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The development of a simulation model of the dense packing of large particulate assemblies

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Abstract

The dense packing of particulate assemblies is an enduring theoretical and practical problem. In spite of its apparent simplicity, this problem still remains challenging. Recent progress in the performance of computers boosted the development and realization of a number of effective packing algorithms. Yet, because of the complexity of the problem, many of existing methods have difficulties in handling large numbers of particles. A simulation model is proposed to overcome this. The model assumes that the centers of the spheres are randomly generated at the intersections of a cubic lattice. The largest possible spheres are packed first; subsequent spheres are limited by the set of minimum diameters, which is specified by the constraints imposed by two major parameters imitating the compaction gradient: a reduction coefficient and the number of packing trials. Importantly, the packing arrangements are not defined by the initially specified particle size distribution (as considered by many existing packing algorithms), but rather the most dense particle size distribution, along with the corresponding value of packing degree, is generated by the proposed model. Based on these criteria, a very fast algorithm was developed for simulating of the dense packing of large assemblies of particulate, spherical material (in the order of millions of particles). Using this approach, the influence of geometrical parameters and model variables on the degree of packing and the corresponding distribution of particles was studied.

Keywords: Simulation model; Packing algorithm; Packing degree; Particle size distribution; Particulate material; Initially pre-packed state

1. Introduction

The problem of the best possible packing of particulate or spherical assemblies arose with the demand for a better understanding of both material structure and also of engineering problems related to the military, trade and transportation [1–5]. Dealing with equally sized spheres, Kepler in 1611 suggested that "no packing of balls can be denser than the face-centered cubic lattice arrangement", which is equal to $\pi/\sqrt{18} \approx 0.74$. Only recently Kepler's conjecture was confirmed by Hales; yet, the validity of Hales' proof is still debated by mathematicians [3–5].

The maximum packing value of randomly packed equally sized spheres was found to be 0.64 [6–9]. An increase in density could be achieved only if spheres of different size are used. In this case, smaller spheres must fit into the cavities between the already packed bigger neighbors—a similar procedure to the small spheres in the three-dimensional representation of the Apollonian problem [9]. By using a wide range and large number of particles, the packing density can theoretically approach very close to unity.

The optimal arrangement of spherical systems has been the subject of many experimental and theoretical investigations [7–12], but, still, the problem of the dense packing of large assemblies of particulate materials of nonuniform sizes requires further attention. This problem has important implications for modeling the behavior of composite materials and also for a number of engineering processes [13–18]. Generally, it is accepted that the improvement of the packing degree of particulate systems can boost the performance of existing materials and technological processes. Better packing of composite materials may advance fundamental engineering properties: strength, modulus of elasticity, creep and shrinkage. Further, it brings valuable savings due to a reduction in the volume of binder.

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The first attempts to provide the "best" particle distribution for spheres of different diameters were based on trials with balls and geometrical calculations [10,15–17,19]. These experiments resulted in the recommendations on sizes and proportioning of balls or optimal distribution curves [16–19]. Some of these findings are currently accepted as standards. One of the early examples is presented by Fuller [20] in a series of curves which are currently used for the optimization of concrete and asphalt aggregates:

$$P = 100\left(\frac{d}{D}\right)^n$$

where P = total percent of particle passing through (or finer than) sieve; D = maximum size of aggregate; d = diameter of the current sieve; and n = exponent of the equation (n = 0.45–0.7).

Because it is relatively simple by using a few (or at least two) sets of particulate materials to achieve the "target" distribution of particles with a minimum deviation [21], this approach is extensively used. Yet in spite of its practical importance, this empirical method cannot predict the packing degree of the particulate mixtures.

A model developed by Aim and Goff [22] and Toufar et al. [23] has provided a useful tool for explaining the packing mechanism. Their model deals with the packing of two groups of equal spheres. Each group of spheres is represented by its characteristic diameter and its eigenpacking degree. After a minor adjustment, it was demonstrated that this model gives quite a good explanation of the experimental results [24]. However, to apply this model, it is necessary to measure or estimate the eigenpacking degree of the individual group of particles. Moreover, real systems are usually better represented by the particle size distributions rather than by the characteristic diameter. These two constraints limit the applicability of this model. Another approach to the optimal packing of the particulate materials is based on the Solid Suspension Model [25].

In spite of several reports emphasizing the valuable contribution of the shape of the particle on packing [16,21,26–29], it is still appropriate to model and represent natural or artificial particulate materials (which are mainly irregular in shape) by using groups of spheres of different diameters. This assumption reflects the existing methods of particle size analysis and helps to simplify the packing calculations [19,29].

With the development of computers, the packing problems of real systems became a challenging subject for engineers [7–12,27–32]. The first computer algorithms were able to pack only about 1000 spheres per hour [29]. Such algorithms are usually based on the modeling of the movement of particles (represented as spheres or ellipsoids) due to rolling or sliding under the compaction gradient. Based on this strategy, the particles in a rigid container are forced to occupy the best vacant positions in the neighborhood. Modern modeling approaches include better insight into the natural packing process and even full-scale modeling of the particulate systems [9,28,33]. The contribution of additional factors (such as friction and deformation) acting at the contact points was found to be essential for modeling the dynamic processes, involving particulate materials [33–40]. To realize such algorithms, each movement of a particle requires the solution of the relevant differential equation; this procedure slows down the calculation process [40]. A comprehensive survey of packing algorithms was recently presented by Jia and Williams [28].

An interesting approach to dense packing was suggested by Anishchik and Medvedev [9]. It involves the solution of

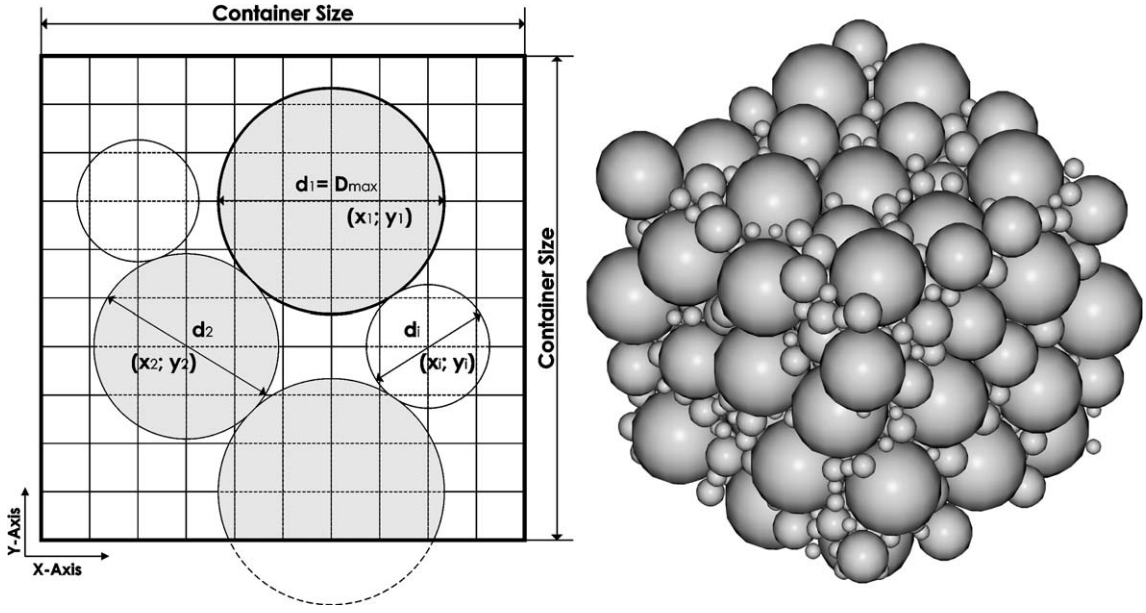

Fig. 1. 2D Representation and the application of the packing model for packing of 1000 spheres with 80% at N = 1M and K = – 3.

the three-dimensional Apollonian problem using the Voronoi–Delaunay method extended to deal with nonequal spheres [9]. As a result of this method, a new sphere is packed into the Voronoi S-region (the region of a volume all points of which are closer to the surface of a given sphere than to the surfaces of other spheres in the packing). Using this approach, a very high packing degree of 90% was achieved using a relatively small number of particles (about 40,000) [9].

2. Importance of the problem

In spite of recent progress in the development of packing algorithms, it is evident that a new approach is needed to deal with large assemblies of particulate materials. On the one hand, the natural packing processes must be simulated; yet on the other hand, the approach must be robust and easily applicable to solve engineering problems. Of special interest for many practical applications is the problem of establishing the relationship between the "best" particle distribution and the degree of packing.

3. Description of the packing model

The improvement of existing packing strategies can be achieved when the "classical" packing problem (involving the finding the degree of packing for given particle size distribution) is transferred to a problem of finding the "best" particle distribution and corresponding degree of packing for given packing conditions [41]. It is obvious that the realization of such an approach would require significantly reduced computational efforts and therefore would be applicable to large assemblies of particulate materials.

It was found that a good approximation to the packing of particulate materials of elementary volume within a container with rigid or periodic boundaries can be achieved when the center of the particle is randomly located at the grid of a cubic lattice [29]. In this case, a thick 3D mesh with an opening size of less than 1/100 of the minimal diameter of the particle must be used to minimize any possible error. The particle is considered as a discrete element which is represented by a sphere. A simplified two-dimensional (2D) representation of the packing algorithm and an example of its 3D output for 1000 spheres are presented in Fig. 1.

The developed algorithm begins with the random generation of a center for the first sphere. Packing starts using a

Table 1
Variable parameters of the simulation model

Total amount of spheres, N_{total}	Maximum sphere size, D_{max}	Number of packing trials, N	Reduction coefficient, K
$5M = 5 \times 10^6$	$10k = 10^4$	$10k = 10^4$	−1
		$100k = 10^5$	0
		$1M = 10^6$	+1

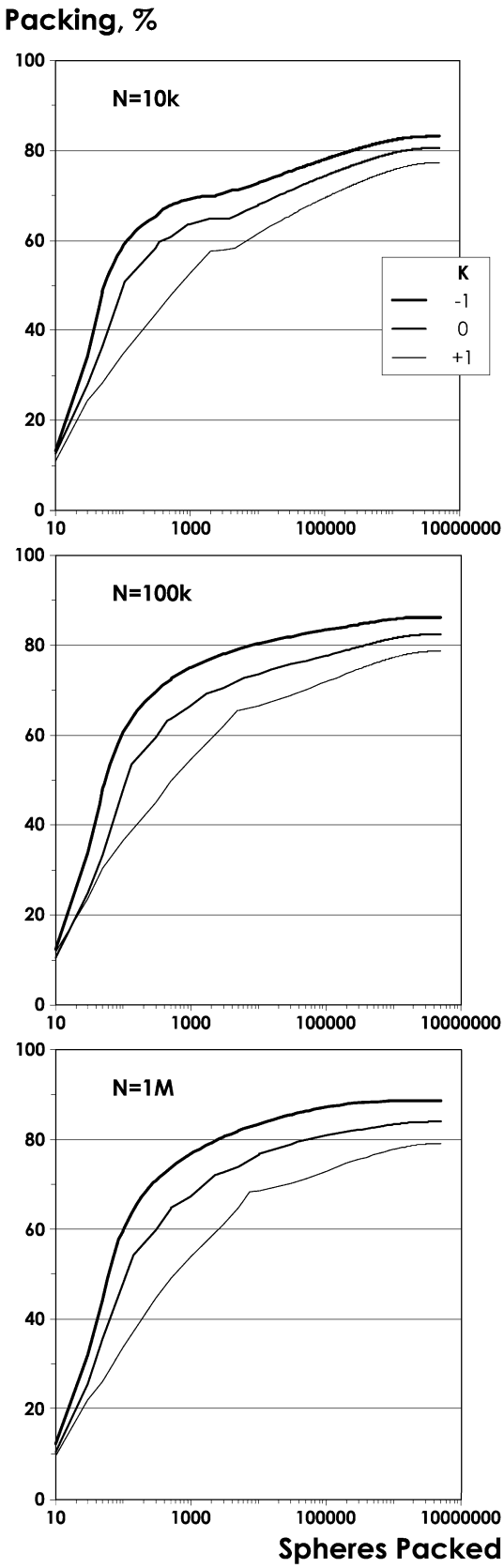

Fig. 2. Development of packing degree.

sphere of the maximum diameter (D_{max}) followed by the placement of the spheres with a diameter larger than or equal to the minimum diameter ($D_{max} \geq d \geq D_{min}$). Overlaps between spheres are not allowed; importantly, a sphere can be packed only if its center is located inside the container. If the generated coordinates are not suitable for the placement of a sphere (with a diameter in a range between D_{min} and D_{max}), then the sphere is discarded and new coordinates of the center are generated. If parts of the accepted sphere are located outside of the container, the corresponding reduction of the volume is provided. After achieving a certain number of packing trials N, D_{min} is reduced using the coefficient K according to the following formula: $D_{min} = D_{min}/(1+10^K)$ [41]. Finally, with the adjustment of the container size/D_{max} ratio, N and K, a very quick pseudo-dynamic packing strategy was realized (Fig. 1).

In this research program, the packing into a container with periodic boundaries was considered in order to represent the elementary volume of particulate assemblies and also to eliminate the wall effect. The ratio of the container size to the maximum diameter of the sphere was fixed at 3.3 (that is, a common assumption related to the density measurements when the wall effect is eliminated). The total amount of spheres used in the packing trials (N_{total}) was set at 5×10^6 (5M) for all trials, and the mesh size was 1/32,766 of the container length.

The variable parameters and their levels are presented in Table 1.

4. Results and discussion

The results of the simulation algorithm are presented in Figs. 2 and 3 and Table 2, where the passing values are given for specific particle sizes that are standard for the sieve analysis; they are determined using the formula: $d_i = D_{max}/2^m$ (where $m>0$).

4.1. Packing process

The development of the packing degree depending on N (number of packing trials) and K (reduction coefficient) is demonstrated in Fig. 2. As expected, the major contribution to packing is provided by the first 10^5 (100k) packed spheres. It is important that the packing of first 100 spheres is represented by the straight line (Fig. 2) and determined only by the reduction coefficient K. in this case, any N results in the densest possible packing; for example, the ~ 60% packing is achieved at $K=-1$. There is almost no significant density increase after the packing of 300k spheres at $K \leq 0$ and $N \geq 100$k. The highest value of packing degree − 88.64% is achieved with a peak value of $N=1$M and the lowest used value of $K=-1$ (Table 2). The specific yield part of the packing curve at $K<2$ and $N<100$k could be attributed to the ineffective cavity-filling process with the limited number of the high- and medium-sized spheres (because of low N) at the range between 1000 and 5000 spheres. This condition is lifted with the consequent exploration of the free space at later stages (Fig. 2). It is observed that an increase of N and a reduction of K serve the same function: it provides the priority for packing spheres of maximum size and the pseudo-dynamic functionality of the algorithm.

4.2. Particle size distribution

The major interest of the model is seen in the distribution curves (Table 2; Fig. 3). The best gradings with 86–88% packing are obtained at $N=10^5-10^6$ (100k–1M) and $K=-1$ (Table 2).

It is observed that the curves representing the densest assemblies ($N=1$M and $K=-1$) are modified Fuller type or "Initially Pre-Packed" gradings (IPP-gradings [41]) with a predominant volume (~ 50%) of the largest particles ranging from D_{max} to $0.85*D_{max}$. This arrangement results in 48.4% of packing. About 34% of the volume is represented solely by the spheres of maximal size (D_{max}) which are responsible for 28% of packing. Still, the relatively narrow range of particle sizes (from D_{max} to $D_{max}/2$) provides about 60% of packing (Table 2; Fig. 2).

This group of particles can be considered as arranged in a manner similar to the "ideal" regular close-packed lattices (Fig. 1) that approaches the condition of maximum possible value for randomly packed systems (jammed state) [8]. Such

Table 2
Results of the simulation

N	K	Packing degree, %	Passing through a sieve with an opening of size $d_i = D_{max}/2^m$ at m									
			0	1/2	1	2	3	4	5	6	7	8
10k	−1	83.2	100	40.84	33.98	25.15	19.33	13.85	8.79	4.53	1.16	0.01
	0	80.63	100	58.74	39.2	28.81	22.63	16.01	10.04	4.98	1.16	0.01
	+1	77.35	100	62.72	54.64	40.27	27.93	19.14	11.73	5.56	1.15	0.01
100k	−1	86.26	100	41.63	32.6	22.18	15.17	10.49	7.08	3.92	1.18	0.02
	0	82.47	100	61.48	37.4	26.23	18.96	13.51	8.94	4.65	1.17	0.01
	+1	78.73	100	61.72	53.66	38.65	26.02	16.97	10.94	5.31	1.16	0.01
1M	−1	88.64	100	43.12	34.11	22.23	14.5	9.18	5.66	3.23	1.19	0.02
	0	83.98	100	62.81	38.44	26.01	17.35	11.52	7.56	4.23	1.18	0.01
	+1	79.12	100	66.23	54.96	39.4	27.28	15.74	10.68	5.26	1.15	0.01

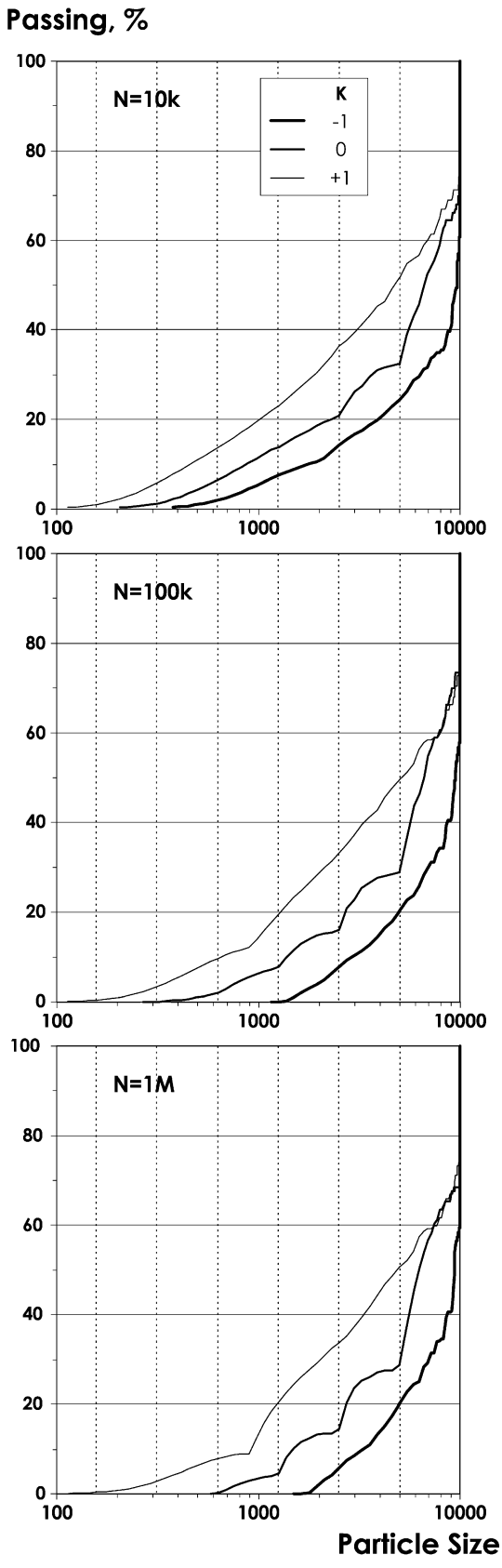

Fig. 3. Particle size distributions corresponding to 75% packing.

dense packing conditions are determined by the combination of high N and low K. In this case, the distribution of particles is obtained by the relatively narrow range of the sizes. To achieve the same packing degree at a less arranged initial structure, a much wider range of sizes is necessary (Fig. 3).

In practice, due to friction between particles and their irregularity, the achievement of these well-arranged initially pre-packed structures is quite difficult using the conventional compaction methods. As a result, many particulate assemblies could be described by those models with $K \geq 2$. This condition is the case of a "Loose Initial Packing" (LIP) arrangement [41], when the largest particles (from D_{max} to $0.85D_{max}$) occupy only 24% of volume and provide 25.8% of packing (Table 2; Fig. 2).

Quite interesting behavior is observed for the particle size distribution curves at $K=2$. In this case there is a gap between D_{max} and D_{min} even at one of early stages of packing process. This results in a loose initial packing, but at the same time, the void filling capability of the algorithm is realized (Fig. 3). Due to this feature, the "Gap-Gradings" are achieved. It is noticeable that with increasing N, the amount of characteristic zones corresponding to the void filling effect increased from three (at $N=10$k) to four (at $N=1$M). At $K>2$, the particle size curves are represented by the continuous distributions involving a wide range of particles that are very close to practically applied Fuller functions. Still, at high N, the void filling feature results in a characteristic zone at particle size of $D_{max}/10$ (Fig. 3).

5. Conclusions

1. For a given number of particles, dense packing is achieved either when dense pre-packing is realized or when a wide range of particle sizes is available. The best packing curves with a 86–88% packing degree are presented by the modified Fuller type or "Initially Pre-Packed", IPP-gradings. The characteristic feature of the IPP-gradings is related to high (60%) values of packing degree obtained by the narrow range of particle sizes from D_{max} to $D_{max}/2$. The IPP condition occurs when the combination of a high number of packing trials and a low reduction coefficient is set.
2. The opposite case is a "Loose Initial Packing" or LIP condition when a high (77–84%) packing degree is obtained due to a wide range of particle sizes. This condition is characteristic of many "real" particulate assemblies which could be presented by models with $K \geq 2$. It was found that the void filling capability of the algorithm is realized at $K=2$. In this case, there is a gap between D_{max} and D_{min}, so many vacancies are left while the program runs; however, due to a void filling capability, these gaps are closed on the later runs. This results in a particle size distribution known as "Gap-Gradings".

3. The predominantly static or pseudo-dynamic model, described in this report, may be further improved if the placed particles are allowed to change their location so as to occupy a possible better vacancy corresponding to a bigger diameter. Alternatively, the performance of the algorithm, especially in the range of medium- and small-sized spheres, could be improved by implementing the self-adjusting (or just sliding) values for a number of packing trials N or a reduction coefficient K in order to keep the tight range of currently packed particles. It is obvious, that only minor adjustments to current model might be necessary to represent virtually any particle size distribution. After such updates, the developed algorithm, when built into a recursive procedure, could even be applicable to solve the "classical" packing problem involving the search for the degree of packing for given number of particles and particle size distribution.

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