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A Packing Computational Method Relating Fractal Particle Size Distribution and Void Fraction in Granular Media

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Abstract. The study of granular systems is of great interest to many fields of science and technology. The packing of particles affects to the physical properties of the granular system. In particular, the crucial influence of particle size distribution (PSD) on the random packing structure increase the interest in relating both, either theoretically or by computational methods. A packing computational method is developed in order to estimate the void fraction corresponding to a fractal-like particle size distribution.

Keywords: granular media, packing, particle size distribution, porosity.

1 Introduction: from particle size distribution to packing

Particulate systems are of great interest in many fields of science and technology (see [1]). Packing of particles affects physical properties of the granular system. The observed and expected influence of particle size distribution on random packing structures increases the interest in relating both, either theoretically or by computational methods.

Modelling of PSD and the packing of particles of granular media produced by grinding has been jointly addressed in [2]. In [3] the effect of type of distributions on packing density is studied using dense random packing of sands, and in [4] a probabilistic approach is used to determine the distribution of the volume of voids between packed spheres once their size distribution is given. In [5] a threedimensional Apollonian packing is used as a model for dense granular systems to investigate the fractal nature of packing. Packing of spheres with lognormal distribution of radii has been studied in [6] by means of computer simulations. Monte Carlo simulations are used in [7] to create the structure made of spherical particles of sizes obeying a given distribution.

Fractal models used for PSD of different granular media may be useful to study the packing structure. The goal of this work is to apply a version of the computational method used in [7] to the fractal PSD model proposed in [8]. In particular, we have been interested in studying the influence of the parameters defining of the fractal model on the resulting void fraction.

2 The particle size distribution model

In practical terms the statistical similarity property for a grain distribution might be defined by the requirement that after sieving some amount of granular material with sieves of different size, the structure of the grain distribution of the material sieved is equivalent (in information terms) to the grain distribution of the initial one.

Let us suppose that the granular material is sieved retaining grains of size greater than r (think r = 1/2). Suppose that the fraction of material sieved is p_1 and the retained part $p_2 = 1 - p_1$

Let w_1 and w_2 be the linear transformations $w_1 = x/2$ and $w_2 = (x+1)/2$ which transform the interval [0,1] into the subintervals [0,1/2] and [1/2,1] respectively.

Following [8], the invariant measure μ verifying

$$\mu(I) = \sum p_i w_i^{-1}(I) .$$
 (1)

is proposed as a model for PSD. The measure of any subinterval J is easily computable using Elton's theorem [9].

3 The packing algorithm

The computer simulation of packing has been done following the algorithm described in [7]. This algorithm, in a first step seeds (according to a uniform distribution) the initial positions of particles within a square domain of area equal to the sum of the areas of the particles multiplied by 4/3. In a second step, a process of rearrangement is iteratively repeating. In this process the relocation of each particle, i, is performed as follows: a search is made of all particles which overlap particle i, then a displacement vector is calculate for each particle j which overlaps i, following the equation:

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$$\boldsymbol{R}_{ij} = \boldsymbol{R}_j + \left(\boldsymbol{R}_i - \boldsymbol{R}_j\right) \left(\frac{\boldsymbol{r}_i + \boldsymbol{r}_j}{\boldsymbol{d}_{ij}}\right). \tag{2}$$

where R_i and R_j are the vectors of the centers of the particles i and j, the parameters r_i , r_j , are the radii of the particles i and j, and d_{ij} is the distance between the centers of the particles i, j. If there are more than one particle which overlaps the particle i, then the arithmetic mean of all R_{ij} is calculated.

The algorithm takes into account the cases when a particle is not in contact with another particle, then that particle is moved to contact its nearest neighbour.

4 Results

Following section 2, different PSD have been generated for different values of p_1 and p_2 . The packing algorithm has been applied with the simulated PSD's with 10 replications for any of them. The influence of these parameters on the porosity have been studied. Figure 1 shows the results of the simulations for two different values of p_1 . The variation of the mean porosity of replications is shown in Fig. 2 as a function of the sample size for three values of p_1 . Mean values and the standard deviation values of the porosity measured over the replications implemented for the p_1 are summarized in Table 1.

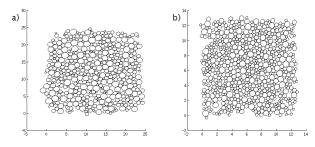


Figure 1: Examples of the results of two simulations for a) $P_1 = 0.1$ and b) $P_1 = 0.7$.

Table 1: Mean values and standard deviation of the porosity for the replications implemented for $P_1=0.1$, $P_1=0.4$ and $P_1=0.7$.

| P1 | Mean Porosity | Standard deviation | Number of Samples |
|-----|---------------|--------------------|-------------------|
| 0.1 | 0.283 | 0.0146 | 10 |
| 0.4 | 0.279 | 0.0130 | 10 |
| 0.7 | 0.259 | 0.0170 | 10 |

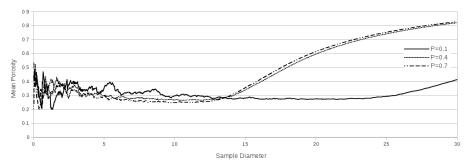


Figure 2: The variation of the mean porosity as function of the sample diameter for $P_1=0.1$ (continuous line), $P_1=0.4$ (dashed line), $P_1=0.7$ (dots and dashed line). (the sample is a circle centered on the mean value of the coordinates of all particles and the unit of length is the same as for the particles).

A first conclusion is the dependence of the variance on the value p_1 : for values showing a great variance, the number of particles used should be increased in order to ensure the reliability of computer simulations in obtaining the representative elemental volume of the porous medium. Results also seem to indicate the relation between porosity and the value p_1 . Further simulations are planned.

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