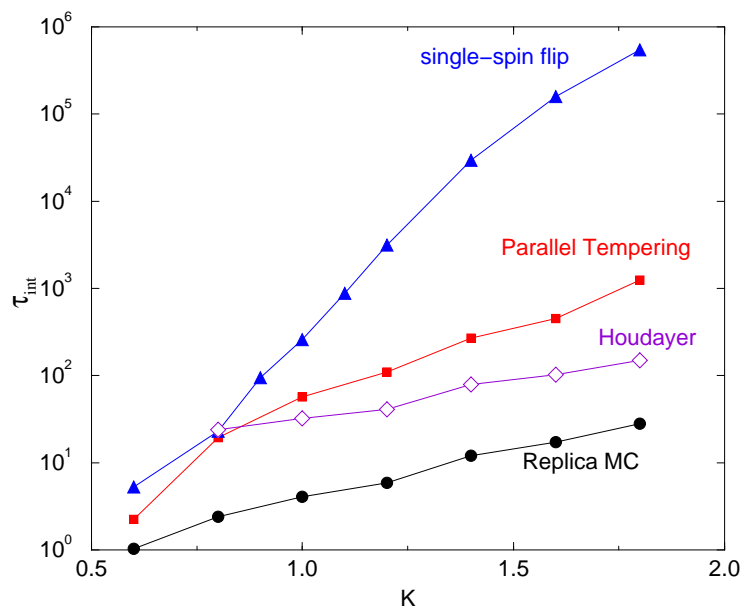


Fig. 3. Comparison of integrated correlation times on a 32×32 lattice for several algorithms. The $K = \beta J$ value is distributed from 0.2 to 1.8 in spacing of 0.2.

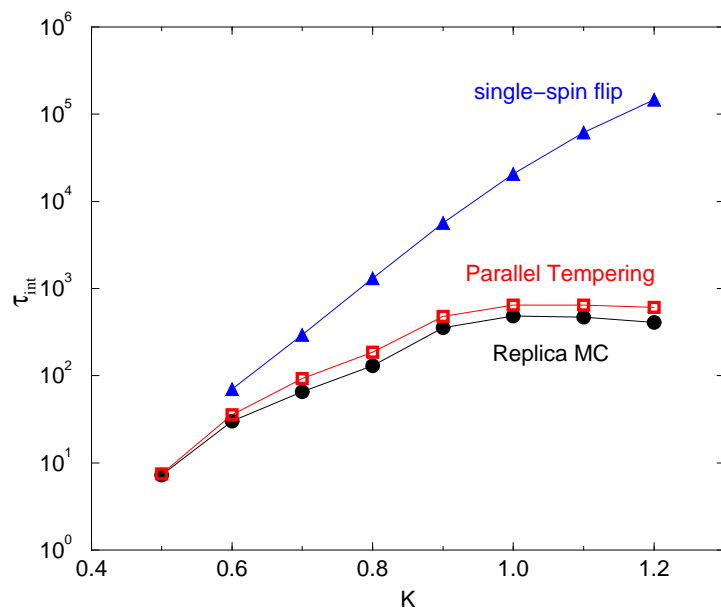


Fig. 4. Integrated correlation time on a $12 \times 12 \times 12$ lattice for single-spin-flip, parallel tempering, and replica Monte Carlo. The βJ value is distributed from 0.1 to 1.2 in spacing 0.1.

a simulation of 2 sets of systems (instead of a large number of sets). A unit time step consists of one Metropolis sweep for all the systems for the two sets, single cluster moves between the sets, and replica exchanges in a set between neighboring temperatures.

In figure 4, we present the correlation times for a three-dimensional $\pm J$ Ising spin-glass system of size 12^3 . The replica Monte Carlo includes moves between the two sets at same temperature. As one can see, the performance of replica Monte Carlo and parallel tempering is nearly the same. This is because in three or higher dimensions, there are essentially only two τ clusters, one with $+\tau$ -spin and other $-\tau$ -spin. Flipping either of them is equivalent to exchange of configurations.

In these correlation time comparisons, we have not fine-tuned the simulation parameters (distribution of temperatures, number of sweeps for each type of move, and number of sets). Future research on the optimal simulation parameters might reveal further improvements in efficiency.

§5. Conclusion

We introduced the replica Monte Carlo algorithm and presented new correlation time data. These results show that replica Monte Carlo algorithm is extremely efficient in two dimensions, and is even much better than parallel tempering. In three dimensions, replica Monte Carlo and parallel tempering are of comparable efficiency.

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