Computer simulation of close random packing of equal spheres

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We have developed an algorithm which generates a random close packing of equal spheres from a random distribution of points. Each point is the center of an inner and an outer sphere. The inner diameter defines the true density and the outer a nominal density. The algorithm eliminates overlaps among outer spheres while slowly shrinking the outer diameter. The two diameters approach each other, and the eventual coincidence of true and nominal densities terminates the procedure. The spheres in the packing, which is inherently homogeneous and isotropic, are close together but not touching. Thus, near neighbors are defined as those within a specified distance, δ, of touching. When the outer diameter is contracted relatively quickly, the number of near neighbors depends strongly on δ. As the contraction rate approaches zero, this dependence decreases sharply. We speculate that the limiting value is exactly 6 for all $\delta \leq 10^{-3}$. Packing fractions between 0.642 and 0.649, which are easily achieved by this method, are higher than any experimental or previously simulated values, but are consistent with Berryman's extrapolation [Phys. Rev. A **27**, 1053 (1983)] from the radial distribution function for hard spheres. The algorithm can also be used for packing hyperspheres in higher dimensions.

I. INTRODUCTION

The packing fraction η for experimental packings of equal spheres varies with the method of packing.[1] The maximum for truly random experimental packings appears to be 0.6366.[2,3] Recently, we obtained this value for a simulated packing which was homogeneous and isotropic.[4] The precise agreement of these values suggested that $\eta = 2/\pi = 0.6366\ldots$ might be the true fraction.[5,6] On the other hand, Berryman[7] noted that experimentally obtainable values need not be maximal and cited evidence that $\eta = 0.64 \pm 0.02$. He suggested $0.642 \leq \eta \leq 0.645$ as the best estimate. Some excess space in our simulated packing also suggested that a denser packing might be possible,[4] but very long simulation times indicated that much greater efficiency would be required.

II. A NEW ALGORITHM FOR CLOSE RANDOM PACKING

One thousand points are generated randomly in a $12 \times 12 \times 12$ cube with periodic boundaries.[4] Each point is the center of an inner and an outer sphere. The inner diameter is set, after each iteration, to the minimum center-to-center distance between any two spheres and defines a true density which is very low initially. The outer diameter is set initially to the arbitrary[8] value $2.4(3/4\pi)^{1/3}$ which yields a nominal value of $\eta = 1$. The algorithm eliminates overlaps while slowly reducing the outer diameter. Thus, the two diameters approach each other and the eventual coincidence of true and nominal densities terminates the procedure.

In each step, the worst overlap is eliminated[4] by moving both spheres an equal distance along the line joining their centers until these centers are separated by one outer diameter. This may introduce new overlaps and change or eliminate others. (A linked-list structure simplifies the bookkeeping.) For intersecting outer spheres, center-to-center distances (called "rods") are calculated, but no rod is placed in the queue if the overlap to which it corresponds would be changed by the elimination of a greater overlap. Subject to this restriction, rods are queued in order of increasing length up to a maximum value of 1.3, corresponding to $\eta = 0.666$.[9] In each step, rods are added to or deleted from the queue according to the criteria described above. A simple example is shown in Fig. 1.

The packing process is a deterministic transition from an approximately Poisson distribution of points to a dense packing of hard spheres. The method appears crude in

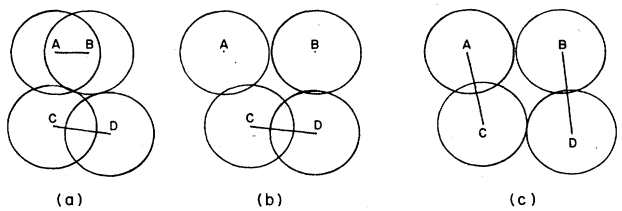

FIG. 1. Stages in the elimination of overlaps in a four-disk system. (a) The worst overlap corresponds to the shortest rod AB. Rod AC is not in the queue because the worst overlap involving A is with B and the worst involving C is with D. (b) The worst overlap is now between C and D. Rods AC and BD are not in the queue because the worst overlap involving C is with D and vice versa. (c) With the elimination of the overlap between C and D, rods AC and BD are placed in the queue.

that each step removes the worst overlap without regard for the consequences. The reality is more subtle. Large shifts in position are needed to fill big holes. The true density fluctuates up and down as the inner radius changes, but there is a subsequence $\{\eta_i\}$, which is monotonically increasing, and a corresponding sequence $\{t_i\}$, where t_i is the minimum value of t for which $\eta(t)=\eta_i$. Thus, the true diameter of spheres measured from "snapshots," at $t_0<t_1<\cdots<t_n$, shows a steady increase with time. Since any configuration in a snapshot is an allowable configuration for a hard-sphere gas, it is impossible, in the absence of a reference length, to tell whether the spheres are increasing in size or simply being pushed closer together. Nevertheless, the relaxation method[4] used here should be much more efficient than the compression of a hard-sphere gas. Overlaps are removed directly by spreading spheres apart and indirectly by shrinking the outer radius. Although the latter process is indispensable, it has the undesirable effect of producing gaps between near neighbors. Thus, the rate of contraction is slowed as the nominal and real densities approach each other.

An iteration consists of spreading two spheres apart, checking the queue for rods and, if overlaps remain, reducing the outer radius slightly according to the equation

$$\lambda^{(i+1)}=\lambda^{(i)}-(\tfrac{1}{2})^j k/M\ , \tag{1}$$

where

$$\lambda^{(i)}=d^{(i)}/d^{(0)} \tag{2}$$

and

$$j=[-\log_{10}\Delta\eta^{(i)}]\ . \tag{3}$$

Here M is the number of spheres (1000 in this work), d is the nominal diameter, $\Delta\eta$ is the difference between the nominal and actual packing fractions, and [ ] is the greatest integer function. The parameter k, which is independent of the size and number of spheres, characterizes the initial rate of contraction of the ensemble.

Figure 2 shows how the true and nominal densities change with the number of iterations N. The final part of the upper curve reflects the slower decrease in the outer diameter in the final stages of packing. The lower curve is concave downwards for $5000<N<30\,000$, but this period of slow growth may be misleading. It appears that keeping the nominal density large helps to spread out the centers and sets the stage for the subsequent period of rapid growth.

Figure 3 indicates that there is an almost exact relationship between the number of iterations N to produce an overlap-free packing and the time constant τ, which is the reciprocal of k. A linear regression of $\log_{10}N$ versus $\log_{10}\tau$ yields

$$E(N)=176.1\tau^{0.9955} \tag{4}$$

($R^2=99.999\%$) which suggests that the relationship is actually linear. Indeed, regression of N versus τ yields

$$E(N)=167.543\tau+12\,000\ , \tag{5}$$

with $R^2=99.9996\%$. Since the iteration time is approximately constant, the computing time t to generate and analyze a random packing is also roughly linear. Regression of t versus τ yields

$$E(t)=0.9082\tau+534.6 \tag{6}$$

($R^2=99.99\%$) where t is the CPU (central processing unit) time (in seconds) on a Digital Equipment Corporation VAX11/780 computer.

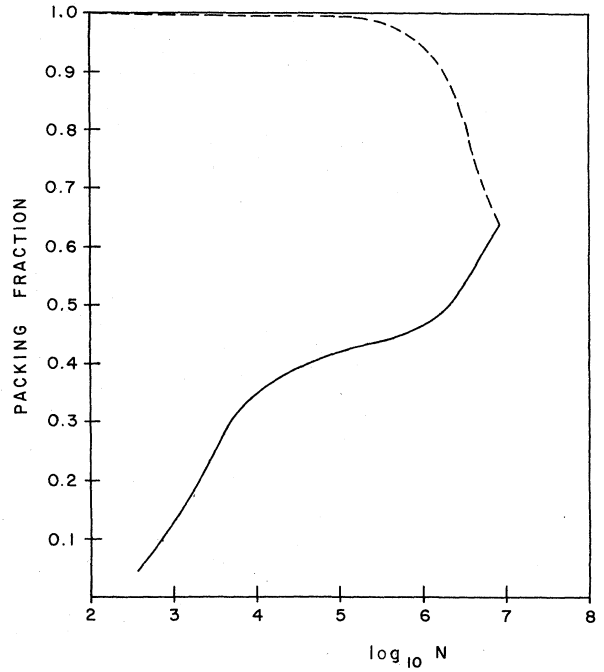

FIG. 2. Variation of nominal and true densities with number of iterations. The upper curve (— — —) shows the decrease in nominal density from its initial value of 1.0 to its final value of 0.648 78. The lower curve (——) shows the increase in true density. The two values coincide after 13 687 449 iterations.

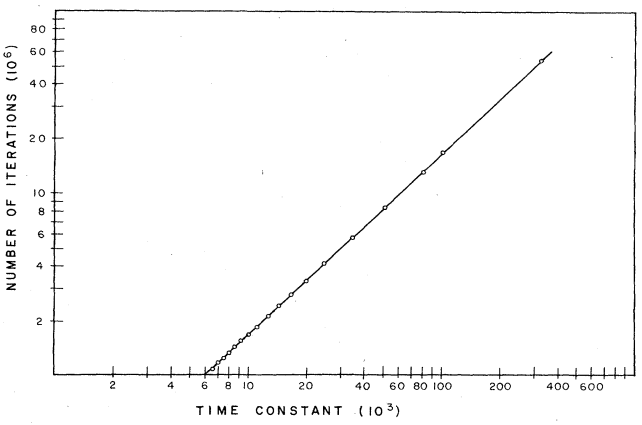

FIG. 3. Variation of number of iterations N with time constant τ. Though N is a random variable (which depends on the initial random configuration), its dependence on τ is almost exactly linear.

TABLE I. Dependence of distribution of number of near neighbors on designated maximum spacing between neighbors ($\eta=0.645\,68$).

Maximum spacing	Number of spheres with designated number of near neighbors[a]												
$-\log_{10}\delta$	0	1	2	3	4	5	6	7	8	9	10	11	12
2	5	2	4	2	53	138	252	276	206	55	6	1	0
3	17	7	9	16	125	239	274	199	95	19	0	0	0
4	38	13	17	38	208	279	233	128	38	8	0	0	0
5	82	42	61	135	252	239	135	42	10	2	0	0	0
6	212	179	203	209	130	57	9	1	0	0	0	0	0
7	689	236	65	8	2	0	0	0	0	0	0	0	0
8	959	30	10	0	1	0	0	0	0	0	0	0	0
9	992	6	2	0	0	0	0	0	0	0	0	0	0

[a]Near neighbors are defined as those within δ of touching. Note that the unit length is absolute while the sphere radius r varies with η. Here $r=0.6434$.

III. RESULTS

The algorithm generates a packing in which only two spheres are actually in contact, but many spheres are nearly touching. Table I shows the distribution of near neighbors for a packing with $\eta=0.6457$. When near neighbors are defined as those within 10^{-7} of touching, most spheres have none and no sphere has more than four. The distribution of neighbors is quite different when the tolerance δ is 10^{-4}. Though there are still some spheres with few neighbors, the mode is five. For larger tolerances, the distributions are similar, with a gradual shift of the peak and a marked decline in the number with few neighbors. For a fixed tolerance, the distribution of neighbors shows a similar shift with increasing η. Table II illustrates this for $\delta=10^{-4}$.

The similarity of these distributions facilitates the use of their means in representing the effect of tolerance and contraction rate on the distribution of near neighbors.

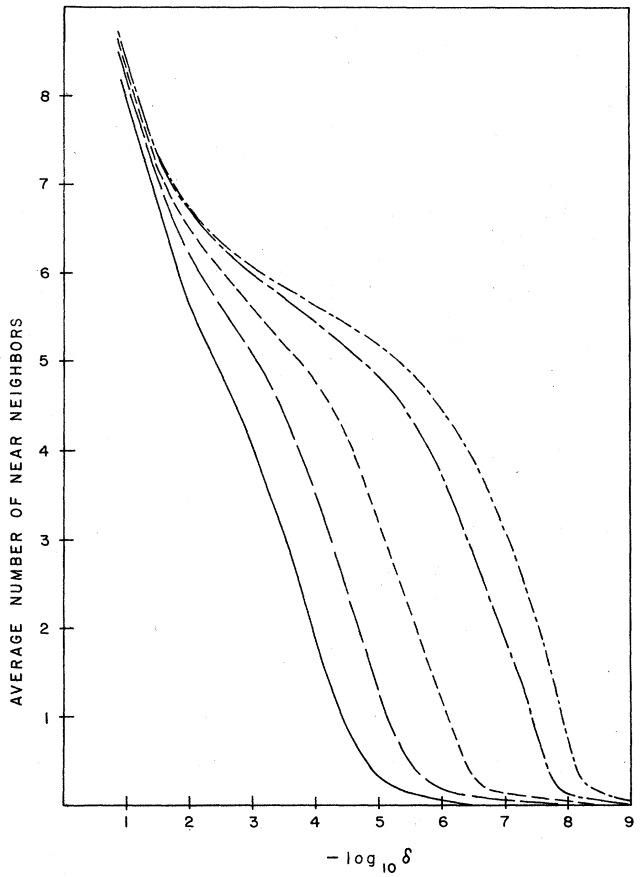

FIG. 4. Dependence of average number of near neighbors on touching tolerance δ and time constant τ. Neighbors within δ of touching are considered to be near. The curves correspond to different values of τ: ——800; ——3200; — — —12 800; —·—102 400; — · —327 680.

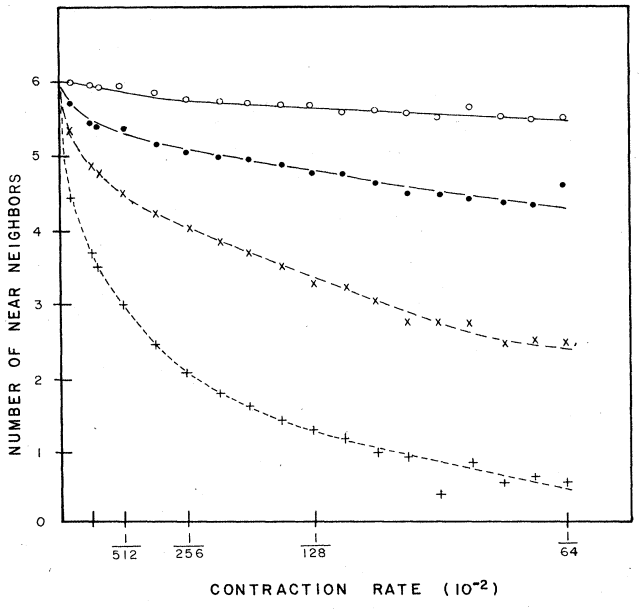

FIG. 5. Dependence of average number of near neighbors on contraction rate k. Neighbors within δ of touching are considered to be near. The symbols (and the curves fitted to them by eye) correspond to different values of δ: ——○——10^{-3}; ——●——10^{-4}; ——×——10^{-5}; — — —+— — —10^{-6}. The leftmost points correspond to $k\simeq 3.05\times 10^{-6}$. The extrapolation to $k=0$ is speculative.

TABLE II. Dependence of distribution of number of near neighbors on rate of contraction.

Time constant	Number of spheres with designated number of near neighbors[a]												
	0	1	2	3	4	5	6	7	8	9	10	11	12
800	206	238	241	178	101	28	6	2	0	0	0	0	0
1600	105	132	154	235	218	110	42	3	1	0	0	0	0
3200	84	69	111	186	227	203	90	27	2	1	0	0	0
6400	45	39	52	101	250	268	177	51	16	1	0	0	0
12 800	35	15	24	89	224	288	218	84	19	4	0	0	0
25 600	38	13	17	38	208	279	233	128	38	8	0	0	0
51 200	20	12	12	33	170	280	240	175	54	4	0	0	0
102 400	27	3	5	20	160	269	274	171	62	7	2	0	0
327 680	19	1	3	9	125	268	281	207	76	10	0	1	0

[a]Near neighbors are those within 10^{-4} of touching. Note that this value is absolute while the sphere radius varies from 0.6424, for $\tau=800$, to 0.6444, for $\tau=327\,680$.

Figure 4 shows how the average number of neighbors varies with δ and the time constant τ. Note that the gaps between near neighbors can be reduced by increasing τ. Figure 5 indicates that the number of neighbors which are very close rises sharply as $k\rightarrow 0$. The data suggest that the limit might be exactly six touching neighbors (consistent with the value for random sequential packing[10,11]), but the small values of k required to confirm or refute this conjecture require a great deal of computing time on a much faster system. (Note that $k=10^{-6}$ would require 10.5 CPU days on the VAX11/780 computer.)

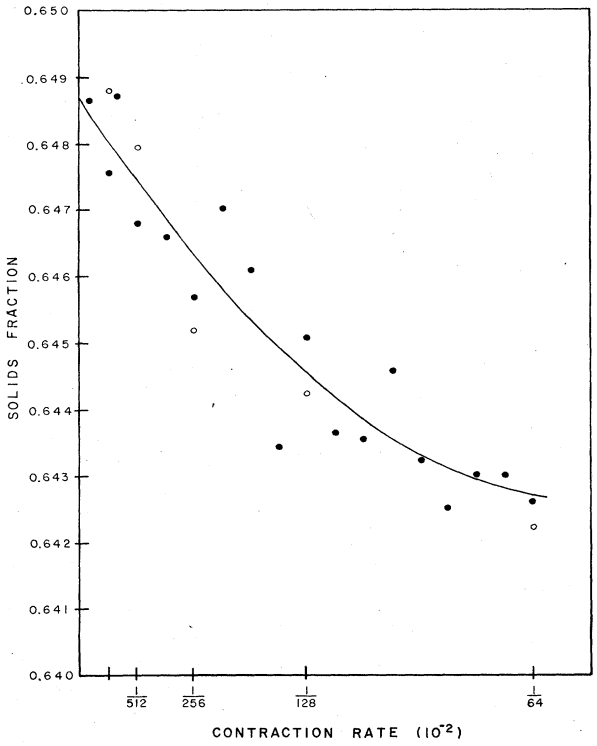

FIG. 6. Variation of solids fraction η with contraction rate, k. The curve, depicting Eq. (7), is the best-fit parabola for the solid circles (normal simulations). The open circles represent tests in which all initial points were generated in a small corner of the cube.

Finally, Fig. 6 shows that we can routinely produce random packings for which $\eta>0.645$. These data are represented reasonably well ($R^2=89.3\%$) by

$$E(\eta)=0.648\,70-6.908k+1967k^2\,. \tag{7}$$

The maximum expected value occurs at $k=0$.

The distribution of points about the regression line, the nature of the distribution of near neighbors (including the complete absence of any spheres with 12 neighbors) and the usual shape of the radial distribution functions (not shown[12]) indicate that the packing is truly random. It is inherently homogeneous and isotropic.[13]

IV. DISCUSSION

The packing fraction η is a random variable which is determined solely by the random-number triples (interpreted as points in $\mathbb{R}^3$) and the value of k. Variations in η arise from differences in the spacings between spheres and from holes in the packing. A comparison of Table I with Table II of our earlier paper[4] shows that more spheres were very close together ($\delta\leq 10^{-6}$) in the previous packing even though η was considerably less. However, the new algorithm produces a packing in which more spheres are fairly close together. It seems likely that the current packing has fewer and/or smaller holes. The essential feature appears to be a long period of vigorous movement. Provided that this occurs, the process is robust: generating all centers in a small corner ($1\times 1\times 1$) of the cube gave results (open circles in Fig. 6) similar to those where the centers were distributed throughout the entire cube. The regression equation based on all points,

$$E(\eta)=0.648\,87-7.416k+2199k^2\,, \tag{8}$$

yields values which differ little[14] from those of Eq. (7).

Equations (6) and (7) yield

$$E(\eta)\simeq 0.648\,70-6.274/(t-534.6) \tag{9}$$

for small k, indicating a very slight gain in $E(\eta)$ for enormous cost. Thus, the optimum strategy for achieving some very high values of η is to do many runs at feasible values of k. This takes advantage of the variability of η

about the regression line ($s_\eta = 7.383 \times 10^{-4}$). However, optimization at this stage would be premature because the effect of the variation of nominal density with time (including the initial value) should be studied further.

In principle, our program can pack spheres in $\mathbb{R}^n$, $n = 2,3,\ldots$. Small-scale runs have been successful in $\mathbb{R}^2$ (though the final packing may not be random) and $\mathbb{R}^4$. Results in $\mathbb{R}^2$ will be published elsewhere; studies in higher dimensions will be completed as suitable computing facilities become available.

ACKNOWLEDGMENTS

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[1]D. P. Haughey and G. S. G. Beveridge, Can. J. Chem. Eng. **47**, 130 (1969).

[2]G. D. Scott and D. M. Kilgour, J. Phys. D **2**, 863 (1969).

[3]J. L. Finney, Proc. R. Soc. London, Ser. A **319**, 479 (1970).

[4]W. S. Jodrey and E. M. Tory, Powder Technol. **30**, 111 (1981).

[5]A. Gamba, Nature (London) **256**, 521 (1975).

[6]E. M. Tory and W. S. Jodrey, in *Advances in the Mechanics and the Flow of Granular Materials,* edited by M. Shahinpoor (Trans Tech, West Germany, 1983), Vol. 1, Chap. 1, pp. 75–106.

[7]J. G. Berryman, Phys. Rev. A **27**, 1053 (1983).

[8]The initial value of the outer diameter must correspond to a nominal value of η much greater than any attainable true value. Our earlier simulation, which gave lower final values of η, did not have this feature.

[9]This target must be slightly greater than any attainable true value.

[10]C. H. Bennett, J. Appl. Phys. **43**, 2727 (1972).

[11]W. S. Jodrey and E. M. Tory, Simulation **32**, 1 (1979).

[12]These curves, which were all basically the same, showed the familiar damping out with distance. A radial distribution based on our previous simulation is shown in Fig. 4 of Jodrey and Tory (cf. Ref. 4).

[13]Results from our previous simulation, (cf. Ref. 4) whose homogeneity and isotropy were similarly inherent, were tested to confirm these properties.

[14]An attempt to show Eq. (8) in Fig. 6 was abandoned when it became clear that the second curve would be too close to the first to be clearly distinguishable.