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Note

Correlational Defects in the Standard IBM 360 Random Number Generator and the Classical Ideal Gas Correlation Function*

Warnings exist that pseudorandom number generators should always be tested to insure that they are sufficiently random for the purposes for which they are to be used [1]. The following is a test which the standard IBM 360 random number generator failed, but which an improved generator suggested by MacLaren and Marsaglia [2] passed.

The standard IBM 360 routine produces pseudorandom odd integers between 1 and 2^{31} by the Multiplicative Congruential method using the formula [3]

$$I_{i+1} = aI_i (\text{mod } 2^{31}), \tag{1}$$

where a is usually taken to be 65539 and I_0 is an odd integer supplied as a seed. These random numbers have a cycle length [4] of 2^{29} when a is 3 or 5 mod 8 and are usually considered random enough for most purposes. However, the serial correlation between successive numbers has been shown to be between the bounds [5, 6]

$$1/a \pm a/2^{31} \tag{2}$$

from which reason a is usually taken to be approximately 2^{16}. This serial correlation is of a particularly nasty type which persists through successive choices of I. The randomness of this type of generator along with that of some of the mixed congruential type were tested by MacLaren and Marsaglia [2]. All were found to do extremely poorly in picking triples of random numbers. They suggested and tested a method whereby two multiplicative random number generators are used with one feeding into a table of numbers and another choosing from the table, with much better results.

This defect of the random number generator shows up dramatically in the following test. A number of configurations were prepared in which 32 particles were placed randomly in a box extending from -1 to 1 in three dimensions. The first particle was placed at the origin, then the next three random numbers between -1 and 1 were used for the coordinates of the second particle, the next three for the third, etc. The 16×31 different distances between the particles were then

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TABLE I
Two-Body Correlation Functions for a Classical Ideal Gas[a]

Spherical shell edges	Expected standard deviation	g_1 $x_{n+1}=65539x_n$ mod 2^{31} $x_0=1812396755$	g_1 $x_{n+1}=3x_n$ mod 2^{31} $x_0=1812396755$	g_2 $y_{n+1}=65549y_n$ $y_0=1812396755$ $x_{n+1}=65539x_n$ $x_0=1475621131$	g_3 $z_{n+1}=65549z_n$ $z_0=1812396755$ $y_{n+1}=65525y_n$ $y_0=1475621131$ $x_{n+1}=65539x_n$ $x_0=1123456791$
	$\chi^2=\sum_{i=1}^{32}(\delta_i/\sigma_i)^2$	1348.6	3.25×10^5	39.37	30.87
0.0478	0.188	2.812	87.53	1.195*	1.160
0.0957	0.071	1.180	12.49	0.919*	1.004
0.1148	0.078	0.863	5.939	1.129*	0.881*
0.1340	0.066	0.813	4.295	1.012	0.900*
0.1531	0.057	0.663	3.218	1.004	0.956
0.1722	0.050	0.509	2.443	0.959	1.005
0.1914	0.045	0.902	2.027	0.997	0.969
0.2105	0.041	1.367	1.726	0.957*	0.961
0.2297	0.037	1.237	1.392	0.980	1.054*
0.2488	0.034	1.202	1.084	1.010	1.099**
0.2679	0.032	1.098	1.040	1.075**	0.992
0.2871	0.030	0.971	0.885	0.999	0.975
0.3110	0.024	0.954	0.724	1.004	1.022
0.3349	0.023	0.862	0.642	0.995	1.009
0.3588	0.021	0.805	0.563	0.996	1.015
0.3828	0.020	1.047	0.481	1.022*	1.025*
0.4067	0.019	1.163	0.444	0.971**	0.987
0.4306	0.018	1.118	0.363	1.011	1.008
0.4545	0.017	1.057	0.348	1.022*	1.004
0.4785	0.016	0.971	0.294	0.976*	1.001
0.5024	0.015	0.928	0.287	0.964**	1.014
0.5263	0.014	0.917	0.259	0.986	0.986
0.5502	0.014	0.844	0.228	0.974*	0.988
0.5741	0.013	1.109	0.214	0.985*	1.022*
0.6220	0.0087	1.067	0.185	1.016*	1.001
0.6698	0.0080	1.006	1.429	1.007	1.005
0.7177	0.0075	0.926	2.211	1.003	0.990*
0.7655	0.0070	1.036	1.212	0.992*	0.997
0.8134	0.0066	1.050	1.855	0.999	1.001
0.8612	0.0062	0.994	1.284	1.000	0.999
0.9091	0.0059	0.932	0.975	1.007*	1.004
0.9569	0.0055	1.037	0.790	0.999	0.999

[a] The expected standard deviation was computed as (the number expected)$^{1/2}$/(the number expected). An asterisk in the last two columns indicates a difference greater than 1 standard deviation, a double asterisk a difference greater than 2 standard deviations.

calculated using periodic boundary conditions so that the smallest distance between particles and their images was used. These distances were then converted to a radial correlation function, $g(r)$, by adding up the number of distances between spherical shells, dividing by the volumes of the shells, and multiplying by the appropriate normalization to make $g(r)$ go asymptotically to 1. If the pseudo-random numbers were truly random, $g(r)$ would be the radial correlation function for the classical ideal gas (one everywhere) with random fluctuations due to the finite number of distances found in each shell. The expected size of these fluctuations for a given number of configurations can be calculated as $\sigma_i =$ (number expected in the ith shell)$^{-1/2}$ for $g(r_i)$. This, along with $\delta_i = g(r_i) - 1$, can then used to calculate $\chi^2 = \Sigma_i(\delta_i/\sigma_i)^2$ which gives a measure of the probability that the deviations, δ_i, noted in a given run could be due to random fluctuations. Thirty-two values of r_i were used in this work which means that χ^2 should be about 32.

Four groups of 1000 configurations were prepared. The first used the standard IBM generator, $I_{n+1} = 65539 I_n$, and exhibited the sawtooth pattern shown in Table I and Fig. 1. The results were quite consistent with a vertical leading edge and period of 0.187. The χ^2 was 1348.6. It being easier to make a worse random

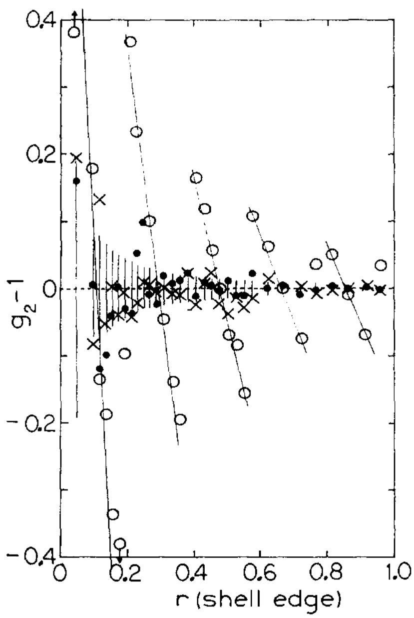

FIG. 1. $g_2 - 1$ vs r for various runs. (○) Run 1, standard IBM random number generator. (×) Run 3, 2 random number generators with a table. (●) Run 4, 3 random number generators with two tables. Light vertical lines indicate expected standard deviations.

number generator than a better one, the next set used $I_{n+1} = 3I_n$. The period of the sawtooth changed to about 0.65 and its magnitude increased drastically—χ^2 went to 3.25×10^5. For the third group, the MacLaren–Marsaglia method was used with a table of 128 numbers chosen according to $I_{n+1} = 65549I_n$ and then numbers from the table according to $I'_{n+1} = 655391I_n'$ with I' normalized to be between 1 and 128. The table was completely refilled before each new configuration was chosen. This group shown as x's in Fig. 1 has a χ^2 of 39.37 which has an acceptable 17% chance of being exceeded in a truly random sample. For the fourth group, the table of random numbers was randomly moved to another table according to $I''_{n+1} = 65525I''_n$. These results are the dots in Fig. 1 and have a χ^2 of 30.87 which has a 53% chance of being exceeded in a truly random sample.

The conclusion is that it is surprisingly easy to introduce correlations into a many-body calculation through the random number generator. In point of fact, the correlations present in the standard random number generator were first suspected through their subtle bias on a much more complex calculation of the correlation function for liquid sodium. The author would like to thank Marvin Pokrant whose knowledge of statistics exceeds his for suggesting the calculation of the various χ^2 values and for finding the probabilities that truly random samples would have χ^2 of these sizes.

References

1. M. Greenberger, *Comm. ACM* **8** (1965), 177.
2. M. D. MacLaren and G. Marsaglia, *J. Assoc. Comput. Mach.* **12** (1965), 83.
3. IBM Corp. System/360 Scientific Subroutine Package, H20–0205–3, New York, 1968.
4. B. Jansson, "Random Number Generators," p. 54, Victor Pettersons Bokindustri Aktiebolung, Stockholm, 1966.
5. J. M. Hammersley and D. C. Handscomb, "Monte Carlo Methods," p. 29, John Wiley, New York, 1964.
6. M. Greenberger, *Math. Comp.* **15** (1961), 383; *Math. Comp.* **16** (1962), 126(c).

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