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Random packings of spheres built with sequential models

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Received 28 February 1992

Abstract. Several models have been introduced to construct random packings of identical spheres. The packings are built on a horizontal basal layer using iterative sequential algorithms in which a new added sphere is always in contact with three other spheres in the packing. In the Bennet model the position with the lowest vertical coordinate is selected. In the 'anti-Bennet' model, only positions that are stable under gravity are considered, and that with the highest vertical coordinate is selected. In the Eden model the new sphere is selected at random among all the possibilities and, in the 'stable Eden' model, the random choice is limited to positions that are stable under gravity. In all cases, the density (packing fraction) is determined within an uncertainty of $\pm 10^{-4}$. The histogram for the number of contacts between spheres, the bond angle distribution and the distance distribution were also determined. The results are compared with corresponding ballistic model results

1. Introduction

Both computer and physical models in which discs or spheres are packed together to form contracting random assemblies have been used extensively to represent the structure of liquids and glasses [1-7], to provide structural models to study phenomena such as electrical conductivity [8-10], fluid flow [11-13], stress distribution [14-17] and other mechanical properties in granular materials. Similar models have also been used to investigate processes such as sintering [10, 18, 19].

In many cases the algorithms used to generate random packings can be viewed as irreversible growth models in which spheres are added sequentially to the packing. Therefore the recent progresses towards understanding irreversible growth and aggregation phenomena [20] can provide interesting new ideas on the construction of random packings and how to study their properties. One of these algorithms, the ballistic deposition model [21-25], has already been extensively studied by us and used to describe penetration [24] and segregation effects [25]. In this paper we describe some other sequential procedures, often inspired by old ideas [3, 26]. The common feature is that, as in the ballistic model, the packing is built sequentially such that the last added sphere is always in contact with three other spheres in the packing. This ensures that the mean number of contacts per sphere is strictly equal to six inside the bulk of all the packings. In all these procedures, we use a 'strip' geometry in which the packing is built from a basal first layer and grows in a direction perpendicular to the plane, with periodic boundary conditions at the edges of the strip. This allows us to build

considerably larger packing than was possible in the past and thus to calculate their characteristics such as density (or packing fraction), contact number histograms, bond angle distribution, with a great accuracy.

2. Description of the models

In all cases, we start from a first layer of size $L \times L$ made of L^2 spheres. The horizontal projections of their centres are disposed on a square lattice with lattice spacing equal to the sphere diameter, taken equal to unity. This first layer is randomly disordered from a purely horizontal plane by adding random vertical displacements to the coordinates of all the spheres. The vertical coordinate z_{ij} of the centre of sphere i, j whose horizontal coordinates are $x = i$ and $y = j$) is taken to be:

$$z_{ij} = \delta \xi_{ij}$$

where ξ_{ij} are random independent variables uniformly distributed between 0 and 1 and δ is a parameter which determines the intensity of the initial disorder. We have observed that all the characteristics of the resulting packings, measured far from the basal layer, do not depend on δ if this parameter is different from zero and smaller than a critical value which would produce some 'holes' in the first layer that would make the procedure described below impossible.

As soon as the first layer is built, the list of coordinates, $x_p(k), y_p(k), z_p(k)$ ($k = 1, 2, \dots, k_m$) for all the k_m possible positions for the centre of a sphere is determined. The coordinates in this list correspond to positions in which a new sphere contacts three spheres of the first layer and sits on these contacting spheres (i.e. the sphere centre must be above the plane made with the centres of the three contacting spheres). One of these positions k_0 is chosen according to a given rule, which depends on the model, and the centre of the next sphere of the packing is placed at $x_p(k_0), y_p(k_0), z_p(k_0)$. We then remove this k_0 position from the list of coordinates as well as all other positions which correspond to a sphere which would overlap the newly added sphere and we add to the list all the other possible positions for a sphere to be in contact with the new sphere and two other spheres of the packing. After the list has been updated and the new k_m value has been calculated, we choose another position in the list according to the adopted rule and we proceed as before: a new sphere is added to the packing at this position, the list of possible positions is updated and so on. During all steps in this iterative procedure, periodic boundary conditions are used in the two horizontal directions.

The most time-consuming part of the algorithm is the updating of the list of possible positions. At this stage, both the spheres of the packing as well as the possible positions which are in the neighbourhood of a given point must be determined. This can be efficiently done by storing both particles of the packings and possible positions in L^2 columns, labelled by i and j integers, both ranging from 1 to L . The coordinates of the centres of spheres of the packing and possible positions for the new spheres are stored into tables with three indices $x(i, j, m), y(i, j, m), z(i, j, m)$ and $x_p(i, j, m), y_p(i, j, m), z_p(i, j, m)$ respectively. When there is something in the column, m runs from 1 to a given, column-dependent, maximum value $mm(i, j)$ of $mm_p(i, j)$. The indices $mm(i, j)$ and/or $mm_p(i, j)$ are set to zero when there is nothing in the i, j column. Additional tables are used to make the correspondence between the one-index lists and the three-index lists for x_p, y_p and z_p . The particles of the packing are stored in

descending order in a given column and are discarded as soon as they are too far from the top to participate in particle addition. Then the search for a particle (or for a position) can be carried out efficiently using only a few columns.

In some of our procedures, the list of possible positions has been restricted to 'stable' positions, i.e. to positions for which, in a horizontal projection, the centre of the new sphere lies inside the triangle formed with the centres of the three contacting particles. The four different procedures that we have considered here are the following:

(1) The 'Bennet' procedure: the lowest vertical position is always selected. This is a variant of a model first introduced by Bennet [3] in a spherical geometry (starting from a 'seed' and choosing the new position nearest to the seed).

(2) The 'anti-Bennet' procedure: always the highest position is selected but the list is restricted to stable positions.

(3) The 'Eden' procedure: the new position is selected at random among all the possibilities (i.e. $k_0 = 1 + \text{int}(k_m \xi)$, where ξ is a random variable lying between zero and one and 'int' denotes the integer part). This is an off-lattice version of a model first introduced by Eden [26] to study the growth of tumours and which has been extensively studied on lattices [20].

(4) The 'stable-Eden' procedure: this is the same as the Eden procedure but the list is restricted to stable positions.

All the results obtained with these models will be compared with similar results obtained with the ballistic deposition model. The algorithm for this model has been described elsewhere [23, 24]. In this model, spheres are deposited along randomly positioned vertical trajectories and follow the path of steepest descent on the packing before reaching their final stable position in contact with three spheres of the packing.

The following general comments concerning these models may be helpful before presenting the results:

(i) The two first procedures (Bennet and anti-Bennet) are entirely deterministic. This means that the randomness of the packings comes only from the randomness originally put in the first layer.

(ii) All procedures, except the Eden model, produce packings that are stable under gravity.

(iii) It is essential to restrict the choice to stable positions in the anti-Bennet procedure. Without this restriction a single column is grown without entirely covering the base.

3. Characteristics of the packings

To make a qualitative comparison between the different models we show vertical cuts of packings built with $L = 30$ in figure 1. The total number of particles is the same in all cases so that the mean height of each packing gives an idea of its density. It is apparent that the Bennet model gives the most compact packing. However, due to surface roughness it is difficult to discern if the least compact packing is obtained with the Eden or the anti-Bennet model. This figure also shows some interesting surface features that we have not quantitatively studied here. While the surface for the Bennet model is almost flat the surface of the anti-Bennet packing exhibits a characteristic conical shape and all the others are quite rough.

The density ρ of each packing has been estimated from five independent simulations made with a lateral size of $L = 60$ up to a height of $3L$. For each model the vertical

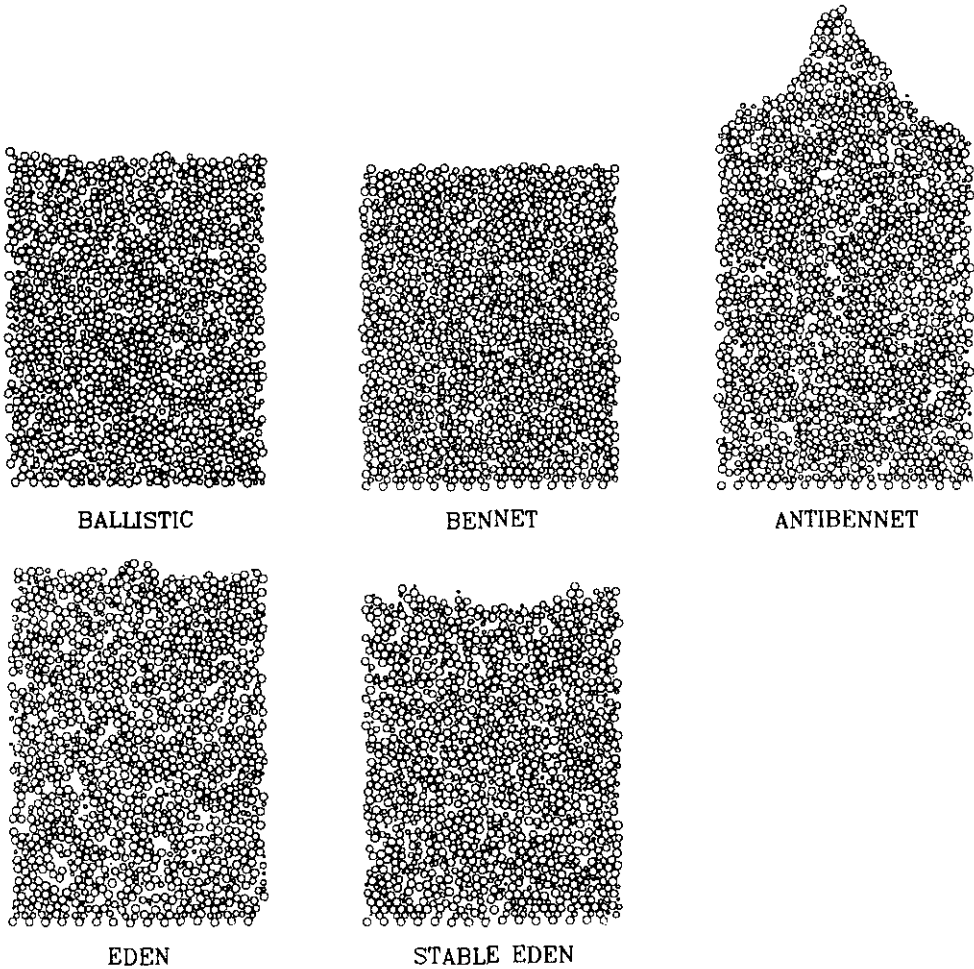


Figure 1. Vertical cuts through packings built with $L = 30$. All packings contain the same total number of particles. In the case of the anti-Bennet model the origin of the coordinate system has been translated so that the peak appears in the centre of the figure.

density profile was measured. Sufficiently far from the top and bottom of the packing this density profile fluctuates about a constant mean value. The mean value in the central part of the profile was taken to be the packing density. The results are reported in table 1. In all cases, the uncertainty is of order 0.0001. The density varies between 0.5447 for the least compact packing (Eden) and 0.6053 for the most compact (Bennet) the order with respect to the density being: Bennet > ballistic > anti-Bennet > stable Eden > Eden.

Table 1. Numerical values of the densities ρ for the different packings.

	Ballistic	Bennet	Anti-Bennet	Eden	Stable Eden
ρ	0.5812	0.6053	0.5745	0.5447	0.5719

We have also calculated the histogram $f(n)$ for the number of contacts, n , per sphere. These histograms have been normalized such that $\sum_n f(n) = 1$ and $f(n)$ is the fraction of spheres having a given number of contacts n with other spheres in the packing. These numbers have also been calculated well inside the bulk, i.e. after eliminating the bottom and top parts of the packing. The results are reported in table 2 and the corresponding histograms are shown in figure 2. In the ballistic case, our values for the $f(n)$ s are very close to older results [22]. It is worth noting that, since each added sphere contacts three previous ones, the mean number of contacts should

Table 2. Numerical values of the fraction $f(n)$ of spheres having n contacts with other spheres in the packing (the corresponding histograms are given in figure 2).

	Ballistic	Bennet	Anti-Bennet	Eden	Stable Eden
$f(3)$	0.0006	0.0006	0.0009	0.0180	0.0016
$f(4)$	0.0381	0.0282	0.0453	0.0992	0.0529
$f(5)$	0.2474	0.2331	0.2508	0.2351	0.2489
$f(6)$	0.4359	0.4749	0.4155	0.3049	0.4000
$f(7)$	0.2329	0.2355	0.2351	0.2243	0.2376
$f(8)$	0.0427	0.0273	0.0489	0.0948	0.0546
$f(9)$	0.0023	0.0004	0.0035	0.0215	0.0042
$f(10)$	2×10^{-5}	6×10^{-7}	6×10^{-5}	0.0022	8×10^{-5}
$f(11)$	0.0	0.0	0.0	9×10^{-5}	0.0
$f(12)$	0.0	0.0	0.0	3×10^{-6}	0.0

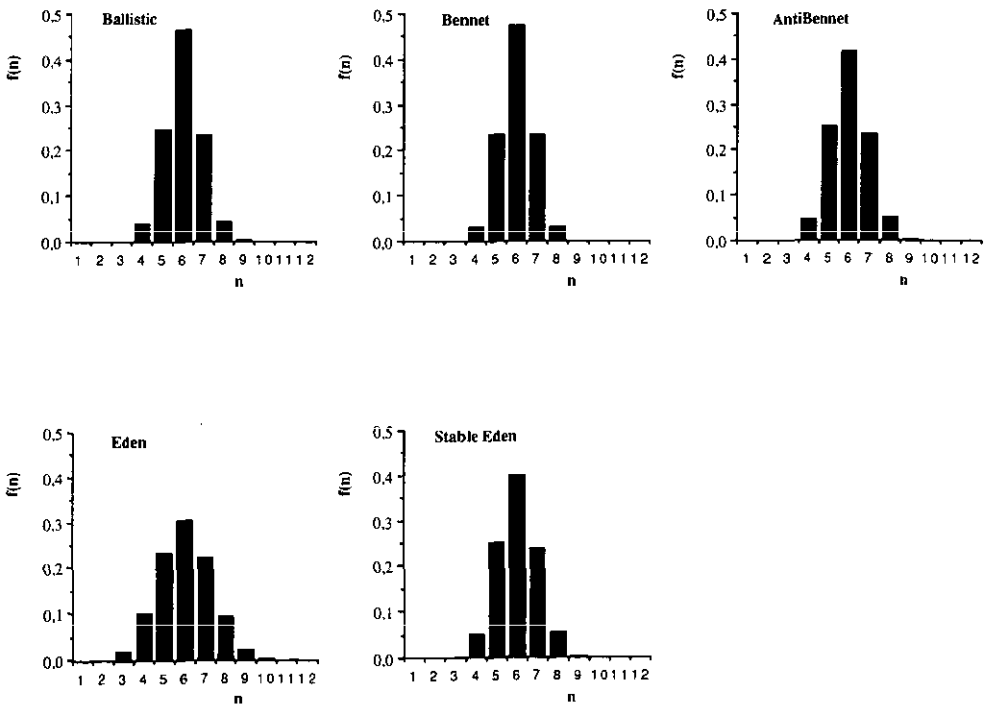


Figure 2. Histograms for the number of contacts. $f(n)$ is the fraction of spheres having n contacts with other spheres in the packing.

be strictly equal to six. This has been verified by our results where for all packings we have found

$$\sum_n nf(n) = 6 \pm 0.001.$$

As expected, since there are at least three contacts per sphere, we have found that, for all packings, $f(1) = f(2) = 0$. It is interesting to observe that there is a finite fraction of spheres with only three contacts. Since the evaluation of the contact populations $f(n)$ has been done within the bulk of the packing, this means that there are cavities (which are stable under gravity) and these spheres sit inside such cavities without any contact with the spheres above. It can be shown on typical examples that such may exist. In particular they can be easily obtained when depositing spheres onto any array of identical spheres whose centres form a weakly disordered horizontal square lattice (i.e. the 100 plane of a slightly disordered face-centred cubic structure).

While it is *a priori* possible to put up to 12 spheres in contact with another one, we have never found more than 10 contacts for any of the packings except in the Eden case where $f(11) \sim 9 \times 10^{-5}$ and $f(12) \sim 3 \times 10^{-6}$. This Eden packing, which is the only one to be unstable under gravity, appears to be quite different from the others since, while its density is very low, the most compact local arrangement ($n = 12$) is sometimes realized. Thus there must exist very large density fluctuations in this packing.

We have observed a direct correlation between the density and the number of spheres with six contacts. This is shown in figure 3 where we have plotted ρ as a function of $f(6)$. However, it appears that there is no simple relationship between ρ and $f(6)$. While all stable packings lie on a quasi-parabolic curve with a minimum around 0.57, the Eden packing appears again to be in a singular situation.

As a further analysis of the contacts between spheres, we have counted, among all spheres having the same number n of contacts, the proportion $x(n)$ of them that can be freely displaced, i.e. that have all their contacts located within a single hemisphere. The sum $X = \sum_n f(n)x(n)$ gives the fraction of single spheres that are unstable when

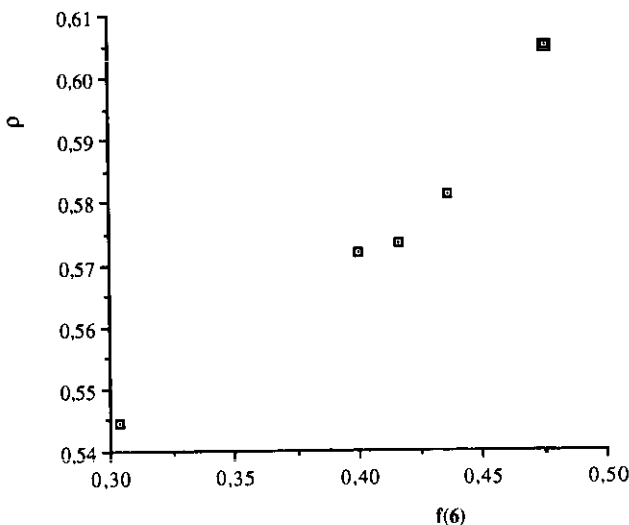


Figure 3. Plot of the density ρ as a function of the fraction of spheres with six contacts $f(6)$. Each point corresponds to a given packing.

turning the packing up-side down (we have not done the same analysis for clusters of spheres). The numerical values for $x(n)$ and X are reported in table 3 for each packing. If we forget the relatively large X value obtained for the least dense Eden packing, all the other X -values are of the order 0.050-0.056 with no clear relation to the density.

We also determined the distribution of angles with the vertical for the lines joining the centres of two spheres in contact, for all pairs of contacting spheres in the packing. This distribution was calculated in two steps. During the growth process (as soon as a new sphere of centre M was put in contact with three spheres of centres M_1, M_2, M_3), we have recorded the three angles φ_i between the vector u and MM_i , where u is the (downward pointing) vertical unit vector, and constructed the histogram for all spheres within regularly spaced ranges of $\cos \varphi$ values. Doing so, we directly obtained the distribution $Q(\varphi)$, ranging between $\varphi=0$ and $\varphi=\pi$, such that the quantity $Q(\varphi) \sin \varphi d\varphi$ is proportional the number of bonds whose angle with the vertical lies between φ and $\varphi+d\varphi$. The distribution $Q(\varphi)$ was normalized to unity:

$$\int_0^\pi Q(\varphi) \sin \varphi d\varphi = 1.$$

Then the final distribution $P(\theta)$ for the angle θ between u and the non-oriented bond direction ($0 < \theta < \pi/2$) can be deduced from $Q(\varphi)$ by

$$P(\theta) = Q(\theta) + Q(\pi - \theta).$$

The distributions $Q(\varphi)$ and $P(\theta)$ are reported in figure 4.

In general, the bond angle distribution $Q(\varphi)$ contains a single maximum whose intensity decreases when going from the most compact to the least compact packing. Each packing has its own characteristics which is reflected by the precise shape of $Q(\varphi)$ and $P(\theta)$. In particular, the anti-Bennet case is very different from the others: the maximum of $Q(\varphi)$ is located at a very low φ value (20°) and there are significant shoulders near 50° and 90° . In the Bennet case, where the density is the highest and where the histogram of contact is remarkably symmetric, the bond angle distribution tends to zero for $\varphi=0$ and $\varphi=90^\circ$ and is strictly equal to zero for $\varphi > 90^\circ$, so that, in this case (and in this case only) there is no difference between $P(\theta)$ and $Q(\varphi)$. This means that, in the Bennet procedure, the lowest position with three contacts never includes 'pointing up' contacts with higher spheres. It is also interesting to observe that the less compact packing, which corresponds to the Eden procedure, is nearly isotropic, since $P(\theta)$ is almost equal to one over the whole range of θ values. However, we have checked, by varying the size and the height of the packing, that the difference

Table 3. Numerical values of the fraction $x(n)$ of spheres with n contacts having all their contacts located within a hemisphere. The value of $X = \sum_n f(n)x(n)$ is reported in the last row.

	Ballistic	Bennet	Anti-Bennet	Eden	Stable Eden
$x(3)$	1	1	1	1	1
$x(4)$	0.4710	0.6352	0.3978	0.7072	0.4010
$x(5)$	0.1069	0.1361	0.1020	0.3407	0.1059
$x(6)$	0.0111	0.0083	0.0114	0.1043	0.0163
$x(7)$	0.0007	0.0004	0.0008	0.0019	0.0008
$x(8)$	0.0	0.0	0.0	0.0004	0.0
X	0.0498	0.0546	0.0498	0.205	0.0561

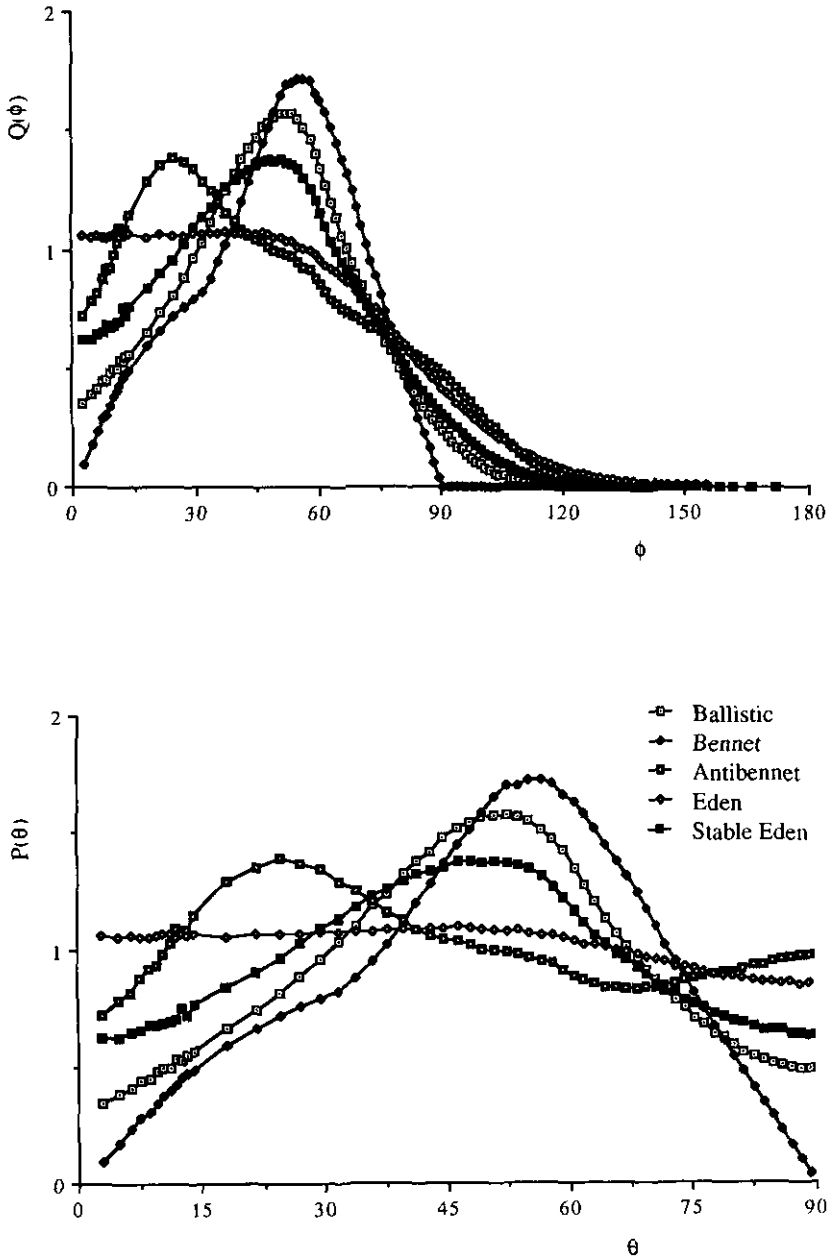


Figure 4. Bond angle distributions $Q(\phi)$ and $P(\theta)$ (see text).

from one is significant, so that, even if the growth rules are isotropic (they do not refer to the direction of gravity) there remain a small but significant anisotropy due to the well defined growth direction determined by the initial conditions.

We have also calculated the inter-distance distribution function $g(r)$ and the results are reported in figure 5 for each packing. We note that $4\pi g(r)r^2 dr$ is proportional to the number of interparticle distances lying between r and $r+dr$. In figure 5, r is measured in units of the sphere diameter and $g(r)$ is normalized in order that $g(r) \rightarrow 1$

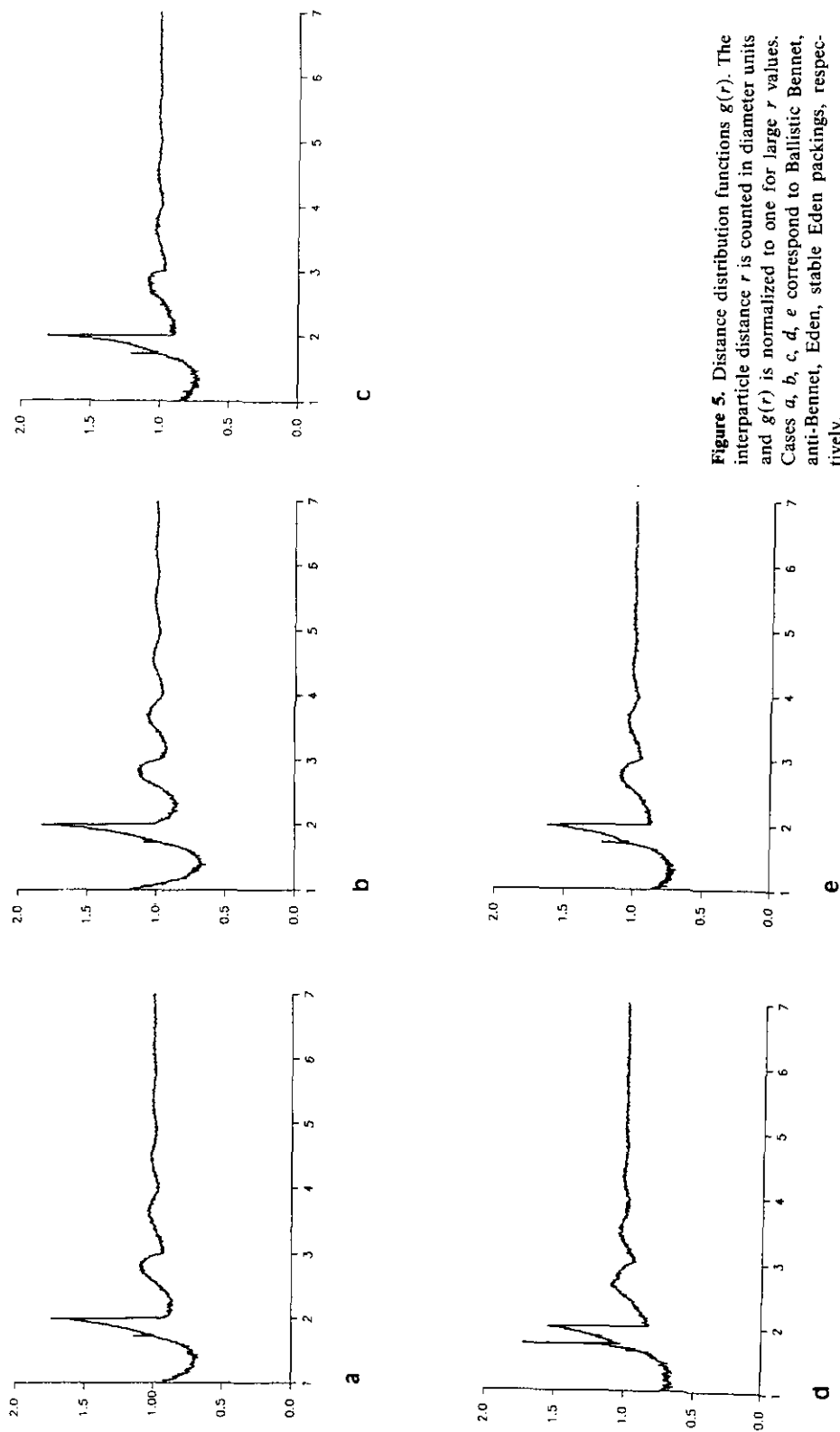


Figure 5. Distance distribution functions $g(r)$. The interparticle distance r is counted in diameter units and $g(r)$ is normalized to one for large r values. Cases a, b, c, d, e correspond to Ballistic Bennet, anti-Bennet, Eden, stable Eden packings, respectively.

when $r \rightarrow \infty$. There is obviously a 'delta' peak at $r = 1$ which cannot be represented on such a plot. When r tends to 1 from above, $g(r)$ tends to a constant whose intensity is larger if the density of the packing is larger. This result can be expected since this constant is related to the number of spheres in close contact to a given sphere: it is a measure of some kind of 'local density'. We always observe a marked discontinuity at $r = 2$ and a smaller one at $r = \sqrt{3}$, except in the Eden case where they are both of the same order of magnitude. The geometrical origins of such discontinuities have been extensively discussed in Bennet's paper [3]. We can also notice that the $g(r)$ oscillations persist up to larger r values in the Bennet case indicating that the correlation length is larger for denser packings.

4. Discussion and conclusion

We have obtained densities ranging from 0.5447 to 0.6053 for different random packings with the same mean coordination number $\langle n \rangle = 6$. These results clearly demonstrate that the density of a random packing does not only depend on the mean coordination number. However, in the literature, there exists a theoretical formula, due to Dixmier [27], which reads

$$\rho = \frac{2\langle n \rangle}{9 + 2\langle n \rangle}.$$

In the case $\langle n \rangle = 6$, this formula gives $\rho = 4/7 = 0.5714$, a value located within the range of values obtained here and very close to the density 0.5719 obtained with the stable Eden procedure which corresponds to the least compact packing that is stable under gravity. We have already extensively discussed the validity of this formula [28] and we have reached the conclusion that it must hold under the following conditions:

- (i) The packing is isotropic.
- (ii) The distribution for the lengths of 'chords' (segments obtained when cutting the spheres by random straightlines) is strictly exponential.

Consequently, the Dixmier's formula cannot apply in our case since all our packings are anisotropic (as shown by the results on the bond angle distributions). However, in the case of the ballistic model, we have numerically found that the chord distribution, calculated for a given chord direction, is remarkably exponential for all chord directions. We intend to extend such calculations to the other packings, and in particular to the most isotropic ones, i.e. Eden and stable Eden. It is expected that the chord distribution of the quasi-isotropic Eden packing should exhibit strong deviations from a pure exponential since its density is considerably lower than $4/7$. Moreover, it would be interesting to understand why the stable Eden packing fits nicely the Dixmier value $\rho = 4/7$.

In reference to the general classification for random packings [29–31], our densities correspond to very loose (in the case of the Eden packing) or loose (in all the other cases) random packings. We have tried to use many other sequential rules to build more compact packings than the Bennet one but did not succeed. It may be that it is necessary to abandon sequential procedures to reach larger densities.

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