Efficient Monte Carlo simulations using a shuffled nested Weyl sequence random number generator

K. V. Tretiakov[1] and K. W. Wojciechowski[1,2,*]
[1]*Institute of Molecular Physics, Polish Academy of Sciences, Smoluchowskiego 17/19, 60-179 Poznań, Poland*
[2]*Abdus Salam International Centre for Theoretical Physics, Trieste, Italy*
(Received 7 July 1999)

The pseudorandom number generator proposed recently by Holian *et al.* [B. L. Holian, O. E. Percus, T. T. Warnock, and P. A. Whitlock, Phys. Rev. E **50**, 1607 (1994)] is tested via Monte Carlo computation of the free energy difference between the defectless hcp and fcc hard sphere crystals by the Frenkel-Ladd method [D. Frenkel and A. J. C. Ladd, J. Chem. Phys. **81**, 3188 (1984)]. It is shown that this fast and convenient for parallel computing generator gives results in good agreement with results obtained by other generators. An estimate of high accuracy is obtained for the hcp-fcc free energy difference near melting.
[S1063-651X(99)09412-X]

PACS number(s): 02.70.−c, 05.10.−a, 61.50.Ah

Fast and easy to use pseudorandom number generators (PRNGs) are important in many areas of scientific research and practical applications. Various algorithms generating pseudorandom numbers and methods of testing them are discussed in detail by Knuth [1]. More brief reviews of the present state of the subject can be found in Refs. [2,3].

Since random number generators are nothing more than deterministic algorithms that produce numbers with certain distribution properties, every generator has to fail in certain simulations, in models which interfere with the particular regularities of this generator [3]. Thus, by definition, perfect PRNG cannot exist. One can introduce, however, a practitioner's definition of a good PRNG saying that this is such a generator that gives correct results for as many applications as possible [3]. One can also distinguish two groups of properties characterizing any generator. The first group, concerning practical aspects, includes such features as the speed of a generator, its memory usage, ease of its implementation, possibility to parallelize (distribute) the calculations using it, and portability of its implementations. The second group concerns theoretical characteristics of a PRNG, such as its (a) period length, (b) structural properties, and (c) correlations. Various methods have been developed to study these quantities [1–3] because they are helpful in choosing, for a given application, the right generator which (a) will correspond to the size of the sample and the planned length of simulations (the period of the generator should not be exceeded during the simulations), (b) will not introduce unwanted side effects caused, e.g., by a specific grid or hyperplane structure of the generator, and (c) will not perturb the simulated system introducing, e.g., an artificial collective behavior caused by specific correlations of pseudorandom numbers.

As no PRNG can work well with all applications, it is meaningful to relate the notion of quality of a given generator to the class of problems to which it is used: a generator is good for a given class of problems if results obtained by applying this generator to this class of problems are correct. Hence, application-specific tests with known (theoretical) results, performed for models that resemble given simulation problems constitute a useful way to test if a given PRNG is good in this sense.

Recently Holian *et al.* have introduced a generator based on the shuffled and nested Weyl sequence, further referred to as the SNWS generator [4]. This PRNG requires very small memory, is easy to implement, very fast [5,6], and convenient to use for parallel computing. Although the SNWS generator was originally designed for large scale molecular dynamics simulations [4], the mentioned advantages encouraged us to apply it to Monte Carlo (MC) simulations. Its structure has been slightly modified by Holian [7] to avoid problems with the finite accuracy of computer implementation of real numbers [8]. Simple tests [7,6] have not revealed any bad feature of this SNWS generator. Moreover, it is worth mentioning that the double precision version of this generator (used in this paper) produces numbers distributed much more smoothly than many other generators, e.g., the well known RAN2 generator [9]; this can be seen in Fig. 1. (The RAN2 generator is a combination of two linear congruencial generators [10] proposed by L'Ecuyer [11] and additionally shuffled by Press and Teukolsky [12] using the Bays-Durham approach [13]. It has a period longer than 2×10^{18} and was considered as ''perfect'' [14] by its authors [9].) Additional tests of the SNWS generator were required, however, to check its behavior for very long sequences.

Extensive simulations of many body systems whose properties are known with high accuracy can be used as a source of data for practical tests of the applicability of the SNWS generator. Recently, a lot of effort has been spent on the investigation of the relative stability of the fcc and hcp crystals of hard spheres [15–19]. We found this problem to be a good example for practical testing of the SNWS generator. This is so because the entropy difference between the two crystalline phases is very small, i.e., the calculations require high accuracy and, hence, should be sensitive on the quality of the generator used. Our interest in this problem was also stimulated by an important mathematical result obtained recently by Hales and Ferguson, who solved the Euler problem of dense packing of hard spheres [20], showing that no pack-

*Author to whom correspondence should be addressed. Electronic address: kww@man.poznan.pl

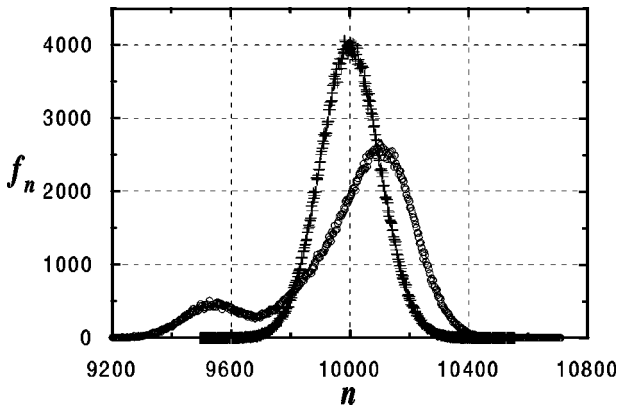

FIG. 1. Smoothness test is performed by dividing the unit interval into M (here $M=10^6$) equal bins, and generating K pseudorandom numbers (here $K=10^{10}$). The number of the bins f_n into which n random numbers were put is then plotted as a function of n. It is easy to show that for random numbers distributed uniformly and continuously on the unit interval (0,1) such a dependence should be Gaussian. In the above figure the results obtained for the SNWS generator (crosses) and for the RAN2 generator (open circles) are shown. The distribution obtained for the SNWS generator is indeed Gaussian [6], whereas it is clearly not Gaussian for the RAN2 generator.

ing of spheres can be denser than that of the fcc packing. Their rigorous result provided a qualitatively new argument supporting the fundamental role of structures forming closely packed stacks of hexagonal layers of hard spheres; the fcc and hcp crystals are the simplest examples of such structures. Although a general consensus has been reached recently about the thermodynamic stability of the fcc structure in the whole density range of existence of the hard sphere solid [15–19], a large quantitative discrepancy remains, however, between the results obtained by Woodcock [15], who used molecular dynamics simulations, and other researchers [16–19], who used MC simulations. It is not obvious if this discrepancy is related to an unknown asymptotic behavior of the hysteresis region of the Hoover-Ree single occupancy model [21], used by Woodcock, or to other reasons. In this context, a study of possible influence of various PRNGs on the entropy difference is of interest.

For the present test we have chosen the method proposed by Frenkel and Ladd [22]. Although this method is considered to be not as accurate as the recently developed methods based on multicanonical distribution [17,19], it is much simpler. We computed the difference [22],

$$\frac{\Delta f(\lambda_{max})}{k_BT} \equiv \frac{1}{k_BT}\int_0^{\lambda_{max}}\left[\frac{\partial f_{fcc}(\lambda)}{\partial\lambda}-\frac{\partial f_{hcp}(\lambda)}{\partial\lambda}\right]$$

$$=\int_0^{\lambda_{max}}\{\langle(\Delta\mathbf{r}_{fcc}^{(N)})^2\rangle_\lambda-\langle(\Delta\mathbf{r}_{hcp}^{(N)})^2\rangle_\lambda\}d\lambda$$

$$\equiv\int_0^{\lambda_{max}}\Delta R(\lambda)d\lambda, \qquad (1)$$

where $f_{lattice}(\lambda)$ denotes the free energy per particle of N hard spheres that interact with their *lattice* sites, $\mathbf{r}_{i,lattice}$, by the harmonic potential $\lambda(\Delta\mathbf{r}_{lattice}^{(N)})^2\equiv\lambda\Sigma_{i=1}^{N}(\mathbf{r}_i-\mathbf{r}_{i,lattice})^2$; lattice=fcc, hcp. The limit $\Delta f(\lambda_{max}\to\infty)$ corresponds to the difference of the free energy per sphere between the hcp and fcc crystals.

TABLE I. Comparison of $\Delta f(\lambda_{max})/k_BT$ computed near melting for $N=13\,824$ hard spheres. The details are described in text.

GLM order	Generator	$10^5\Delta f(\lambda_{max})/k_BT$
10	SIMGEN	-8 ± 27
10	RAN2	88 ± 22
	DRAND48	108 ± 21
	SNWS	111 ± 23
20	RAN2	116 ± 16
	DRAND48	95 ± 15
	SNWS	93 ± 15
40	RAN2	107 ± 11
	DRAND48	92 ± 10
	SNWS	97 ± 10

The simulations were done for $N=13\,824$ hard spheres (24 hexagonal layers of 24 rows, each containing 24 spheres; this system is slightly larger than the largest studied in the literature in this context) for $\lambda_{max}=632.026$ [22] and the relative density $\rho/\rho_{cp}=0.736$, which is close to the melting point of hard spheres [21]. The integration was performed using the 10-, 20-, and 40-point Gauss-Legendre method (GLM) for a few PRNGs. For given order of the GLM, the simulations of a given structure (fcc or hcp) were performed sequentially starting from the largest λ and decreasing it in subsequent runs. Each run corresponded to 1.4×10^5 MC cycles after equilibration. The simulations were conducted on SGI Power Challenge, IBM SP2, and HP workstations using overall some 2000 hours of CPU time.

To check if the simulation results are sensitive to the quality of the generator used, we performed a 10-point run with a very simple PRNG described in [23], further referred to as SIMGEN. This matrix linear congruencial generator with the modulo being the power of 2 [24] has the cycle of only 2^{22} numbers and its smoothness test shows significant departure from a Gaussian already for $M=10^4$ bins ($K=10^8$). As can be seen in Table I, the obtained result has a different sign than the data obtained using other generators, which proves sensitivity of the simulations on the PRNG used.

The main tests have been done for three generators: (i) SNWS, (ii) RAN2, and (iii) DRAND48 [25]. (The latter generator is a linear congruencial one with the period 2^{48}. We do not know any incorrect results obtained by using this generator except the most recent Gärtner's calculations of some particular determinants [26]. We should note that the outcome of the smoothness tests for DRAND48 is indistinguishable from those obtained for the SNWS [6].) The results shown in Table I reveal good agreement between the data obtained by using these three generators. Using all the results obtained (except that for SIMGEN), one can obtain quite an accurate estimate for $\Delta f(\lambda_{max})/k_BT=(100\pm5)10^{-5}$. An analysis of the λ dependence of $\Delta R(\lambda)$ suggests that for large λ it is negative and its absolute value decays exponentially. This makes it possible to estimate the correction to the difference of the free energies per sphere of the hcp and fcc lattices which comes from the integration of $\Delta R(\lambda)$ between λ_{max} and ∞ in Eq. (1). This correction is

$(7\pm10)10^{-6}k_BT$. Thus, the difference of the free energies is estimated as $(99\pm6)10^{-5}k_BT$, which agrees with the most recent result $(91\pm5)10^{-5}k_BT$ obtained by the lattice-switch MC method [19]. Taking into account that the free energy difference increases by about $0.0002k_BT$ when the density is increased from the melting one to $\rho/\rho_{cp}=0.7778$ [27], we should notice, however, that the present result differs by a statistically significant amount from the value $(86\pm3)10^{-5}k_BT$, obtained for the latter density in [17]. We do not know the origin of this discrepancy.

In conclusion, we showed that: (i) the used SNWS PRNG gives, within the Frenkel-Ladd method, the same results for the free energy difference of the hcp and fcc crystals of hard spheres near melting as some other (well tested) generators, (ii) the Frenkel-Ladd method enables one to obtain quite an accurate estimate of this free energy difference, and the value of the latter one is in fair agreement with the most recent result obtained by Mau and Huse by the multicanonical distribution method [19]. The results presented above indicate also that the discrepancy between the calculations of Woodcock and others is not related to generators of pseudorandom numbers used in MC simulations.

Recently, exploiting the advantages of the SNWS generator, we were able to perform other extensive simulations, computing elastic constants of various model systems [28,29]. Those simulations also have not revealed any statistically significant differences between the data obtained by using the SNWS generator and other generators. This encourages one to apply this fast generator in MC simulations of many body systems.

We are grateful to Professor B. L. Holian and Professor W. G. Hoover for helpful correspondence and to Dr. J. Martinek for useful remarks. One of the authors (K.W.W.) is grateful to Professor Yu Lu and Professor S. Shenoy for hospitality. This work was supported by the (Polish) Committee for Scientific Research (KBN) by Grant No. 8T11F01214. Part of the calculations were performed at the Poznań Computer and Networking Center (PCSS).

[1] D. E. Knuth, in *The Art of Computer Programming* (Addison-Wesley, Reading, MA, 1998), Vol. 2.
[2] P. L'Ecuyer, Ann. Oper. Res. **53**, 77 (1994).
[3] P. Hellekalek, Math. Comput. Simul. **46**, 485 (1998).
[4] B. L. Holian, O. E. Percus, T. T. Warnock, and P. A. Whitlock, Phys. Rev. E **50**, 1607 (1994).
[5] In particular, for Hewlett Packard 735 and J282 workstations, the double precision version of the Holian *et al.* generator is more than six times faster [6] than the generator DRAND48 [25]. This results in speeding up the calculations discussed in this paper by a factor close to 2. The SNWS generator is also up to two times faster than the RAN2 generator [9], depending on the computer used [6].
[6] K. V. Tretiakov and K. W. Wojciechowski, Pro Dialog **5**, 97 (1997) (in Polish).
[7] B. L. Holian (private communication).
[8] A generic pseudocode for the SNWS generator we used can be written as

length = 1 000 003; bign = mod(exp(1.),1.)*10^7; do n = 1, number; iseed = iseed + 1; seed = mod(sqrt(iseed),1.); if (seed .eq. 0.) then; iseed = iseed + 1; seed = mod(sqrt(iseed),1.); endif; do k = 1, length; x =mod(k*mod(k*seed,1.),1.)*bign + 0.5; x = mod(x*mod(x*seed,1.),1.); enddo; enddo,

where (for brevity) semicolons represent ends of statements.

Holian noticed also that with HP workstations a substantial increase of the speed is reached when to introduce a user defined function frac(x) = x − int(x), which is used instead of mod(x,1.) [7].
[9] W. H. Press *et al.*, *Numerical Recipes in FORTRAN*, 2nd ed. (Cambridge University Press, Cambridge, England, 1992), p. 272.
[10] Linear congruencial generators (LCGs) are defined by the linear congruence: $y_{n+1}=(ay_n+c)\mathrm{mod}\ m$, where $n\geqslant 0$, and the multiplier a, the modulo m, and y_0 are positive integers; the additive term c is either zero (for multiplicative LCGs) or positive integer (for nonmultiplicative LCGs). Pseudorandom numbers are obtained by the normalization $x_n:=y_n/m$. When y_n, y_{n+1} and a, c denote vectors and matrices, respectively, the above generator is called a matrix LCG, and the pseudorandom numbers are obtained by normalizing one of the components of y_n.
[11] P. L'Ecuyer, Commun. ACM **31**, 742 (1988).
[12] W. H. Press and S. A. Teukolsky, Comput. Phys. **6**, 522 (1992).
[13] C. Bays and S. D. Durham, ACM Trans. Math. Softw. **2**, 59 (1976).
[14] The meaning of ''perfect'' is that $1000 has been proposed to the first person who could convince the authors of Ref. [9] otherwise, by finding a statistical test that RAN2 would fail in a nontrivial way, excluding the ordinary limitations of a machine floating point representation. We do not know if there was a winner.
[15] L. V. Woodcock, Nature (London) **385**, 141 (1997); **388**, 236 (1997).
[16] P. G. Bolhuis, D. Frenkel, S.-Ch. Mau, and D. A. Huse, Nature (London) **388**, 235 (1997).
[17] A. D. Bruce, N. B. Wilding, and G. J. Ackland, Phys. Rev. Lett. **79**, 3002 (1997).
[18] R. J. Speedy, J. Phys.: Condens. Matter **10**, 4387 (1998).
[19] S.-Ch. Mau and D. A. Huse, Phys. Rev. E **59**, 4396 (1999).
[20] T. C. Hales and S. P. Ferguson, http://www.math.lsa.umich.edu/~hales/countdown/.
[21] W. G. Hoover and F. H. Ree, J. Chem. Phys. **49**, 3609 (1968).
[22] D. Frenkel and A. J. C. Ladd, J. Chem. Phys. **81**, 3188 (1984).
[23] W. G. Hoover, *Computational Statistical Mechanics* (Elsevier, Amsterdam, 1992), p. 81.
[24] Arguments against using moduli being powers of 2 are presented in Ref. [2].
[25] *HP-UX 10.20 Reference Manual Series 700 J Class* (Hewlett Packard, USA, 1997), Vol. 3, Sec. 3.
[26] B. Gärtner, DMV Mitteilungen, No. 2 (1999) (in German).
[27] See Fig. 2 in [18].
[28] K. W. Wojciechowski and K. V. Tretiakov, Comp. Phys. Commun. (to be published).
[29] K. W. Wojciechowski and K. V. Tretiakov (unpublished).