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Maximum packing densities of basic 3D objects

LI ShuiXiang*, ZHAO Jian, LU Peng & XIE Yu

State Key Laboratory for Turbulence and Complex Systems, College of Engineering, Peking University, Beijing 100871, China

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Numerical simulation results show that the upper bound order of random packing densities of basic 3D objects is cube (0.78) > ellipsoid (0.74) > cylinder (0.72) > spherocylinder (0.69) > tetrahedron (0.68) > cone (0.67) > sphere (0.64), while the upper bound order of ordered packing densities of basic 3D objects is cube (1.0) > cylinder and spherocylinder (0.9069) > cone (0.7854) > tetrahedron (0.7820) > ellipsoid (0.7707) > sphere (0.7405); these two orders are significantly different. The random packing densities of ellipsoid, cylinder, spherocylinder, tetrahedron and cone are closely related to their shapes. The optimal aspect ratios of these objects which give the highest packing densities are ellipsoid (axes ratio = 0.8 : 1 : 1.25), cylinder (height/diameter = 0.9), spherocylinder (height of cylinder part/diameter = 0.35), tetrahedron (regular tetrahedron) and cone (height/bottom diameter = 0.8).

packing, particle, nonspherical particle, cylinder, cone, spherocylinder, tetrahedron

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To pursue the densest packing has never lost its attraction to human beings. The earliest history of studies on packing problem can be traced back to the famous Kepler Conjecture (the problem of maximum packing density of identical spheres, 1661) and the debate between Newton and Gregory (the problem of maximum coordinate number of identical spheres, 1694). In 1900, Hilbert further presented the packing problem, especially the densest packing of spheres and regular tetrahedra, as the 18th problem in his celebrated list of 23 mathematical problems [1]. For centuries, packing problem has always been attractive since it is not only a basic problem of mathematics and physics, but also extensively applied to many branches of science, engineering and even in daily life. These applications range from the macroscale of celestial body motions to the microscale of molecular arrangements. According to the packing structures, packing problems can be classified into ordered packing and disordered packing. For ordered packing, Hales proposed a proof of the Kepler Conjecture in 1998 [2]. However, it still leaves a long way to the solution of the Hilbert's 18th problem. For disordered packing, random packing which is closely related to matter structure has been investigated extensively. The first systematic study on random packing was undertaken by Bernal in 1950s on the random packing of spheres [3]. Nowadays, numerical simulation has become the main means of random packing researches. Zhao et al. [4] gave a summarization and classification of numerical simulation approaches available on random packing. In respect of particle shapes, sphere is the most comprehensively studied particle shape on random packing, and the packing results are accepted widely within the academic community. Nonspherical particles are often simplified to equivalent spheres in engineering applications. However, recent investigations indicated that the packing properties of nonspherical particles are considerably different from spherical particles, and even a slight deformation on particle shape will increase the packing density notably. Nevertheless, because of the complexity of both particle model and computation, only the packings of a few kinds of nonspherical particles have been investigated. Knowledge on the packing of nonspherical particles is quite limited, especially the particle shape influences on packing density. Packing densities of nonspherical particles were predicted by the sphericity of particles [5], but further studies [6] demonstrate that the

*Corresponding author (email: lsx@pku.edu.cn)

prediction is not correct.

Researches on packing problem have far-reaching significance in both theory and practice [7]. Packing of basic 3D objects can be observed frequently in nature and ordinary life (such as the packing of M&M's candies [8]). It is also a fundamental problem in many disciplines of science and engineering (such as why tetrahedral concrete blocks are used in river damming [7,9]). Moreover, objects of arbitrary shape can be theoretically generated from basic 3D objects (such as basic 3D objects can build a much more complicated 3D solid by Boolean operations in a CAD system; any 3D solid can be separated into an assembly of tetrahedra by Delaunay triangulation technique). Densest packing means best utilization of space, and it has been one of the most important packing problems for centuries. This work summarizes available results thus far on the packing densities of basic 3D objects. The orders of maximum packing densities of basic 3D objects both on ordered and disordered packing are presented, and the optimal aspect ratios of these objects that give the highest packing densities are determined. Current analytical particle models and packing algorithms have difficulties on the simulation of angular particles. In consequence, only the particle shapes with smooth surface, such as sphere, ellipsoid and spherocylinder are well studied, while the packing researches of other particle shapes are extremely lacking. In this work, sphere assembly model and relaxation algorithm [10] are applied to simulating the random packings of spheres, cones, cylinders, spherocylinders, tetrahedra and cubes. The results should fill some blanks in the research area and the comparison of packing densities can be achieved from it. It should be mentioned that only geometric packings of identical 3D particles with periodic boundary condition are concerned in this work.

1 Sphere assembly model and relaxation algorithm of nonspherical particles

The sphere assembly model represents the shape of a nonspherical particle with the contour of overlapping or tangent spheres, and it has the ability to approach any particle shape with enough component spheres [11]. With the model, the contacts between nonspherical particles can be treated as contacts of spheres. Compared with the current analytic models of nonspherical particles, contact detection in sphere assembly model is much simpler, especially for angular particles or particles with complicated shapes. It is a burdensome task to compute the exact surface area and volume of the particles represented by the sphere assembly model since they have rough surfaces. Fortunately, the surface area and volume can be inquired from an AutoCAD system. The sphere assembly models of basic 3D objects are shown in Figure 1. From left to right, they are cylinder, spherocylinder and cube in the upper row, tetrahedron and cone in the lower row.

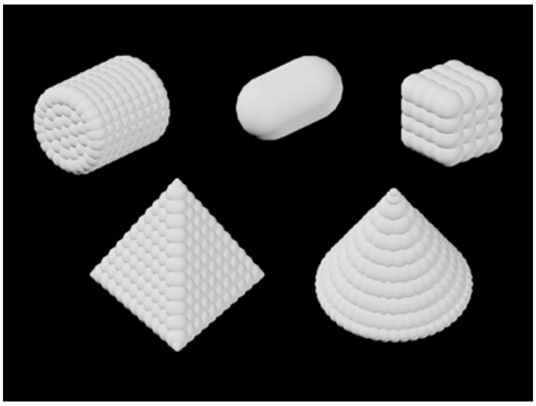

Figure 1 Sphere assembly models of basic 3D objects.

Relaxation algorithm which belongs to collective rearrangement algorithm has been widely applied in sphere packing simulations. Li and Zhao [10] improved the algorithm by introducing torque and rotation of nonspherical particle and extended the original algorithm to simulate the packing of nonspherical particles. The relaxation algorithm gains an advantage over other algorithms by its simple principle and low computation cost. The algorithm begins with randomly placed large overlapping configuration of nonspherical particles in a cubic region. Afterwards, iterations of relaxation procedure are carried out to gradually reduce the overlaps of the particles. Boundary of the packing region is enlarged at the end of each iteration. The final packing is achieved when the maximum overlap rate of all component spheres is below a predefined value.

2 Sphere

The Kepler Conjecture in 1661 is the first investigation on the densest packing of spheres. Kepler believed that the face-centered cubic lattice is the densest packing structure of identical spheres, and the packing density is $\pi/\sqrt{18} \approx 0.7405$. However, it is not easy to prove the conjecture until Hales gave a proof with the help of computer program in 1998. It should be noted that the face-centered cubic lattice is not the only structure of the densest sphere packing [12]. The problem of sphere packing was well studied and the theoretical analysis, numerical simulation and experimental results were consistent with each other. Weitz [13] summarized some important sphere packing densities: the maximum density of ordered packing is about 0.74, the packing density of random close packing is about 0.64, and the packing density of random loose packing is about 0.56. The random close packing of identical spheres was simulated by the relaxation algorithm, and the packing density obtained is 0.6404 [14].

3 Cone

Packing of cones was rarely studied. Trovato et al. [15] investigated the ordered packing of cones and truncated cones. They found a high packing density of $\pi/4 \approx 0.7854$ for ordered cone packing which is independent of cone shape. Chen et al. [16] studied the self-organized structure of cones with sphere assembly model and Monte Carlo approach, though their model called ice-cream cone is not an exact cone. In this work, we simulate the random close packing of cones with sphere assembly model and relaxation algorithm, and the results are illustrated in Figure 2. Numerical simulation results show that the peak value of packing density of cones is 0.6664, while the aspect ratio of cone is 0.8. The aspect ratio of cone is defined as $w = H/D$, where H is the height and D is the bottom diameter.

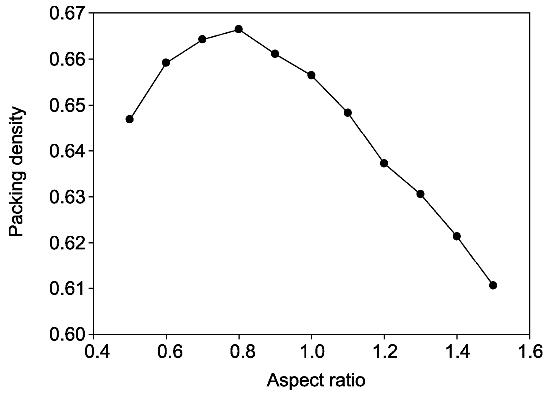

Figure 2 Random packing density versus aspect ratio of cones.

4 Tetrahedron

The problem of the densest packing of tetrahedra was first introduced by Hilbert (1900) and has been remaining as an unsolved problem till now. The packing density of spheres was generally considered as the lowest among all convex objects (Ulam's conjecture), but Conway and Torquato [17] pointed out that the maximum ordered packing density for regular tetrahedra was only 0.717455, which is much smaller than that of spheres (0.7405). Accordingly, they believed the Ulam's conjecture was not true, and they suggested the regular tetrahedron might be the convex body with the smallest packing density. Recently, higher densities of 0.7786 and 0.7820 of regular tetrahedra packings were constructed by Chen [18] and Torquato et al. [19] respectively. For random packing, Chaikin et al. [20] declared that the optimal packing density of tetrahedron which they measured in experiments was above 0.75, while the packing densities in experiments of Dong and Ye [9] were all less than 0.5. Latham et al. [21] found from numerical simulation that the random loose packing density of tetrahedra was 0.416. Random close packings of tetrahedra were simulated with sphere assembly model and relaxation algorithm [22], and the results are shown in Figure 3. The simulation results indicate that the peak value of packing density of tetrahedra is 0.6817 which is higher than that of spheres, while the tetrahedra are regular (the height is 10 and the edge length of bottom regular triangle is 12.2474). If we define the aspect ratio of tetrahedron as $w = H/D$, where H is the height and D is the circumcircle diameter of bottom triangle, then the packing density reaches its maximum when $w \approx 0.7$.

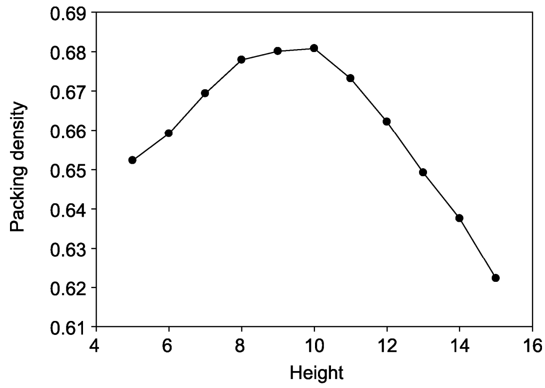

Figure 3 Random packing density versus height of tetrahedra (regular bottom triangle with edge length of 12.2474).

5 Spherocylinder

Spherocylinder is a capsule like object which consists of a cylinder and two hemispheres on both sides. Spherocylinder is one of the most studied nonspherical particles. The geometric model of spherocylinder has smooth surface with no angularity, and therefore it is easy to describe by either mathematical function or sphere assembly model. Spherocylinder was also a substitute for cylinder in some packing studies. The densest ordered packing of spherocylinders is the same as cylinders, it can be considered as the densest ordered packing of circles in 2D when the aspect ratio of spherocylinder is large enough, and the maximum packing density is about 0.9069. In respect of disordered packing, Williams et al. [6] simulated random packing of spherocylinder with aspect ratio w in the range of 0–160, where $w = H/D$, H is the height of the cylinder part, and D is the diameter. They found that the maximum packing density was 0.695 when $w = 0.4$. Charlles et al. [23] simulated random packing of spherocylinder with aspect ratio in the range of 0–3.5, and they found that the maximum packing density was 0.655 when $w = 0.5$. However, these numerical simulations were carried out in a wide range of aspect ratio and only a few points around the peak were obtained. Hence, the optimal aspect ratios which give the maximum packing density may be not accurate enough. In this work, we simulate random close packing of spherocylinder with sphere assembly model and relaxation algorithm. Results and comparisons are shown in Figure 4. The maximum packing density obtained is 0.6896, while w = 0.35. The peak value we obtained is a bit smaller than that of ref. [6] but is larger than that of ref. [23]. As can be seen from the figure, except a slight difference in the peak position, the tendencies of the curves generated by the three algorithms are consistent well.

6 Cylinder

The densest ordered packing of cylinders in 3D can be regarded as the densest ordered packing of circles in 2D, and the maximum packing density is $\pi\sqrt{3}/6 \approx 0.9069$. Random packing of cylinder has been systematically studied since 1970s. Researches have been done for random packing of cylinders with aspect ratio from 1 to 100 through experimental studies. The aspect ratio of cylinder is defined as $w = H/D$, where H is the height and D is the diameter. Most researches agreed that the packing density decreases with the increase of aspect ratio. Zou and Yu [24] even gave a fitting function describing the relationship between packing density and aspect ratio of cylinders. Packing densities measured in these experiments are within 0.6–0.71. Few numerical simulations of random packing of cylinders have been reported, and most of these simulations can only generate a loose packing configuration [25]. Zhang et al. [25] simulated random close packing of cylinders with aspect ratio from 1 to 100. The maximum packing density they obtained is 0.66, while w =1.2. In this work, random close packings of cylinders are simulated with the sphere assembly model and relaxation algorithm, and the results are shown in Figure 5. Simulation results show that the packing density reaches a peak at 0.7185 when w = 0.9. As for $w > 1$, the packing density declines with the increase of w which agrees with the experimental results.

7 Ellipsoid

The geometric model of ellipsoid has smooth surface with no angularity, and is easy to describe with mathematical function. Thus, ellipsoid surfaces and their patches have been often used to approximate the actual surface of particles. Packings of ellipsoid have been comprehensively studied. The most representative work belongs to the research team in Princeton University led by Professor Torquato, who has carried out a series of theoretical analyses [26], numerical simulations [8,27] and experimental studies [28] on both ordered and disordered packing of ellipsoids. Their researches have revealed the principles of ellipsoid packing. Furthermore, their results have been an important reference on ellipsoid packings. For ordered packing of ellipsoid, Donev et al. [26] found that the maximum packing density reached about 0.7707 when the axes ratio was $1:\sqrt{3}:1$ or

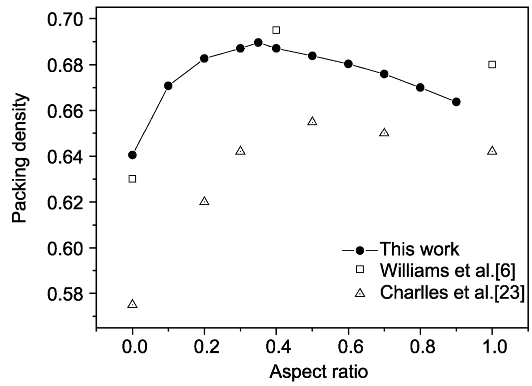

Figure 4 Random packing density versus aspect ratio of spherocylinders.

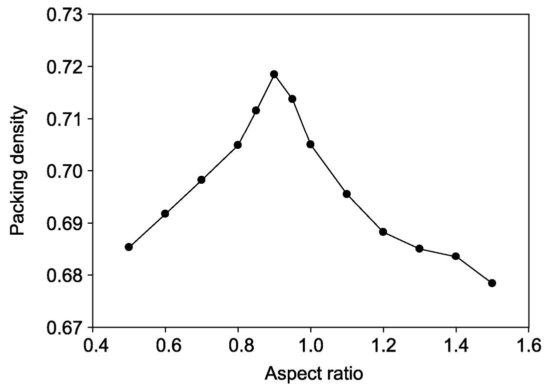

Figure 5 Random packing density versus aspect ratio of cylinders.

$1:1/\sqrt{3}:1$. For disordered packing of ellipsoid, investigations [8,27] indicated that the maximum packing density reached 0.735 when the axes ratio was 0.8:1:1.25. The packing density of randomly packed ellipsoids with axes ratio $w^{-1}:1:w$, as a function of aspect ratio w, is shown in Figure 6.

8 Cube

The maximum packing density of orderly packed cubes is 1. It means that the orderly packed cubes can take up the entire space with no gaps. Very few studies on random packing of cubes can be found in literatures. One reason for this is that cube is a typical angular convex body, the orientation and the contact of edges and corners of angular particle may bring some difficulties to simulation algorithms. Additionally, the boundary between the definitions of ordered and disordered packing is not so clear, and the parameters to quantify the randomness of packings are not appropriate [29]. These factors caused some puzzles in the studies of random packings of cubes. Differences between experimental results on random packing of cubes are remarkable.

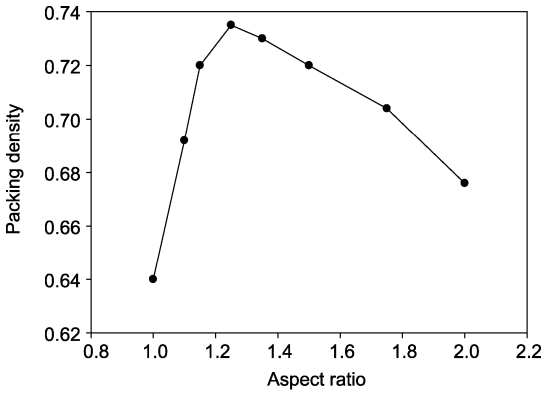

Figure 6 Random packing density versus aspect ratio of ellipsoids [8].

The packing density of random close packing of cubes given by Dong and Ye ranges from 0.64 to 0.74 [9]. Yu et al. [30] reported that the packing density of cubes they measured was about 0.57; Fraige et al. [31] simulated and measured the cube packings in a cubic container with gravity and the packing density obtained was about 0.67. Random close packings of cubes were simulated with sphere assembly model and relaxation algorithm [14], and the maximum packing density we obtained was 0.7755.

9 Conclusions

Numerical simulation results show that the upper bound order of random packing densities of basic 3D objects is cube (0.78) > ellipsoid (0.74, axes ratio is 0.8 : 1 : 1.25) > cylinder (0.72, w=0.9) > spherocylinder (0.69, w=0.35) > tetrahedron (0.68, regular tetrahedron) > cone (0.67, w=0.8) > sphere (0.64), while the upper bound order of ordered packing densities of basic 3D objects is cube (1.0) > cylinder and spherocylinder (0.9069) > cone (0.7854) > tetrahedron (0.7820) > ellipsoid (0.7707) > sphere (0.7405). The two orders of ordered packing and disordered packing respectively are significantly different. It should be noted that the maximum packing densities mentioned in this work are the known optimal values so far. Moreover, except the ordered sphere packing, there are no rigorous mathematical proofs for the maximum packing densities of other 3D objects. Hence, these optimal values may be updated in further researches.

The relationship between particle shape and packing density has always been the forefront of packing researches. Nevertheless, little was known on the relationship up to the present. Sphericity is one of the most common parameters describing particle shape. Researches indicated that random packing density is not always incremental with the increase of sphericity. All the sphericity-packing density curves have a peak point, but the peak position of each curve varies significantly between different particle shapes. Zou and Yu [32] described the particle shape-packing density relationship by a sphericity-packing density fitting function, but the function does not have universal validity. Thus, the single parameter of sphericity may not be enough to reflect the complexity of the shape effects of nonspherical particles on the packing density. Wouterse et al. [33] presented that the packing density reached its maximum when the particle's aspect ratio was about 1.25. However, only a few kinds of nonspherical particles were studied in their work. Review with the simulation results in this work, the proposition is not completely true. The packing study of basic 3D objects is an important component of the research on particle shape-packing density relationship. The final solution to the problem may depend on the joint efforts of academia on various academic disciplines.

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