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Original Research Paper

SPATIAL STATISTICS FOR SIMULATED PACKINGS OF SPHERES

ALEXANDER BEZRUKOV[1], DIETRICH STOYAN[1] AND MONIKA BARGIEŁ[2]

[1]Institut für Stochastik, TU Bergakademie Freiberg, 09596 Freiberg, Germany, [2]Institute of Computer Science, AGH Krakow, al. Mickiewicza 30, 30-059 Krakow, Poland
e-mail: stoyan@orion.hrz.tu-freiberg.de
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ABSTRACT

This paper reports on spatial-statistical analyses for simulated random packings of spheres with random diameters. The simulation methods are the force-biased algorithm and the Jodrey-Tory sedimentation algorithm. The sphere diameters are taken as constant or following a bimodal or lognormal distribution. Standard characteristics of spatial statistics are used to describe these packings statistically, namely volume fraction, pair correlation function of the system of sphere centres and spherical contact distribution function of the set-theoretic union of all spheres. Furthermore, the coordination numbers are analysed.

Keywords: contact distribution, coordination number, pair correlation function, simulation, sphere packing, volume fraction.

INTRODUCTION

Random packings of spheres with constant and random diameters play an important role in many branches of physics and engineering. Simulated packings serve as models for real packings of particles, *e.g.* in the context of particle science, where, however, the assumption that the particles are spheres is often a simplification. Also many porous media can be represented as packed arrangements of spheres.

In these and other cases, the characteristics of the simulated packings should be at least similar to those of the real structures investigated. This concerns primarily mean value characteristics such as porosity and mean coordination number and, additionally, functions such as coordination number distribution, pair correlation function and spherical contact distribution function.

There is a wide variety of sphere packing algorithms. This paper uses the force-biased algorithm (Mościński *et al.*, 1989; Mościński and Bargieł, 1991), and the Jodrey-Tory sedimentation algorithm (Jodry and Tory, 1979). The first algorithm starts with a very dense configuration of large spheres which can even overlap. It reduces stepwise the diameters and moves the spheres in order to reduce the degree of overlappings. The second algorithm simulates the successive packing of a container with spheres falling in the gravitational field. A sphere with three contacts with earlier packed spheres is considered as being in its final position. While the first algorithm is able to produce very dense nearly isotropic packings, the second one yields loose packings of volume fraction V_V = 0.58 in the case of equal spheres, which show a light gradient in vertical direction. Other known packing algorithms use the discrete element method (Stroeven and Stroeven, 2000).

For the physicist, engineer and statistician then the question arises which of these algorithms to choose. The decision should be based on statistical properties of the packings produced, i.e. as said above, the model characteristics should be as close as possible to the empirical counterparts and the diameter distributions should be identical. Therefore, this paper presents results of the two algorithms for some interesting cases of diameter distributions and packing densities.

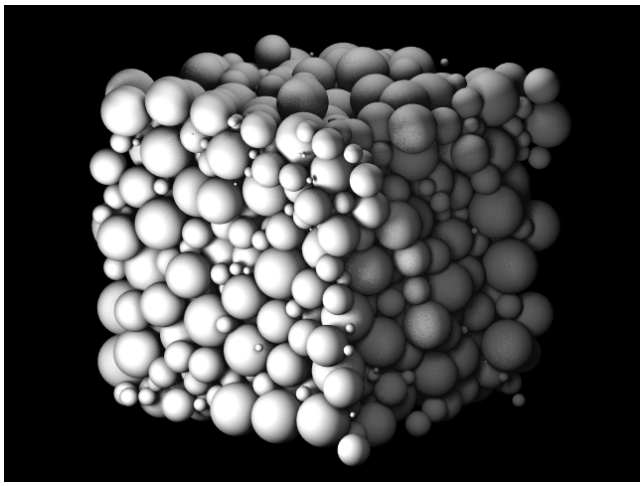

Fig. 1. *A simulated sphere packing with a lognormal diameter distribution and volume fraction* V_V*=0.70.*

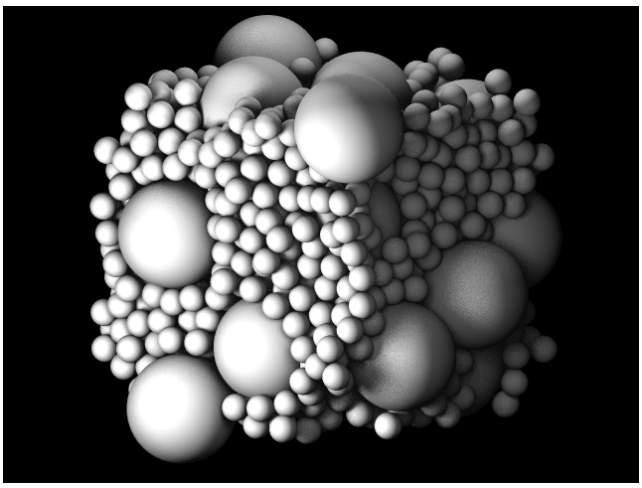

Fig. 2. *A simulated sphere packing with bimodal diameter distribution with diameters 1 and 10 and V_V=0.80.*

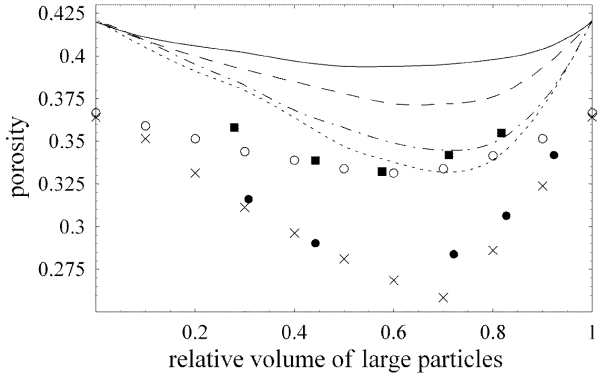

Fig. 3. *Porosity versus relative volume v of smaller spheres. The curves result from simulations with the sedimentation algorithm, the points are experimental data taken from Sohn and Moreland (1968). Size ratio 1 : k: ○, —— 0.5; ■, – – – 0.39; ●, – · – 0.29; ×, · · · · · 0.25.*

POROSITY

First the most important parameter of sphere packings is considered, packing density or volume fraction V_V of the space occupied by the spheres for two important cases, lognormal and two-point distributions. The case of a two-point distribution is of particular interest since in the literature just such packings were studied experimentally for real spheres (Sohn and Moreland, 1968; Yu and Standish, 1987). Here one diameter is assumed to be 1 and the other is k. The probabilities of occurrence of these values are $p_1 = p$ and $p_k = 1 - p$. Fig. 3 shows porosity $\eta = 1 - V_V$ as a function of k and v for packings obtained by the sedimentation algorithm, where

$$v = \frac{p}{p + k^3(1-p)}\,. \qquad (1)$$

It is interesting to compare these results with the empirical results, which are also shown in Fig. 3.

It is not surprising that the empirical porosities are clearly smaller, since the sedimentation algorithm does not include any compression and rearragement step. For the force-biased algorithm a similar figure is not presented, since it is possible to find program parameters which yield just the empirical values given in Fig. 3. In the lognormal case two parameters play a role: μ and σ^2, where the mean is given by $m = \exp(\mu + \sigma^2/2)$. It can be observed that volume fraction V_V depends only little on the mean-value parameter μ but heavily on the variance parameter σ; V_V increases with σ.

PAIR CORRELATION FUNCTION AND SPHERICAL CONTACT DISTRIBUTION

The classical descriptor of spatial variability with respect to a homogeneous system of spheres with mean number λ of spheres per volume unit is the pair correlation function $g(r)$; (see Stoyan *et al.*, 1995, p. 129). We have determined $g(r)$ statistically by means of the method described in Stoyan and Stoyan (2001) for many of the simulated packings.

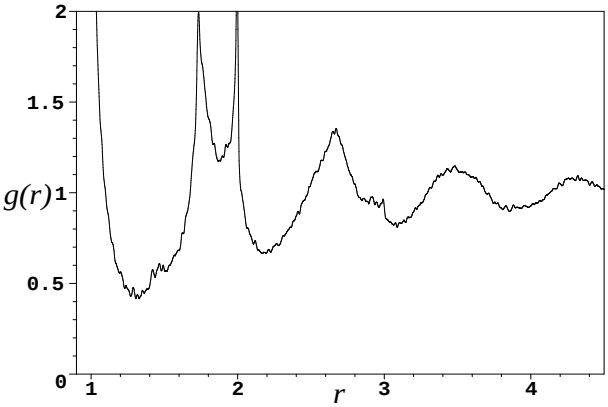

Fig. 4. *Pair correlation function for a dense random packing of spheres with equal diameters and V_V=0.65.*

For the case of packings of spheres of constant diameter obtained by the force-biased algorithm the result is similar to the function shown in Fig. 4.10 of (Stoyan *et al.*, 1995) if $V_V = 0.64$, while in the case of $V_V = 0.70$ the higher order is clearly expressed by peaks much sharper as those shown in Fig. 4. For two-point distributions the number of peaks is smaller, and they result only from pairs of small spheres.

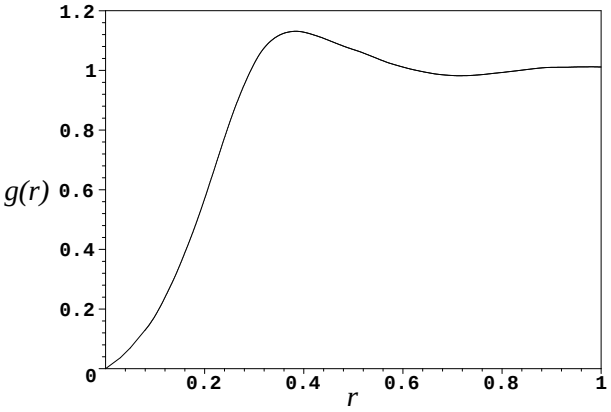

Fig. 5. *Pair correlation function for the case of a lognormal diameter distribution and V_V=0.70.*

Finally, Fig. 5 shows the pair correlation function in a typical lognormal case. The given mixture of spheres of different diameters leads to the effect that this curve does not have any striking peak; it looks like the pair correlation function of a so-called soft-core point process.

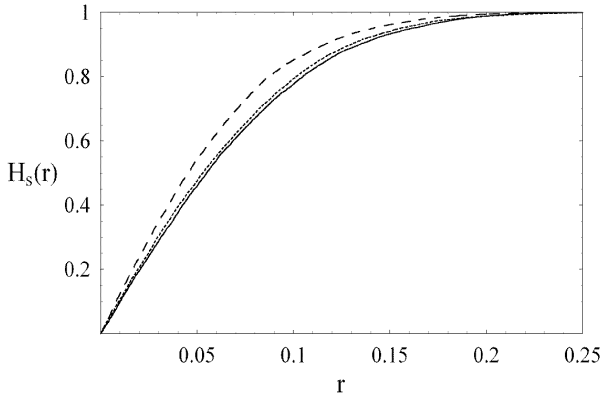

Fig. 6. *Spherical contact distribution functions.*
—— *equal spheres, V_V=0.64; – – – equal spheres, V_V=0.70; ····· lognormal diameters.*

The spherical contact distribution function $H_s(r)$ is a descriptor for sphere systems of a quite different nature; it describes the size of the pore space between the spheres; $H_s(r)$ is the distribution function of the random distance from a random test point in the pore space to the nearest sphere surface point (Stoyan *et al.*, 1995, p. 206).

Fig. 6 shows $H_s(r)$ for equal spheres with V_V = 0.64 and 0.70 and for the lognormal case with V_V = 0.70. The different porosities and diameter distributions lead of course to different spherical contact distribution functions, but also the different arrangement of the spheres plays a role.

COORDINATION NUMBER

A very important feature of sphere packings are the contacts between spheres. They determine, for example, the topological connectivity of the system of spheres or the transfer of forces in mechanically loaded systems of hard spheres.

In the literature there are reports on the distribution of the number of contacts or coordination number c of a randomly chosen sphere and its mean $\overline{c}$. It is clear that these characteristics depend on the diameter distribution as well as on porosity. For real packings of equal spheres, in Bernal and Mason (1960) the value of $\overline{c}$ = 6.4 is given for a 'random close' packing and $\overline{c}$ = 5.5 for a 'loose' random packing, with V_V = 0.62 and 0.60, respectively. For packings obtained by the sedimentation algorithm values around $\overline{c}$ = 6 were observed.

Fig. 7 shows the histogram of contact numbers c for the case of equal spheres and force-biased algorithm with V_V = 0.64 and 0.70. Clearly, in the denser packing there are more contacts. The same figure also shows the empirical contact number distribution for the case of lognormal diameters as in Fig. 1.

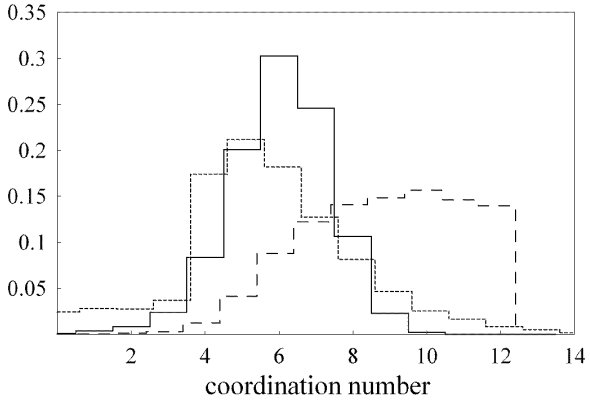

Fig. 7. *Distribution of the number of contacts of the spheres in three packings.*
—— *equal spheres, V_V = 0.64; – – – equal spheres, V_V = 0.70; ····· lognormal diameters, V_V = 0.70.*

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