Fractal Properties of Dense Packing of Spherical Particles

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Abstract

Two computer models were developed to realize the algorithms of random Apollonian and Apollonian packings of the spherical particles in a unit cube. A genetic algorithm was developed for the latter packing model. The upper and lower bounds of a fractal dimension were computed using various numerical methods. It was observed that for both models the fractal properties were not essentially affected by the configuration of initial spheres.

1. Introduction

The quest to obtain the densest possible randomly packed arrangement for particles of varying shapes and sizes is an ongoing and challenging problem; it also has exceptionally wide applications in science and engineering. The hard-sphere packing model is one of the simplest representations of many non-crystalline systems. Examples of systems that are well described by dense random packing of spherical particles include composite materials, colloids, amorphous metals, and simple liquids.

The packing density of spheres is characterized either by packing fraction η, or by porosity $\varepsilon = 1 - \eta$, which is a fraction of unoccupied volume. As Kepler conjectured - and Hales proved [2, 3] - the optimal packing of equal hard spheres is the face-centered cubic (fcc) arrangement with a maximal density of $\pi / \sqrt{18} \approx 0.7405$. As it was shown by Schaertl and Sillescu [1], increasing polydispersity raises the maximum packing fraction η of a hard-sphere system. The particle size distribution is a basic parameter which describes a polydispersity of a hard-sphere system that, for a given η, depends on the selected sphere-packing algorithm. However, for static polydisperse space-filling packings, Aste [4] has analytically proved that the size distribution for the spheres of small radius r ($r < r_{\max}/5$) follows the power

law: $N(r) \propto r^{-\alpha}$, where $N(r)$ is a number of particles. Further, Aste [4] demonstrated that in the case of static polydisperse packings there is an upper and lower bounds of α, which depends on a certain sphere-packing algorithm. The Apollonian packing (AP) algorithm [5] provides the lowest bound of α. The upper bound of α is defined by the "random Apollonian packing" [6]. The "random Apollonian packing" (RAP) is realized by a process that starts with an initial population of hard-spheres of a specified radius with new spheres added one at a time into the packing's unoccupied space. Therefore the center of newly packed sphere is randomly selected and the sphere's size is determined by extending the radius of a sphere until it touches its closest sphere. According to Aste [4], "random Apollonian packing" is defined by $\alpha = d + 1$, where d is a number of dimensions. Recently Dodds and Weitz [6] have shown that some dynamic packing algorithms, where the growing spheres are seeded by a random injection in time and space, could be portrayed as a variation of static packing. They explored the "random Apollonian packing" algorithm and the "packing-limited growth" algorithm using various scenarios of growth dynamics (heterogeneous, exponential, linear). With scaling theory and a numerical simulation they analytically obtained $\alpha \approx 3.8$ for $d = 3$.

The classical Apollonian packing is a two-dimensional case of more general osculatory packings, where two-dimensional osculatory packing of the unit circle is presented by three pairwise externally tangent circles that are all internally tangent to the first one. These circles are called the initial circles of the packing. In the n-dimensional setting, the number of initial spheres is $n + 2$ [7]. Apollonian packings are self-similar [5] and are characterized by a fractal dimension D, which is related to α as $D = \alpha - 1$ [8]. Boyd in his remarkable theorem proved that D is the same for all osculatory packings [9]. It is assumed that D cannot be obtained analytically. Borkovec et al. constructed two fundamentally different numerical methods and computed the fractal dimension of the classical 3-dimensional Apollonian packing to be 2.4739465 [7]. More recently Baram and Herrmann developed an algorithm to construct classical 3-dimensional Apollonian packing with various configurations of initial spheres [10]. Investigating all possible configurations corresponding to Platonic Solids (tetrahedron, cube, octahedron, dodecahedron and icosahedron) and computing the fractal dimensions for these solids, they demonstrated that the fractal dimension D depends on the packing configuration of initial spheres. According to the reported results, D varies from 2.474 for the tetrahedron and up to 2.588 for the bichromatic (octahedron-based) configuration of initial spheres [10]. A few articles report the fractal properties of Apollonian packing with the random distribution of initially prepacked spheres (lately named Apollonian packing or AP). Anishchik and Medvedev [11] proposed a computer model of 3-dimensional Apollonian packing of the hard spheres based on the Voronoi-Delaunay method that was applied to study the dense packing of equal spheres [12]. Anishchik and Medvedev used the Voronoi-Delaunay approach to determine the centers of largest spheres inscribed between the spheres for a relatively narrow range of the sphere sizes (in their work the particle radii differ by less than 10 times). They obtained the fractal dimension $D = 2.45$ which is somewhat less than that for the classical 3-dimensional Apollonian packing with a tetrahedron configuration of the initial spheres ($D =$

2.474). This contradiction can be attributed to the limitations of the Voronoi-Delaunay method applied to pack the spheres of different sizes.

In our study we propose computer simulation models for 3-dimensional Apollonian and random Apollonian packing algorithms to evaluate the upper and lower bounds of α for space-filling polydisperse packings. Our approach is based on a computer model described by Manna [8] for 3-dimensional random Apollonian packing (RAP) of hard spheres. A 3-dimensional Apollonian packing (AP) was realized using the same model enhanced by a genetic algorithm (GA). A GA searches the free space to inscribe the maximum-sized spheres among the previously packed spheres. Few articles deal with the sphere-packing problem using GA. Franck-Oberaspach et al. employed a GA for the solution of two-dimensional packing problem of different rigid objects [13]. In their work an arbitrary number of points is arranged within a given two-dimensional connected region in a such way that their mutual distances and the distance from the region boundary reaches a maximum [13]. Cornforth applied a GA for the placement of overlapping grids for input space quantization in machine-learning algorithms [14]. The AP is often visualized in a three-dimensional space with the task of fitting the maximum number of oranges (represented by equal spheres) into a box. Therefore, Cornforth applied a GA for a sphere-packing problem to achieve the maximum density of equal spheres in a given space [14]. Much of the existing models cannot be employed in the case of AP because of their lack of dimensionality and diversity of packing objects.

2. Computer Simulation Models

The RAP model is described as a predecessor of AP model. The developed algorithm of RAP starts with the random placement of the hard spheres of an initially specified configuration into the cube with periodic boundaries. The particle size distribution of an initial configuration of spheres is set by the Gauss's Law. Further, the packing is provided by placing new spheres (one at a time) into the cube by a random selection of a fixed point (as the center of a new sphere) within the free space and extending its radius r_l to meet the closest sphere. In the case of the AP model, the latter step includes the search for the center of a new sphere so that the new sphere can occupy the maximum volume within the available free space left between the previously packed spheres. This step represents a global numerical optimization problem, where $max(r_l)$ is an objective function defined by the search space $S \subseteq R^3$, which is the finite internal region in the 3-dimensional Euclidean space. The search space is restricted to a feasible region (F, where $F \subseteq S$) by a set of constraints imposed by the restriction for the spheres' overlapping: $(x_i - x_l)^2 + (y_i - y_l)^2 + (z_i - z_l)^2 \geq (r_i + r_l)^2$, where x_i, y_i, z_i are the coordinates of packed (i) and new (l) spheres, $(x, y, z) \subseteq R^3$, $i = 1,...,N-1$, $l = i+1,...,N$ and N is a total number of the spheres.

The Genetic Algorithms (GAs) can be employed for solving a wide range of global numerical optimization problems [15]. The advantage of GA is that it does not require a consideration of the landscape of a search space nor the shape of an

optimized function [15]. Therefore, GA is a universal tool for a number of optimization problems. To realize GA, a "genetic pool" of solutions (i.e. the spheres with various radii) is transformed by random "mutations" of their respective codes (a binary string with a length L representing the solution of GA) with a probability p_m and "crossovers" with a probability p_c. New solutions are then evaluated by a "fitness function" (objective function), in such way that only the best solutions "survive". This procedure is applied either for a certain number of generations (N_{gen}), or until the "pool" of solutions statistically reach a fixed point. The quality of a solution with reasonable computational cost (a number of runs for evaluation of function that is directly proportional to a number of generations) is usually a trade-off. Coello, comparing several constraint-handling approaches of GAs, showed that the best results are usually obtained with high computational costs [16]. For the packing problem a computational cost (T) can be represented as $T \propto N^2$, where N is the number of packed spheres; therefore, a constraint-handling method that provides a minimum runs for evaluation of function, but with reasonably high quality of a solution should be applied. For AP the constraint-handling method proposed by Amirjanov [17] was selected. This method, named CRGA (changing range GA), adaptively shifts and shrinks the search space by employing feasible and infeasible solutions in the population to reach the global maximum. CRGA significantly improves the speed of convergence to the global maximum with reasonable precision [17]. According to the method, an elite subset (h_s) of ranking individuals (solutions) from a whole population (N_{pop}) is selected in every generation. Individuals are ranked using stochastic ranking [18] which balances between preserving feasible individuals (satisfied constraints) and rejecting infeasible ones (unsatisfied constraints). This balance is derived from a stochastic bubble-sort algorithm. A probability P_f was introduced for comparing any pair of two adjacent individuals to determine a better fit [18]. Next, for every variable (x, y, z) the center of attraction (or reference point) is identified by calculating mean of a variable from a subset of the ranking individuals [17]. Finally, the size of the search space is shrunk relative to the previous size using coefficient k_r and is shifted to the center of attraction. The shrinking of the size of the search space (the domains of the variables) is continued within every generation until the size of the region becomes greater or equal to t_r of an initial size of the search space. The shrinking and the shifting mechanisms allow the concentration of the search space to a certain cell of a cube. Consequently, the number of evaluations required to examine the set of constraints (overlapping spheres) is significantly reduced [17].

3. Computational Results

Both RAP and AP packings are simulated within a unit cube with periodic boundary conditions. An initial configuration consisting of 100 spheres is seeded according to Gauss's Law with a mean value $\bar{r} = 0.5$ and standard deviation $\sigma = 0.05$ (first experiment) and $\sigma = 0.15$ (second experiment). All experiments were repeated 10 times (N_s). The following values were established for the best performance of GA to simulate AP: $N_{pop}=50$, $p_c=0.85$, $p_m= 0.02$, $L=15$ *bits*, $P_f =0.42$, $h_s=0.2$, $k_r=0.475$, $t_r=0.0025$, $N_{gen}=150$.

The experimental details and the results of a simulation for both models are summarized in Table 1.

Figure 1 illustrates the initial configuration of spheres seeded according to Gauss's Law, where spheres are placed in the cube one at a time by randomly choosing the center of a new sphere in the matrix's free space and expanding its radius r_i to touch the closest neighbor (as per as 3-dimensional RAP approach). Figure 2 demonstrates the sequence of the 3-dimensional Apollonian packing of the spherical particle. As shown in Figure 2 (from step 1 to step 4) the GA searches the packing's free space within the cell in order to place a new sphere with the largest possible radius.

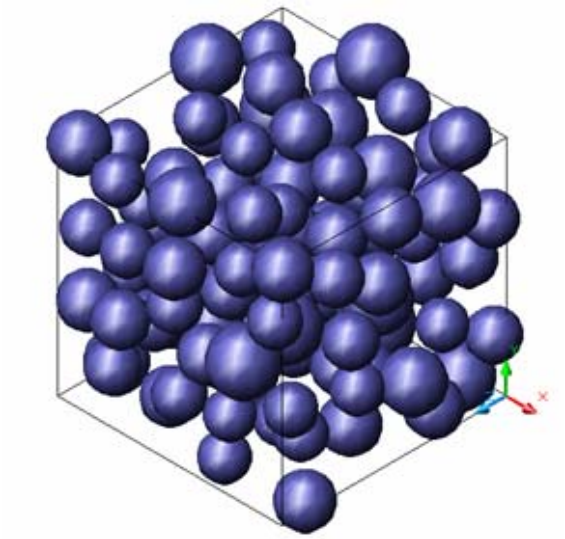

Figure 1. Initial configuration of spheres seeded according to a Gauss's Law ($\sigma = 0.05$)

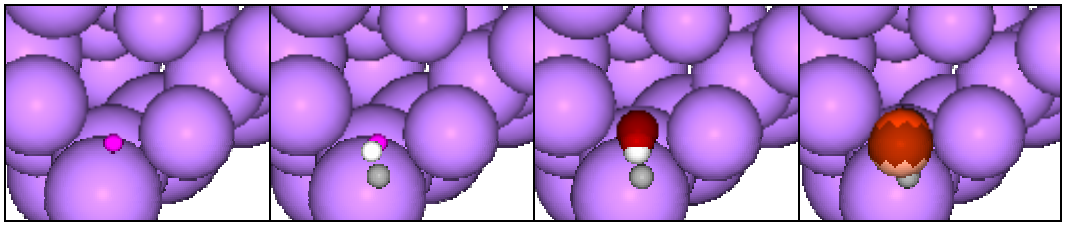

Figure 2. GA search for 3-dimensional Apollonian Packing (AP)

Figure 3 represents the frequency distribution $N(r)$ of the first experiment (double-logarithmic plot) in order to demonstrate the differences in α for both RAP and AP models (where mean values are presented). The straight lines specify the exponent α for RAP and AP. The inset of Figure 3 shows the frequency distribution $N(r)$ vs. r at a wider range, up to cutoff radius $r_c = 0.002$, where RAP and AP simulations involved 10^7 and 10^6 spheres, respectively (N_{total}). It can be observed that a significantly higher number of spheres are required to occupy the packing's free space when the sphere's size is approaching the cutoff radius r_c.

Table 1. Experimental details and results of the simulation for RAP and AP

Parameters	Experiment 1 $\sigma = 0.05$		Experiment 2 $\sigma = 0.15$	
	RAP	AP	RAP	AP
N_s	10	10	10	10
N_{total}	10^7	10^6	10^7	10^6
η_{ini}	0.3524	0.3524	0.5023	0.5023
α @ $N(r)$	3.710 ± 0.009	3.51 ± 0.01	3.712 ± 0.009	3.49 ± 0.01
α @ $\varepsilon(n)$	3.727 ± 0.001	3.4518 ± 0.0006	3.729 ± 0.002	3.4237 ± 0.0004
η	0.803	0.909	0.839	0.923

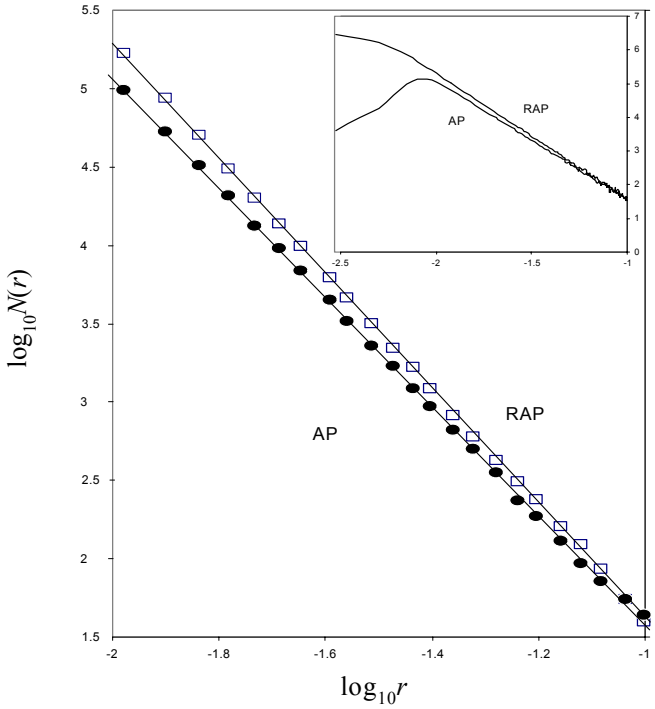

Figure 3. Frequency distribution function $N(r)$ vs. r for the Experiment 1 at $\sigma = 0.05$

The best-fit estimation for the exponent α is given with 95% confidence interval. The estimation of α using a frequency distribution $N(r)$ for RAP closely agrees with the scaling theory proposed by Dodds and Weitz [6]. The curves of a frequency distribution $N(r)$ for the Experiment 2 are shifted to the left as can be seen in Figure 4 (RAP1 vs. RAP2) since the volume fraction of the initial spheres (η_{ini} in Table 1) is greater in the Experiment 2.

The estimation of α using a frequency distribution $N(r)$ for AP shows that value of α in both experiments occur within the range described by Baram and Herrmann [10]. The estimated lower bound of α in both experiments is found to vary from 3.48 to 3.52 (or within the limits specified by Baram and Herrmann [10] for

classical Apollonian packings with various configurations of initial spheres). This means that the various topologies of classical Apollonian packing with different fractal dimensions can be realized by the packing process of AP with a random configuration of initial spheres. For 3-dimensional classical Apollonian packing, Baram and Herrmann [10] proved that the fractal dimension D (or α) depends on a configuration of initial spheres. For 3-dimensional Apollonian packing based on random distributions and various configurations of the initial spheres we found no significant difference in the value of exponent α; still more experiments might be necessary to strengthen this assumption.

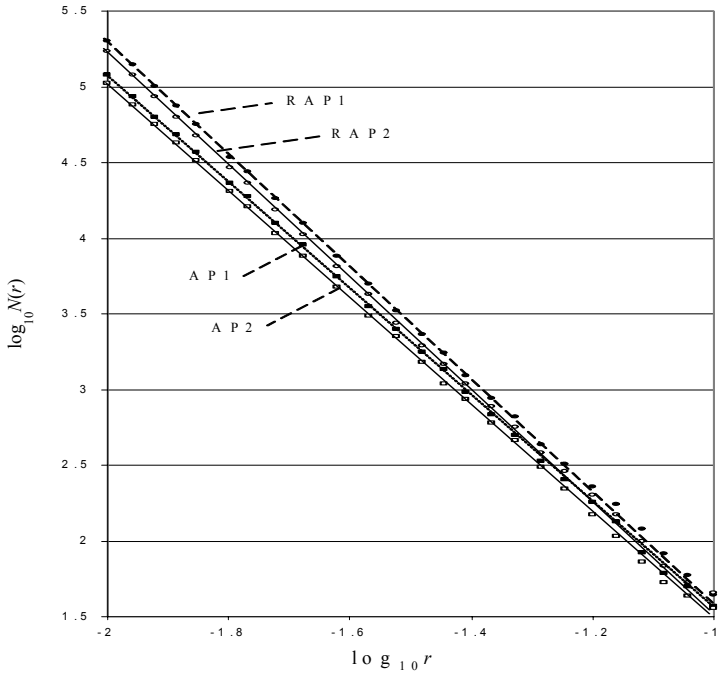

Figure 4. Behavior of the $N(r)$ function for the Experiments 1 and 2

The effect of porosity on the fractal properties of the models was also studied based on the presented approach. The exponent α corresponding to the porosity is given in Table1. Figure 5 represents the double-logarithmic function of porosity $\varepsilon(n)$ vs. n. The relative volume of porous space (or porosity) for both models follows the power law [6, 19]: $\varepsilon(n) \propto n^{-\beta}$, where n is a number of particles. For RAP Dodds and Weitz [6] developed the scaling theory of the distribution of spheres; they determined that $\alpha = (d+1+\beta)/(1+\beta)$. Figure 5 represents the porosity function of $\varepsilon(n)$ versus n for the Experiment 1 and 2 (RAP1 and RAP2). Both curves are in alignment within the zone corresponding to the particles of small radii. The agreement in α values calculated from $\varepsilon(n)$ and $N(r)$ is considered to be satisfactory (the difference is less than 3%). This similarity in values of α governing the functions of $\varepsilon(n)$ and $N(r)$ can be presented as an additional proof of the scaling theory. Based on the relation described by Herrmann et al. [19] : $\varepsilon(r) \propto r^{-D+3}$, for 3-dimensional Apollonian packing the exponent α is specified as

$\alpha = 4/(1+\beta)$. For the spheres of small radii the curves corresponding to AP1 and AP2 are also aligned (Figure 5).

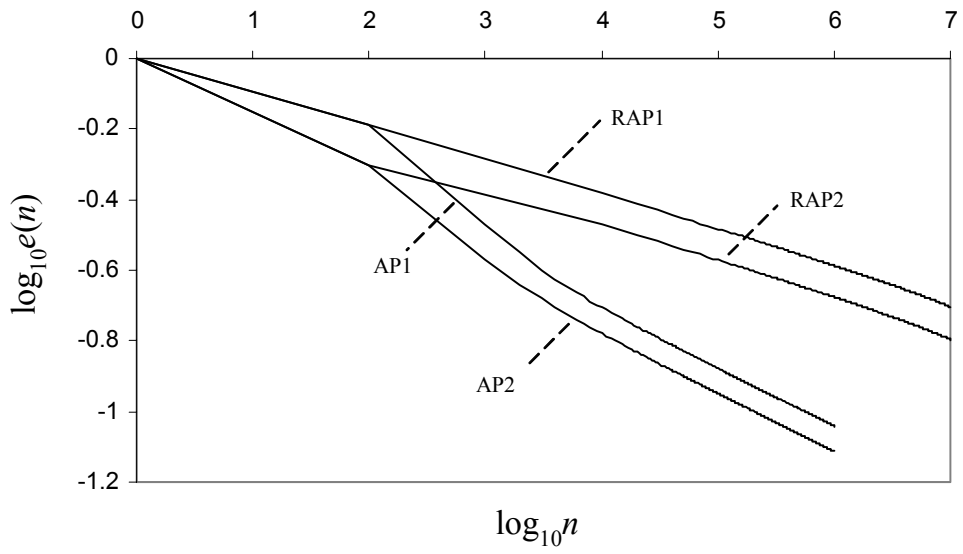

Figure 5. The double-logarithmic function of porosity $\varepsilon(n)$ vs. n

4. Conclusion

Computer models were developed to investigate the fractal properties of 3-dimensional random Apollonian packing and Apollonian packing. The latter was represented as a numerical optimization problem resolved by a genetic algorithm. These models were used in extensive numeric simulations to estimate the lower (AP) and upper (RAP) bounds of an exponent α. The upper bound of α were numerically estimated for $N(r)$ and $\varepsilon(n)$; the experimental results have provided an additional support to the scaling theory proposed by Dodds and Weitz [6]. The anticipated lower bound of α were found to be within the range from 3.48 to 3.52, that is to say within the limits reported by Baram and Herrmann [10] for classical Apollonian packing with various configurations of initial spheres. This means that different topologies of a classical Apollonian packing with different fractal dimensions may be achieved during the packing process of AP at a random configuration of the initial spheres. It was shown that the exponent α was not significantly affected by the configuration of the initial spheres used in both models. When applied the developed models may predict the particle size distributions for a wide range of densities depending on the packing algorithms.

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