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CLUSTER-FLIPPING MONTE CARLO ALGORITHM AND CORRELATIONS IN "GOOD" RANDOM NUMBER GENERATORS

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Monte Carlo simulations of the two-dimensional Ising model at criticality are performed using the cluster-flipping Wolff algorithm. Correlations found recently in a widely used "good" random number generator are observed to depend strongly and systematically on the size of the Monte Carlo system. Rather long-range correlations seem to cause trouble, in growing clusters of specific size in a biased way.

To overcome critical slowing down near the phase transition in Monte Carlo simulations of Ising models, cluster-flipping algorithms have been developed.[1, 2] For instance, in the Wolff algorithm, clusters are generated on a lattice by connecting bonds from a randomly chosen starting point to successive nearest neighbors with a probability

$$p = 1 - \exp(-2J/k_BT), \tag{1}$$

where J is the energy of a bond and T is the temperature. All spins belonging to a cluster are flipped.

However, it has recently been noted that supposedly "good" random number generators (RNGs) show important correlations when applied to the Wolff algorithm, leading to incorrect results [3]. In particular, the widely used shift register algorithm of Kirkpatrick and Stoll, the R250, was shown to give wrong results for the two-dimensional Ising model with $L \times L = 16 \times 16$ spins, subject to full periodic boundary conditions, at criticality, $k_BT_C/J = 2/\ln(1+\sqrt{2})$. The R250 is based on the recursion [4]

$$X_n = X_{n-A} \text{ XOR } X_{n-B} \tag{2}$$

with $(A, B) = (103, 250)$. Other pairs of numbers have been also advocated. The R250 had passed very successfully a number of statistical tests; see, for example, a recent comparative study of RNGs [5].

In contrast, the supposedly rather poor linear congruential RNG, CONG,

$$X_n = (16807 \cdot X_{n-1}) \bmod (2^{31} - 1), \tag{3}$$

reproduced well, within the error bars, the exact values of the energy E and specific heat C of that Ising model [3].

Independently, pronounced deviations from correct results have been noted by using the R250 for another cluster growth problem, generating self-avoiding walks on a cubic lattice [6].

In our simulations of the two-dimensional nearest-neighbor Ising model, applying the Wolff algorithm, we extended the prior work to different lattice sizes, $4 \leq L \leq 64$. We implemented both the R250 (with variants, see below) and the CONG. Simulations were done at T_c. For each lattice size, the system was equilibrated in 10^6 updates. Averages were computed from the following 10^7 clusters. Internal energy E and, from energy fluctuations, specific heat C were computed. Each run was subdivided, evaluating data after each $5 \cdot 10^5$ clusters, to determine statistical errors in the standard way.

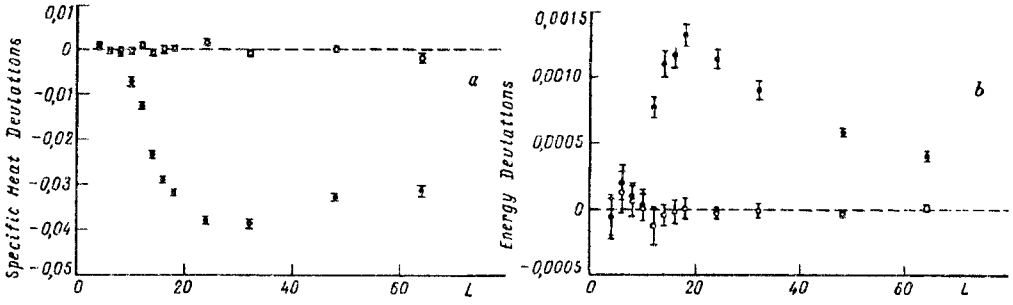

Fig.1. Deviations of the Monte Carlo data from the exact values, eq. (4), as a function of the size of the lattice, $L \times L$, for (a) specific heat, C and (b) energy E. The open circles refer to the CONG and the solid diamonds refer to the CONG

Figure 1 shows results for the deviations from the exact values, Δ, defined by, for the specific heat,

$$\Delta = (C_{MC} - C_{\text{exact}})/C_{\text{exact}}. \tag{4}$$

$C_{exact} = C_{exact}(L, T_c)$ follows from Ref.[7]. The analoguous definition has been used for the internal energy, $-E$.

Obviously, the CONG yields accurate results, within the error bars, for all sizes studied. On the other hand, the R250 gives correct results only for small lattices sizes, $L \leq 8$. The maximal deviations occur for L around 20, for the energy, or 30, for the specific heat. There the results deviate from the exact values by about 20 or 40 standard deviations, in agreement with the findings of Ferrenberg et al [3]. However, the disagreement becomes less pronounced when the system size is increased furthermore.

It is important to note that the choice of the starting point of a cluster has no significant influence on the data. It may be fixed or chosen randomly. Similarly, the order of choosing subsequent bonds to generate the cluster plays no important role.

To get a further clue on the correlations in the R250, we looked at the effect of systematically destroying short-range correlations. In growing the cluster, only each Nth random number was used, with N ranging from 1 to 5. The system size was fixed, $L = 16$. As shown in Fig. 2, there is an interesting non-monotonic behavior at $N = 4$. For $N = 5$, the deviations are rather small.

We also looked at the effect of introducing randomness in the use of the R250, motivated by the implementation of that random number generator in the cluster-algorithm special-purpose computer by Talapov et al [8, 9] In particular,

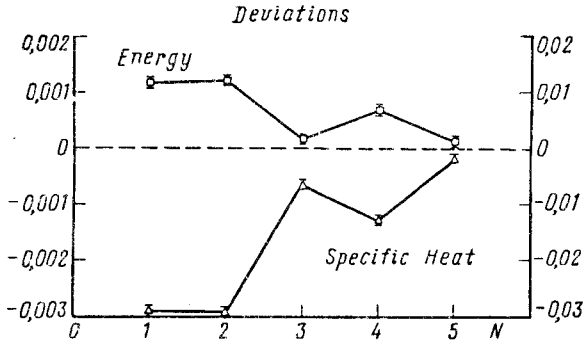

Fig.2. Deviations from exact values, $L = 16$, as a function of discarded random numbers, N, in the R250. Energy scale is shown by the left axis. Right axis describes specific heat scale

at each step of the growing cluster, we called at least four (up to ten) random numbers, while at most three were actually used. For $4 \leq L \leq 64$, the deviations from the exact values follow quantitatively a similar trend as before (Fig. 1), but they are appreciably smaller.

In summary, our results indicate that the R250 fails to generate clusters of specific sizes, being dominant for L around 20 to 30, in the proper way. This observation agrees with the recent explanation of Grassberger [10] of the correlations in the R250 for self-avoiding random walks. They are of rather long range, with a typical range of a few hundreds. If the dominant clusters in the simulations are of corresponding size, their structures are expected to be correlated and biased. Such long-range correlations may be overlooked by standard statistical tests of RNGs. The non-monotonic behavior for the deviations from the exact values with the number of discarded random numbers agrees with the interpretation that short-range correlations do not primarily cause the trouble. The observed behavior may help to pinpoint the weakness of the R250. By randomly perforating the R250, as is done for the cluster-algorithm special-purpose computer, large lattice sizes are expected to be simulated rather accurately. The simple CONG showed best results in this study on clusters in Ising models of moderate sizes.

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