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Physical Tests for Random Numbers in Simulations

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We propose three physical tests to measure correlations in random numbers used in Monte Carlo simulations. The first test uses autocorrelation times of certain physical quantities when the Ising model is simulated with the Wolff algorithm. The second test is based on random walks and the third on blocks of n successive numbers. We apply the tests to show that recent errors in high precision Ising simulations using generalized feedback shift register algorithms are due to short range correlations in random number sequences.

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The Monte Carlo (MC) simulation method is a standard technique in physical sciences [1]. The key ingredient in its successful application lies in the quality of random numbers used, which are usually produced by deterministic pseudorandom number (PRN) generator algorithms. Several tests for PRN generators have been suggested [2–4] and conducted [3–6] to test PRN generators, but none of them can prove that a given generator is reliable in *all* applications. Sometimes the inevitable correlations in their output can lead to erroneous results, as recently demonstrated in high-precision MC simulations for some commonly used generators combined with special simulation algorithms [7–11].

In this Letter, our purpose is to introduce physical tests which allow more precise characterizations of correlations which may cause problems in simulations. These tests are then used to demonstrate that for some generators there exist nontrivial *local* correlations which are present in rather short subsequences of random numbers and cannot always be detected by conventional test methods [2,3,6]. We start by generalizing the Ising model simulations of Refs. [7,10,11] to show that the local correlations lead to *deviations in the cluster formation process* of the Wolff algorithm [12] which explains the errors observed in Refs. [7,10,11]. As a test of random numbers, we show that *integrated autocorrelation times* [13] of certain

physical quantities are particularly sensitive measures of local correlations. We then introduce *random walk* and *n-block* tests and show how these tests can be used to precisely measure the length of correlations in PRN sequences.

The PRN generators tested in this work include generalized feedback shift register (GFSR) algorithms [14], which are of the form $x_n = x_{n-p} \oplus x_{n-q}$, where \oplus is the bitwise exclusive OR operator. They are denoted by R_p ; recommended values for p and q ($p > q$) can be found, e.g., in Ref. [15]. Other generators include a linear congruential generator $x_n = (16807 \times x_{n-1}) \bmod(2^{31} - 1)$ [16] known as GGL (CONG in Ref. [7]), RAN3 [17], which is a lagged Fibonacci generator $x_n = (x_{n-55} - x_{n-24}) \bmod 2^{31}$, and a combination generator RANMAR [18]. The GFSR generators were initialized with 32-bit integers produced by GGL. Other initialization methods including the one in Ref. [19] were also checked, but the results were unaffected.

In Refs. [7,10,11] problems with GFSR generators arose when the two-dimensional Ising model was simulated on a square lattice with the Wolff algorithm [12]. We carried out analogous simulations for an Ising model of linear size $L = 16$ at $K_c = \frac{1}{2} \ln(1 + \sqrt{2})$, for a variety of generators listed in Table I. Our implementation of the single cluster search algorithm follows Ref. [20]. We

TABLE I. Results of simulations for the Ising model at criticality with the Wolff algorithm. The number of samples is $N = 10^7$, and k is the decimation parameter. The errors shown correspond to σ [13]. The most erroneous results are in boldface. See text for details.

Generator	k	q	$\langle E \rangle$	$\langle \hat{\chi} \rangle$	$\langle c \rangle$	τ_E	$\tau_{\hat{\chi}}$	τ_c
R31	1	3	1.46774(7)	0.564(2)	0.5664(3)	1.233(4)	1.058(3)	0.507(2)
R250	1	103	1.45509(7)	0.548(2)	0.5474(2)	1.333(4)	1.143(4)	0.589(4)
	3	103	1.45302(7)	0.545(2)	0.5452(2)	1.446(6)	1.226(5)	0.628(5)
R521	1	168	1.45379(7)	0.546(2)	0.5461(2)	1.384(5)	1.182(5)	0.604(4)
R1279	1	418	1.45312(7)	0.545(2)	0.5454(2)	1.426(5)	1.215(4)	0.622(3)
R2281	1	1029	1.45311(7)	0.545(2)	0.5456(2)	1.439(5)	1.226(5)	0.627(5)
R4423	1	2098	1.45303(7)	0.545(2)	0.5454(2)	1.441(5)	1.226(5)	0.624(4)
R9689	1	4187	1.45313(7)	0.546(2)	0.5455(2)	1.444(5)	1.229(5)	0.625(4)
R19937	1	9842	1.45294(7)	0.545(2)	0.5452(2)	1.434(5)	1.220(5)	0.624(4)
R44497	1	21034	1.45292(7)	0.545(2)	0.5452(2)	1.434(5)	1.219(5)	0.622(2)
RAN3			1.45254(7)	0.545(2)	0.5446(2)	1.447(5)	1.231(5)	0.630(3)
GGL			1.45309(7)	0.545(2)	0.5454(2)	1.436(5)	1.221(5)	0.622(4)
RANMAR			1.45303(7)	0.545(2)	0.5452(2)	1.443(5)	1.227(5)	0.624(4)

calculated the energy E , the magnetic susceptibility $\hat{\chi}$, and the (normalized) size of the flipped clusters c . We then calculated the corresponding *integrated autocorrelation times* τ_E , $\tau_{\hat{\chi}}$, and τ_c , by first calculating the autocorrelation functions,

$$C(t) = \frac{\langle A(t_0)A(t_0 + t) \rangle - \langle A(t_0) \rangle^2}{\langle A(t_0)^2 \rangle - \langle A(t_0) \rangle^2}, \quad (1)$$

and then following the procedure in Ref. [13].

A summary of the results in Table I shows that based on this test, the generators can be classified into two categories. For the energy $\langle E \rangle$, for example, deviations from the exact result of $\langle E \rangle = 1.45312$ [21] for R31, R250, R521, and RAN3 are much larger than 3σ , where σ is the standard deviation [13]. In particular, $\langle c \rangle$ reveals that in the erroneous cases the *average flipped cluster size* is biased. Most striking, however, is the behavior of the integrated autocorrelation times. For generators, which show no significant deviations in $\langle E \rangle$, $\langle \hat{\chi} \rangle$, or $\langle c \rangle$, results for the τ 's agree well with each other. However, for R31 and R250 the integrated autocorrelation times show errors of about 8%. We thus propose these quantities as particularly sensitive measures of correlations in PRN sequences.

To compare with Refs. [7,10] we also used the autocorrelation time test to study the decimation of the output of R250, i.e., we took every k th number of the PRN sequence. For $k = \{3, 5, 6, 7, 9, 10, 11, 12, 24, 28\}$ the correlations vanish in agreement with $k = 5$ in Ref. [7] and $k = 3, 5$ in Ref. [10]. On the other hand, for $k = 2^m$ with $m = \{0, 1, 2, 3, 4, 5, 6, 7, 8\}$ the sequences fail. These findings agree with the theoretical result of Golomb [22], who showed that the decimation of a maximum-length GFSR sequence by powers of 2 results in equivalent sequences.

The errors in the average cluster sizes for some of the GFSR generators suggests that there must be

correlations present within the $\mathcal{O}(L^2)$ successive PRN's which are used in the single cluster formation of the Wolff algorithm. To quantify the range of correlations we propose the following *random walk* and *n-block* tests.

In the *random walk test* [23], we consider random walks on a plane which is divided into four equal blocks, each of which has an equal probability to contain the random walker after a walk of length n . The test is performed N times, and the number of occurrences in each of the four blocks is compared to the expected value of $N/4$, using a χ^2 test with three degrees of freedom. The generator fails if the χ^2 value exceeds 7.815 in at least two out of three independent runs. This should occur with a probability of only about $3/400$.

Results for a group of generators with this test are presented in Table II with $n = 1000$. They are in agreement with the autocorrelation time test. No correlations for either GGL or RANMAR were observed. R250 and R521 pass the test with $k = 3$, but fail with values $k = \{1, 2, 2^6\}$, whereas R1279 passes with all k tested. The failure of RAN3 with

TABLE II. Results of the random walk test with $N = 10^6$ samples. See text for details.

Generator	k	q	Result
R31	1	3	FAIL
R250	1,2,64	103	FAIL
R521	1,2,64	168	FAIL
RAN3	1		FAIL
R250	3	103	PASS
R521	3	168	PASS
R1279	1,2,3,64	418	PASS
R4423	1	2098	PASS
RAN3	2,3		PASS
GGL			PASS
RANMAR			PASS

$k = 1$ is consistent with previous test results [4,6]. It is notable that all the failures in this test were very clear, since even the smallest χ^2 values exceeded 40. However, RAN3 passed the test when every second or third number was used.

The main difference between the failing generators R250 and R521 (with $k = 1$) and the successful ones R1279 and R4423 lies in the lag parameter p which is less than n for the former and larger than n for the latter. We studied this for various values of p with the random walk test by locating the approximate value n_c , above which the generators fail. The test was performed for R31, R250, R521, and R1279 with $N = 10^6$ samples. The results for n_c were 32 ± 1 , 280 ± 5 , 590 ± 5 , and 1515 ± 5 , respectively, where the error estimate is the largest distance between samples close to n_c . An example of the χ^2 values is given in Fig. 1. These results demonstrate that the correlations are *local*, in the sense that they have a range very close to p .

In order to further quantify the nature of correlations we present the *n-block* test [24]. In it we take a sequence $\{x_1, x_2, \dots, x_n\}$ of uniformly distributed random numbers $0 \leq x_i < 1$, whose average \bar{x} is calculated. If $\bar{x} \geq 1/2$, we choose $y_i = 1$; otherwise $y_i = 0$. This is repeated N times. We then perform a χ^2 test on variables y_i with one degree of freedom. Each test is repeated 3 times, and the generator fails the test with fixed n if at least two out of three χ^2 values exceed 3.841, which should occur with a probability of about 3/400.

In cases of GGL, RANMAR, and RAN3, we observed no correlations up to $n = 10^4$ for $N = 10^6$. For R31, R250, and R521 we performed an iterative study by varying n . When $N = 10^6$ samples were taken, the resulting correlation lengths n_c were 32 ± 1 , 267 ± 5 , and 555 ± 5 , re-

spectively. With better statistics $N = 10^8$, we observed no change for R31, whereas the estimate for R521 reduced to 525 ± 1 , and that of R250 to 251 ± 1 . The latter value was confirmed with $N = 10^9$ also. Typical values of χ^2 for R250 are shown in Fig. 2, where a sharp onset of correlations at n_c is visible.

The results of our Ising simulations show that the origin of the errors observed here and in Refs. [7,10,11] must be due to the appearance of local correlations in the probability distribution. It is important to realize that in our Ising simulations it is the single cluster search [20] in the Wolff algorithm, where $\mathcal{O}(L^2)$ successive PRN's are used in cluster formation that makes the system especially sensitive to correlations; if, e.g., GFSR generators with $p \gg L^2$ ($q \approx p/2$) are used, the results improve considerably. Furthermore, the random walk and n -block tests are powerful enough to accurately pinpoint the range of correlations. For the GFSR generators, these two tests reveal that the dominant correlations appear very close to p , which supports the idea that these are triple correlations as suggested in Refs. [9,25,26].

In conclusion, we have presented three simple physical tests for detecting correlations in PRN sequences. We have demonstrated the quality of these tests by being able to unravel correlations in GFSR generators that have recently been shown to produce erroneous results in Monte Carlo simulations. In particular, we have shown that the errors in Ising simulations lie in local correlations present in the cluster formation process of the Wolff algorithm. For GFSR generators, the dominant correlations are of triple type as revealed by the random walk and n -block tests. This supports the idea of Grassberger for errors observed in the case of another depth-first algorithm [9]. It

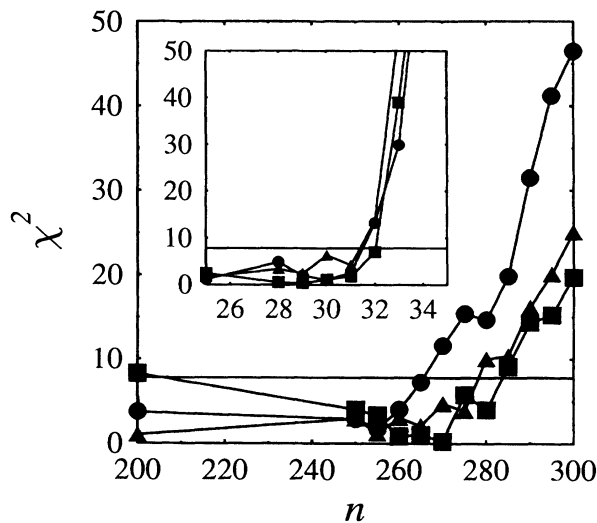


FIG. 1. The χ^2 values for R31 (inner figure) and R250 in the random walk test as a function of walk length n . Three independent runs in both cases are denoted by different symbols. The horizontal lines denote $\chi^2 = 7.815$.

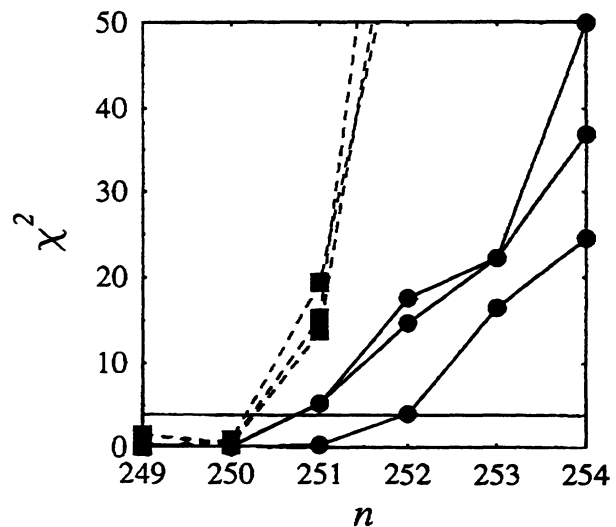


FIG. 2. The χ^2 values for R250 in the n -block test. Curves with circles and squares correspond to $N = 10^8$ and $N = 10^9$ samples, respectively. In both cases three independent runs have been performed. The horizontal line denotes $\chi^2 = 3.841$.

is remarkable that these correlations cannot be seen in either careful statistical [6] or bit level tests [4].

Finally, we would also like to note that we have preliminary results for applying the tests presented here for GFSR generators with four "taps" of the form $x_n = x_{n-9689} \oplus x_{n-471} \oplus x_{n-314} \oplus x_{n-157}$ [27], which is basically a 3 decimation ($k = 3$) of the generator $x_n = x_{n-9689} \oplus x_{n-471}$ [26]. For these generators correlations appear to be very weak as expected, but for smaller lags errors can again be found [28].

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