Using random number generators in Monte Carlo simulations

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One of the standard tests for Monte Carlo algorithms and for testing random number generators is the two-dimensional Ising model. We show that at least in the present case, where we study the two-state clock model, good random number generators can give inconsistent values for the critical temperature. [S1063-651X(98)05110-1]

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There has been rapid growth in the use of Monte Carlo techniques in several areas following the development of more powerful computers. Of course, with this development came the necessity of developing routines for more sophisticated random number generators (RNG's). Long sequences of random numbers are required in numerous applications, in particular statistical mechanics and particle physics. Monte Carlo simulations are subject to statistical and systematic errors [1,2]. Statistical errors are *less* serious in the sense that one can control the error bars associated with each measurement. However, poor random number sequences lead to systematic errors in the Monte Carlo simulations [1,3], which, in many cases, are impossible to evaluate. Even using high-quality RNG's we can get into trouble depending on the Monte Carlo method used, e.g., a single-spin-flip algorithm such as Metropolis or a cluster algorithm such as Swendsen-Wang or Wolff embedding. Ferrenberg *et al.* [1], studying the Ising model where exact results are known, have shown that high-quality RNG's may lead to systematic errors for some algorithms due to the existence of unexpected large correlations. In this work we have used two different Monte Carlo (MC) algorithms and two distinct RNG's to study the continuous clock model, with $n=2$ (CM2), defined by the Hamiltonian [4]

$$H=-J\sum_{i,j}\cos(\theta_i-\theta_j)-h_n\sum_i\cos(n\theta_i). \tag{1}$$

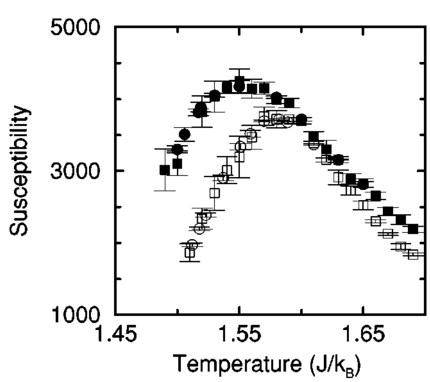

FIG. 1. Magnetic susceptibility for $L=20$. Empty and filled symbols correpond to RAN2 and RANLUX, respectively. Circles are for hybrid and squares for Metropolis algorithms.

Here J is a coupling constant, h_n is a local field, and θ_k is an angle associated with the site k. The parameter n sets the symmetry of the Hamiltonian, $n=0$ is the pure planar rotator model, $n=1$ corresponds to an external field, $n=2$ has Z_2 symmetry, which corresponds to the Ising universality class for any $h_2\neq 0$, and so on. We have determined the critical temperature T_c and the critical exponents for $h_2=1$. Surprisingly, we obtained different values for T_c depending on the RNG used. The results seem to be independent of the MC algorithm.

All the simulations were carried out on an IBM SP2 [5] parallel machine and in a three 200 MHz Pentium PRO cluster [6]. We have used lattices of size $L=4$, 6, 8, 10, 16, 20, 40, 60, and 100 in order to make a reasonable finite size scaling analysis. Steps in temperature were of size $\delta T=0.01$ (temperature is measured in units of J/k_B). Each point is the result of averages over 10^5–(2.5×10^6) independent configurations. Close to the maxima of the specific heat and susceptibilities we have used 2.5×10^6 configurations, so that the calculated error bars were never greater than 0.5% for the hybrid algorithm discussed below (circles in Fig. 1). For the location of the extrema of susceptibility and specific heat we have used the single histogram technique, which allows us to extract the maximum information from our data [7].

We have used an algorithm that is a combination of the cluster Wolff embedding with Metropolis realignments, which was successfully used to study the three-dimensional

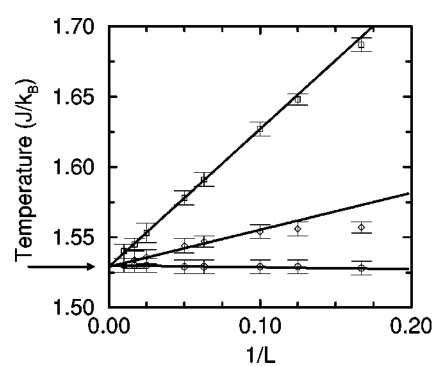

FIG. 2. Shown from top to bottom are the size dependence of the location of the extrema for the magnetic susceptibiltity, the specific heat, and Binder's fourth-order cumulant. In all cases we used the RAN2 random number generator.

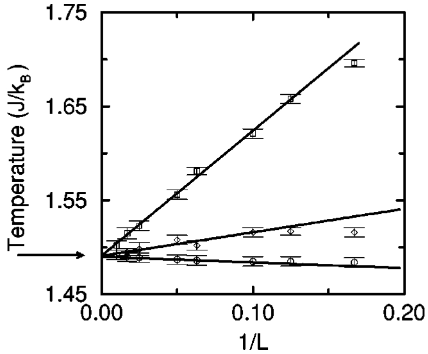

FIG. 3. Symbols are the same as in Fig. 1. Here we have used RANLUX.

Heisenberg model [8] and also the two-dimensional *XY* model [9]. We have also calculated some points using the Metropolis algorithm. Results for the magnetic susceptibility are presented in Fig. 1 for comparison. For each of the MC methods we have used two distinct RNG's: a multiplicative congruential (RAN2) [10] and RANLUX, which uses the algorithm developed by Lücher [11] based on an algorithm introduced by Marsaglia and Zaman [12] and implemented by James [13]. RANLUX has four *luxury* levels and we have used the fourth level, which has passed all known statistical tests [13].

It is well known that CM2 has a second-order phase transition [4]. However, the value of the critical temperature is not known. From Fig. 1 it is already evident that the critical temperature will be estimated differently when using different RNG's. Figures 2 and 3 show the size dependence of the locations of the extrema of different thermodynamic quantities when using RAN2 and RANLUX, respectively. Individually, each simulation seems to be reliable. However, they give different values for T_c. The difference between the two estimated critical temperatures is about 2%, much higher than the intrinsic errors from the MC method. The question of deciding which is the correct one is not an easy task. Suppose, for example, that we expect the system to be in some particular universality class. Then we can assume that we will get the correct critical exponents at the critical temperature. Having this in mind, we also estimated the critical exponents using both RAN2 and RANLUX. The results are presented in Table I. They clearly show that both RNG's give the correct Ising exponents in spite of the estimated critical temperatures being different by about 2%. This striking behavior was not reported in the extensive work by Ferrenberg *et al.* in Ref. [1], where they studied the Ising model. The fact that CM2 is a continuous model seems to play an important role. We do not know the cause of this behavior, but certainly it comes from a different source from that suggested by Ferrenberg *et al.*

TABLE I. Estimated critical temperatures and exponents using RAN2 and RANLUX.

Method	T_c	α	β	γ
RAN2	1.529(5)	0.05(4)	0.13(4)	1.75(9)
RANLUX	1.491(6)	0.00(3)	0.14(6)	1.71(7)
exact		0	0.125	1.75

In conclusion, we performed a careful Monte Carlo simulation of the continuous clock model with Z_2 symmetry that is in the same universality class as the Ising model where the critical exponents are exactly known. We used two different random number generators. Although, we found the correct exponents using both generators, a discrepancy of 2% was found in the critical temperature, which seems to be independent of the used Monte Carlo algorithm. The problem we have found with the RNG's raises concern about other generators. The kind of inconsistency we have observed imposes a potential danger for simulations. In particular this means that it is not enough to test RNG's only in Ising models as is the standard practice in the simulational community.

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[1] Alan M. Ferrenberg, D. P. Laudau, and Y. Joanna Wong, Phys. Rev. Lett. **23**, 3382 (1992), and references therein.
[2] Alan M. Ferrenberg, D. P. Laudau, and K. Binder, J. Stat. Phys. **63**, 867 (1991).
[3] M. N. Barber, R. B. Pearson, D. Toussaint, and J. L. Richardson, Phys. Rev. B **32**, 1720 (1985).
[4] J. V. José, L. P. Kadanoff, S. Kirkpatrick, and D. R. Nelson, Phys. Rev. B **16**, 1217 (1977), and references therein.
[5] Centro Nacional de Processamento de Alto Desempenho para Minas Gerais e *o* Centro Oeste (CENAPAD-MG/CO) Brazil.
[6] Laboratório de Simulação, Departamento de Física, Universidade Federal de Minas Gerais, Brazil.
[7] P. Peczak, A. M. Ferrenberg, and D. P. Landau, Phys. Rev. B **43**, 6087 (1991); A. M. Ferrenberg and D. P. Landau, *ibid.* **44**, 5081 (1991).
[8] H. G. Evertz and D. P. Landau, Phys. Rev. B **54**, 12 302 (1996).
[9] B. V. Costa, J. E. R. Costa, and D. P. Landau, J. Appl. Phys. **81**, 5748 (1997); J. E. R. Costa and B. V. Costa, Phys. Rev. B **54**, 994 (1996).
[10] *Numerical Recipes in C*, 2nd ed., edited by William H. Press, Saul A. Teukolsky, William T. Vetterling, and Brian P. Flannery (Cambridge University Press, Cambridge, 1992), p. 282.
[11] Martin Lücher, Comput. Phys. Commun. **79**, 100 (1994).
[12] G. Marsaglia and A. Zaman, Ann. Appl. Prob. **1**, 462 (1991).
[13] F. James, Comput. Phys. Commun. **79**, 111 (1994).