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Computer Simulation of Random Sphere Packing in an Arbitrarily Shaped Container

S.X. Li[1], L. Zhao[1] and Y.W. Liu[2]

Abstract: Most simulations of random sphere packing concern a cubic or cylindric container with periodic boundary, containers of other shapes are rarely studied. In this paper, a new relaxation algorithm with pre-expanding procedure for random sphere packing in an arbitrarily shaped container is presented. Boundaries of the container are simulated by overlapping spheres which covers the boundary surface of the container. We find 0.4∼0.6 of the overlap rate is a proper value for boundary spheres. The algorithm begins with a random distribution of small internal spheres. Then the expansion and relaxation procedures are performed alternately to increase the packing density. The pre-expanding procedure stops when the packing density of internal spheres reaches a preset value. Following the pre-expanding procedure, the relaxation and shrinking iterations are carried out alternately to reduce the overlaps of internal spheres. The pre-expanding procedure avoids the overflow problem and gives a uniform distribution of initial spheres. Efficiency of the algorithm is increased with the cubic cell background system and double link data structure. Examples show the packing results agree well with both computational and experimental results. Packing density about 0.63 is obtained by the algorithm for random sphere packing in containers of various shapes.

Keyword: sphere packing, random packing, computer simulation, relaxation algorithm, containers.

[1] State Key Lab for Turbulence and Complex System Study, College of Engineering, Peking University, Beijing, China. E-mail: lsx@pku.edu.cn (S.X. Li)

[2] Institute of Mechanics, Chinese Academy of Sciences, Beijing, China

1 Introduction

The packing of spheres has long been of interest since the Kepler's conjecture in 1611. It is not only a basic problem of mathematics and physics, but also has been extensively applied in many branches of science, engineering and even in ordinary life. These applications range from atomic level to celestial bodies. With the rapid progresses in computer technology, computer simulation has been widely used in the study of random sphere packing and become a powerful means besides theoretical and experimental research. Bernal (1959) was among the first to simulate random packing of equal spheres using computer. Comprehensive remarks and classification of simulation models have been given by Yu *et al.* (2003), He, Ekere and Cai (1999) and other scholars.

In the light of new approaches reported in recent years, the simulation models of random sphere packing can be classified into four categories, sequential addition [Visscher and Bolsterli (1972); Han, Feng and Owen (2005); Santiso and Muller (2002)], collective rearrangement [Li, Zhao and Zhou (2008); Yu *et al* (2003); He, Ekere and Cai (1999); Yang, Miller and Turcoliver (1996); Clarke and Wiley (1987); Nolan and Kavanagh (1993); Lubachevsky and Stillinger (1990); Kansal, Torquato and Stillinger (2002); Yang, Zuo and Yu (2000); Stroeven and Stroeven (1999)], advancing front [Lohner and Onate (2004); Feng, Han and Owen (2003)] and optimization approaches [Sutou and Dai (2002); Li and Ng (2003)]. The sequential addition models have a high packing speed but give low packing density (<0.6) and mean coordinate number (about 4). The collective rearrangement models give high packing density (>0.62) and reasonable coordinate number (5.6∼6), but are rel-

atively slow. Mostly used models of collective rearrangement are relaxation approach [Li, Zhao and Zhou (2008); He, Ekere and Cai (1999); Yang, Miller and Turcoliver (1996); Clarke and Wiley (1987); Nolan and Kavanagh (1993)], L-S approach [Lubachevsky and Stillinger (1990); Kansal, Torquato and Stillinger (2002)] and discrete element method [Yang, Zuo and Yu (2000); Stroeven and Stroeven (1999)]. The idea of advancing front comes from mesh generation in finite element method. The advancing front approaches have a very high packing speed but generally give a packing density less than 0.5. The optimization approaches provide global optimized solution of sphere locations by optimization algorithm, however it can only be applied to a small number of spheres so far.

Most simulations of random sphere packing concern a cubic or cylindric container with periodic boundary, containers of other shapes are rarely studied. Although infinite domain is studied in some cases and periodic boundary simplifies the boundary treatment, practical packings of spheres usually involve a real container with more complex shape. Sphere packing in polytope is studied by Sutou, Dai (2002) and Li, Ng (2003). In these researches, boundary of the polytope is represented by a set of inequalities. However, inequalities can be hardly established for the containers of irregular shapes.

To simulate random sphere packing in a real container, sequential addition approaches are not suitable because no obvious dropping direction can be found. Advancing front approaches have been applied to fill the space in complex shaped containers with spheres. Although high speed packing is attractive, fairly low packing density may be unacceptable for some applications. Moreover, optimization approaches heretofore do not have the ability to simulate packings of large amount spheres. Therefore, collective rearrangement approaches are considered as a better choice to simulate random sphere packing in a real container. Since only geometric packing and hard sphere model are involved, the relaxation approach is applied in this study.

2 Boundary simulation

Boundary treatment is the main problem for sphere packing simulation with nonperiodic boundaries. In previous study [Han, Feng and Owen (2005)], special detecting algorithm is developed to deal with the collision between spheres and boundaries. It can be more complicated in a corner, where two or more boundaries are contacted with a sphere. In this paper, hard nonperiodic boundaries of real containers are simulated by overlapping spheres. Therefore, collisions with boundary can be treated in the same way as collisions with spheres. In this way, spheres are classified into boundary spheres and internal spheres. Boundary spheres are introduced to confine the internal spheres within a specified domain. They can be overlapped but are fixed in position. Internal spheres can be adjusted in position and they construct the final packing. Only internal spheres are calculated in packing density and coordinate number.

Definitions of packing density and coordinate number should be redefined in the hard nonperiodic boundary composed of overlapping spheres. Figure 1 shows the definition of packing density with nonperiodic boundary in 2D case. The boundary of the container is simulated by overlapping boundary spheres. The packing density is defined as $\sum_{i=1}^{n} V_i/V$, where n is the number of spheres, V_i is the volume of each sphere, V is the volume of the container (hatch area in Figure 1). Although this definition is simple and easy to calculate, the small gaps between boundary spheres will increase the packing density since the internal spheres may take up these small spaces. High overlap rate of the boundary spheres will decline this tendency.

The mean coordinate number is the average contact number of the internal spheres. If the smallest distance between two spheres is less than 0.2% of the sum of their radii, we consider that they contact each other [He, Ekere and Cai (1999)]. The contact number includes the contacts between internal spheres and also the contacts between internal spheres and boundary spheres.

The overlap rate of two spheres is defined as

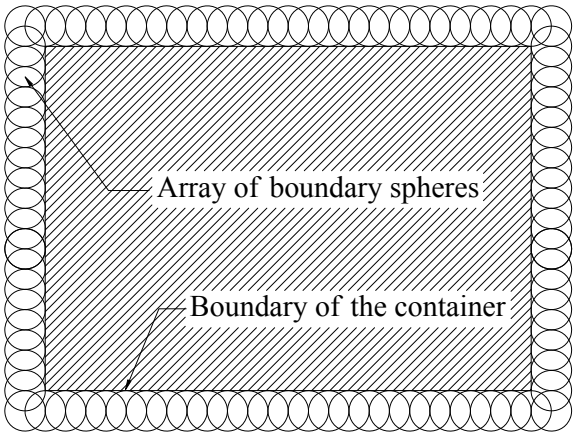

Figure 1: Definition of packing density with non-periodic boundary

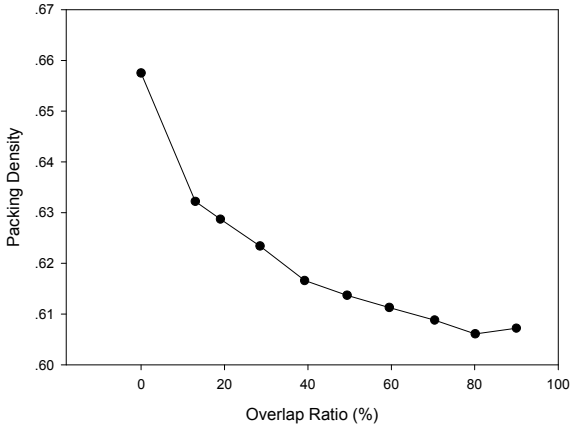

Figure 2: Packing density vs. overlap rate

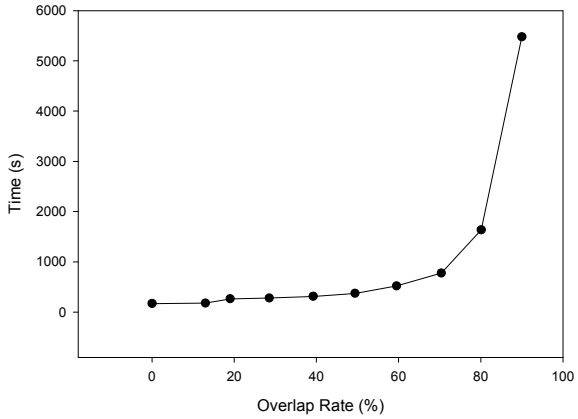

Figure 3: CPU time vs. overlap rate

$\frac{r_i+r_j-d_{ij}}{r_i+r_j}$, where r_i and r_j are the radii of sphere i and j respectively, d_{ij} is the distance between the centers of sphere i and j. The overlap rate of boundary spheres is an important parameter and should be carefully chosen. Large overlap rate is preferred since tightly arranged boundary spheres prevent the boundary crossing of the internal spheres more effectively. Moreover, large overlap rate decreases the gaps between boundary spheres and lead to a more precise value of packing density. Figure 2 shows the relationship between the overlap rate and the packing density. Unfortunately, large overlap rate increases the number of boundary spheres and the CPU time cost as well. Figure 3 gives the relationship between the overlap rate and the CPU time. The figure demonstrates the computing time will increase rapidly when the overlap rate is larger than 60%. When the overlap rate reaches 90%, the number of boundary spheres will be 45 times than the internal spheres, and the CPU time cost is 15 times comparing to 50% of the overlap rate. Hence, we believe 40% to 60% of the overlap rate of boundary spheres is a proper value since the CPU time cost can be afforded. From Figure 2, we know there is only 1% increment in the packing density from 90% of the overlap rate to 50%. Therefore, the overlap rate of the boundary spheres is set to 50% in this paper, and the precision of the packing density is acceptable.

3 Relaxation algorithm with pre-expanding

Relaxation algorithm [He, Ekere and Cai (1999); Yang, Miller and Turcoliver (1996); Clarke and Wiley (1987)] takes a geometric consideration of spheres packing and was successfully applied in periodic boundary condition. The initial stage of the algorithm is a small cubic region with large overlapping spheres. A relaxation algorithm is applied to gradually reduce the overlaps between spheres, and the cubic space expands at the end of each step. When there are no overlaps between spheres, the algorithm stops and the final packing is achieved. However, some difficulties arise when applied in the nonperiodic boundary condition. One is the "overflow" problem. The boundaries of the container are simulated by boundary spheres in the nonperiodic boundary condi-

tion. In the initial stage, density of the internal spheres is much higher than that of the boundary spheres. The initial packing density is 0.86 for random close packing in the study of He, Ekere and Cai (1999). Therefore, some of the internal spheres near the boundary will be pushed out of the boundary by repulsions of others, and this leads to failure of the sphere packing. Another problem is the real boundary does not allow expanding. For a substitution, the internal spheres are shrunk at each step.

Pre-expanding procedure is presented in this study to overcome the "overflow" problem. The procedure begins with a random distribution of small internal spheres and there are large spaces between spheres. Radius of the small internal spheres is set to 10% of the radius of internal spheres in final packing which can be estimated by Eq. (5). Then each internal sphere expands by

$$r^{(k+1)} = [1.0 + \frac{0.2}{\lg(k+2)}]r^{(k)} \tag{1}$$

$r^{(k+1)}$, $r^{(k)}$ are radii of the spheres at step k+1 and k respectively. Following the expansion, a specified number of relaxation iterations are applied to rearrange each internal sphere. The relaxation procedure relocates a sphere by repulsions from spheres which overlap with it. A new position of sphere i is calculated by

$$\mathbf{R}_i^{new} = \frac{1}{n_i}\sum_{j=1}^{n_i}\mathbf{R}_{ij} \tag{2}$$

where $\mathbf{R}_i^{new}$ is the aggregate vector indicating the new position of sphere i, n_i is the number of spheres overlapping with sphere i, $\mathbf{R}_{ij}$ is the vector indicate the position of sphere i repulsed by sphere j. $\mathbf{R}_{ij}$ is calculated by

$$\mathbf{R}_{ij} = \mathbf{R}_i + (\mathbf{R}_j - \mathbf{R}_i)\frac{r_i + r_j}{d_{ij}} \tag{3}$$

where $\mathbf{R}_i$, $\mathbf{R}_j$ are vectors of the centers of sphere i and j. The expansion and relaxation procedures are performed alternately to increase the packing density of the internal spheres. The pre-expanding procedure stops when the packing density reaches φ_0. φ_0 is the initial packing density and is set to 0.68 for random close packing in this study. It is not necessary to completely eliminate the overlaps in this stage.

After the pre-expanding procedure, relaxation iterations and sphere shrinking are carried out alternately. Each internal sphere shrinks by

$$r^{(k+1)} = r^{(k)}(1.0 - molr \cdot \beta) \tag{4}$$

where $molr$ is the maximum overlap rate of internal spheres at step k, β is the shrinking factor which is set to 0.015 in this study after a number of tests. The algorithm is completed when the $molr$ is below 2.0×10^{-4} [He, Ekere and Cai (1999)]. Figure 4 shows the packing process of the internal spheres with this algorithm. The process is demonstrated with three stages which are the initial stage of the pre-expending procedure, the finial stage of the pre-expending procedure and the final packing of the internal spheres from left to right in Figure 4.

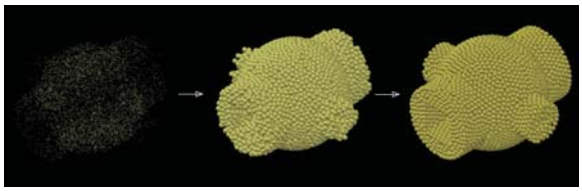

Figure 4: Packing process of the internal spheres

The benefits coming with the pre-expanding procedure are in two aspects. One is the reduce of initial packing density which drops from 0.86 [He, Ekere and Cai (1999)] to 0.68 in this study. Low initial packing density avoids "overflow" of the internal spheres. Another benefit is the internal spheres are well distributed after the pre-expanding procedure, and this will speed up the following packing procedures.

4 Contact detection and data structure

Contact detection is the operation to identify the overlaps between two spheres. It is the most time consuming operation in the algorithm. The efficiency of the contact detection is one of the main contributions to the efficiency of the algorithm, especially when large number of spheres

are involved. A background system of cubic cells is used in this study to register both boundary spheres and internal spheres to cells. The background system is constructed within the minimal enclosing box of the container and is divided into cubic cells. Size of the cubic cell should be slightly larger than the diameter of the spheres in final packing. A sphere is register to a cell when its center is in the cell. With this system, there will be no need to search through all the spheres for detecting the overlaps of a sphere. Instead, only $27(3^3)$ neighborhood cells should be examined since the overlap only occurs in these cells.

Date structure is also a main factor to the efficiency of the algorithm. In the relaxation algorithm, positions of the internal spheres are adjusted in each iteration, and they are frequently pushed into another cell by repulsions of others. Therefore, inserting and deleting operations in the sphere list of cells are frequent. To eliminate the location search in the inserting and deleting operations, a double link data structure is presented. Figure 5 shows the data structure of the background system. It can be regarded as a two-dimensional array, the first dimension stores head addresses of sphere lists of each cell, and the second dimension is implemented by a double link with forward and backward pointer in each element. Hence, the location search can be avoided in the inserting or deleting of an element, only pointer adjustment is required. The algorithm is implemented by C++ codes and compiled with Microsoft Visual C++.

With the cubic cell background system and the double link data structure, time complexity of the algorithm is $O(N)$ in both random close packing and random loose packing, where N is the number of spheres. Figure 6 shows the time complexity of the algorithm. It costs 217s of CPU time to achieve a packing density of 0.64 for 10,000 equal spheres in random close packing with periodic boundary on an AMD Athlon 3200+ PC.

5 Generation of initial spheres

The shape of a real container can be very complicated. Analytical description of a real container is usually unavailable. In this study, containers are modeled in an AutoCAD system and initial spheres are generated using Brep (Autodesk boundary representation library) functions.

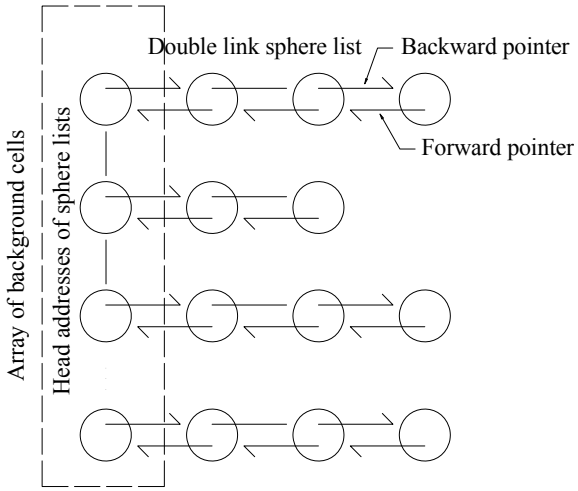

Figure 5: Data structure of the background system

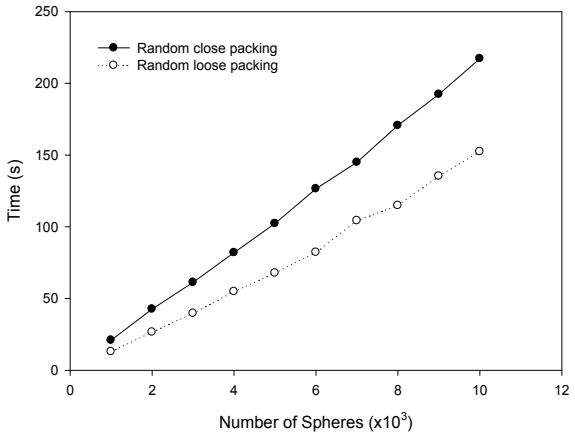

Figure 6: Time complexity of the algorithm

Boundary spheres should be uniformly distributed and cover the whole surface of the container. Positions of boundary spheres are obtained from the nodes of triangles on surface mesh of the container. The positions can also be derived from STL (stereolithography) file which can be generated by most CAD software [Bechet, Cuilliere and Trochu (2002)]. Size of the surface mesh should be set to a proper value to ensure the overlap rate of boundary spheres is 50%. Radius of the boundary spheres should be equal to radius of the internal spheres in the final packing. The radius

can be estimated by

$$r_{bs} = \left(\frac{3\varphi V}{4\pi n}\right)^{\frac{1}{3}} \tag{5}$$

Where r_{bs} is the radius of the boundary spheres, V is the volume of the container, n is the number of spheres in packing, φ is the final packing density which is about 0.64 for random close packing. Position and radius of the boundary spheres are both unchangeable in the packing procedures.

Positions of internal spheres are randomly generated in the region of the background system. The sphere inside the container is reserved, otherwise it will be deleted. A function of Brep is applied to determine the inclusion or exclusion of a point to the container. For the relaxation algorithm with pre-expanding, the radius of the initial internal spheres is set to 10% of the radius of the final spheres which can be estimated by Eq. (5). Figure 7 gives a local view of initial internal spheres and boundary spheres in a cube.

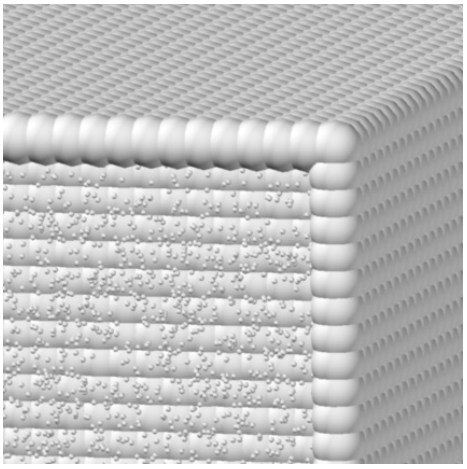

Figure 7: Local view of initial internal spheres and boundary spheres in a cube

6 Examples

A number of examples applying the proposed simulation approach have been worked out for evaluation. These examples also demonstrate the ability of the algorithm to fill containers of any shape with random packed spheres as well. Random close packing with equal spheres is simulated in these examples.

Example 1 is a cube packed with 10,000 equal spheres. This example is presented to evaluate the results with previous studies. Figure 8 shows the cube and its final packing of internal spheres. The packing density of random close packing obtained by the algorithm mentioned above is 0.633. This value agrees well with the simulation results of He, Ekere and Cai (1999) (0.627), Yang, Miller and Turcoliver (1996) (0.637) and Nolan and Kavanagh (1993) (0.64), and also the experiment results of Scott (1960) and Ye, Han and Zeng (1986) (0.633∼0.634). For comparison, the packing density obtained by advancing front method under nonperiodic boundary condition is 0.552 [Lohner and Onate (2004)]. The mean coordinate number of this study is 0.5781 which is close to the value of He, Ekere and Cai (1999) (5.68), but is lower than the value of Yang, Miller and Turcoliver (1996) (6.0).

Example 2 is a gourd packing with 10,000 equal spheres. The gourd is a revolved object with cross sections of various radii. Figure 9 shows the gourd and its final packing of internal spheres. The packing density reaches 0.629 and the mean coordinate number is 5.656.

Example 3 is a typical civil engineering structure with columns and floors which have many right angles. This example is come from Lohner and Onate (2004). The object is packed with 41,883 equal spheres. The packing density obtained in this study is 0.623 while the result from advancing front method is 0.505 [Lohner and Onate (2004)]. The mean coordinate number of this study is 5.563 which is close to the value of advancing front method (5.71) [Lohner and Onate (2004)]. Figure 10 and Figure 11 show the object and its final packing of internal spheres.

Example 4 is an axle sleeve with complex external and internal boundary. The object is packed with 10,000 equal spheres. This example is designed to evaluate the algorithm applying to the objects with holes and detail boundaries. The packing density is 0.607 which is 3% lower than other examples. This is due to the detail bound-

aries on surface of the object. The mean coordinate number is 5.72. The example indicates that complex and detail boundaries may reduce the packing density. Figure 12 shows the axle sleeve and its final packing of internal spheres, Figure 13 shows a cross section view of the final packing.

Example 5 is a button with four cylindric holes. The object is also packed with 10,000 equal spheres. Packing density of 0.628 is reached by the algorithm and the mean coordinate number is 5.703. Figure 14 shows the button and its final packing of internal spheres. Figure 15 gives a local view of sphere packing around a hole.

Table 1 gives the results of the five examples. These results indicate the algorithm gives reasonable packing configurations of spheres in the containers of various shapes.

Table 1: Results of random sphere packing in containers of various shape

Examples	Number of spheres	Packing density	Mean coordinate number
cube	10000	0.633	5.781
gourd	10000	0.629	5.656
civil structure	41883	0.623	5.563
axle sleeve	10000	0.607	5.720
button	10000	0.628	5.703

7 Conclusions

A new relaxation algorithm with pre-expanding procedure is presented to simulate sphere packing in an arbitrarily shaped container. The pre-expending procedure avoids overflow of the internal spheres and generates a more uniform distribution of initial spheres comparing to random distribution. Boundaries of the container are distributed and simulated by overlapping spheres. Definition of packing density and coordinate number under nonperiodic boundary condition is presented. The overlap rate of boundary spheres is suggested to 40%$\sim$60% and the radius can be estimated. A cubic cell background system and double link data structure are applied to increase

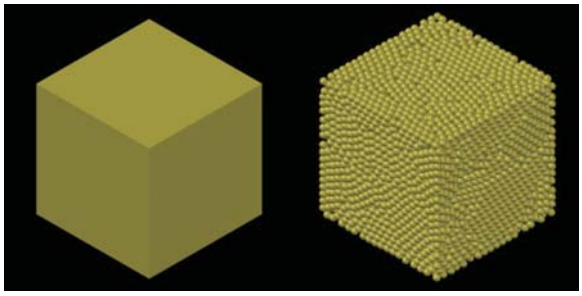

Figure 8: Cube and its final packing of internal spheres

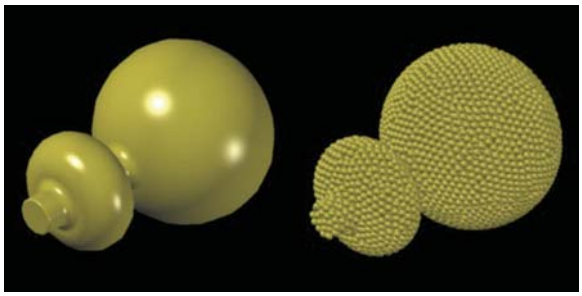

Figure 9: Gourd and its final packing of internal spheres

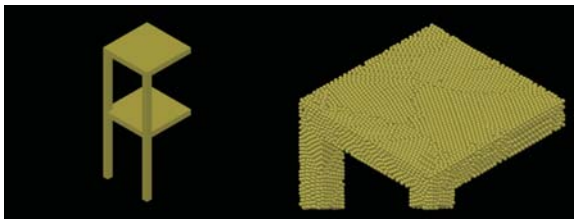

Figure 10: Civil engineering structure and its final packing of internal spheres (upper part)

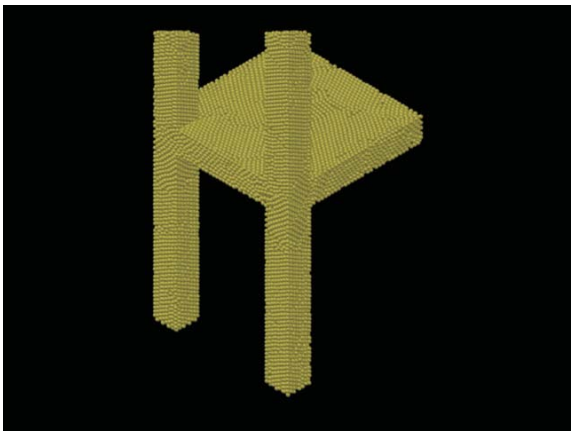

Figure 11: Final packing of internal spheres of civil engineering structure (lower part)

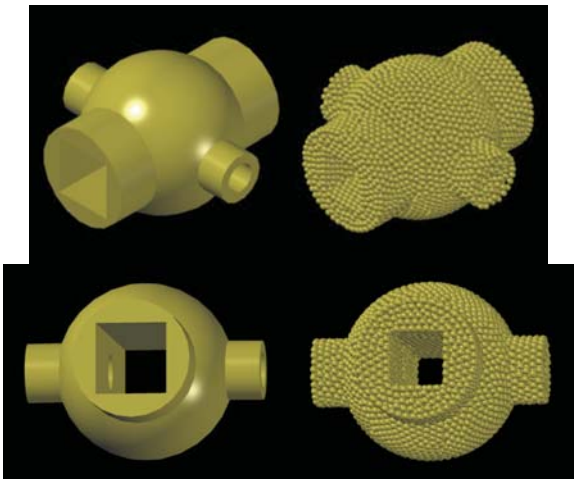

Figure 12: Axle sleeve and its final packing of internal spheres

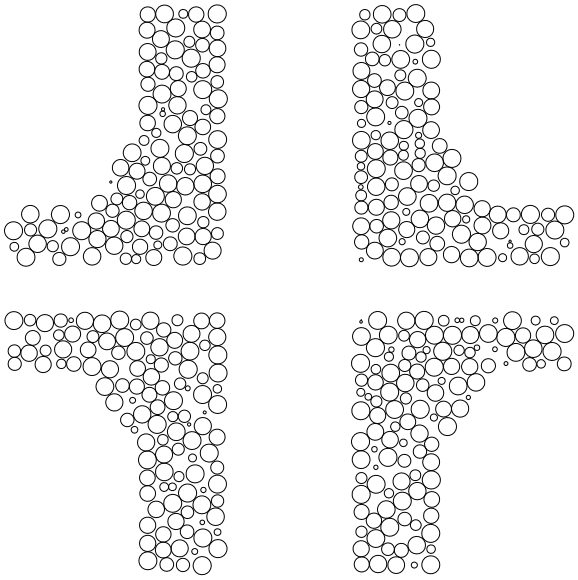

Figure 13: Cross section view of the final packing of axle sleeve

the efficiency of contact detection. Time complexity of the algorithm is $O(N)$, where N is the number of spheres in packing. Examples show the simulation results are in good agreement with previous studies, and packing density about 0.63 is obtained by the algorithm for random sphere packing in containers of various shapes. The final packing of the algorithm gives a description of the packing structure in a real container which is considerablely important in many research fields

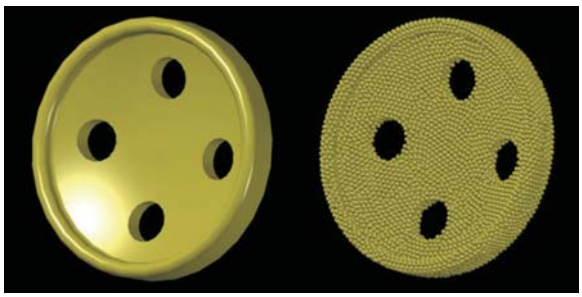

Figure 14: Button and its final packing of internal spheres

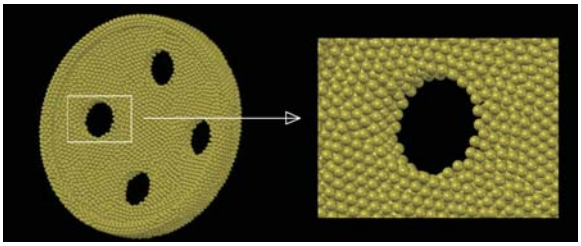

Figure 15: A local view of sphere packing around a hole

of physics and mechanics. It also provides the optimized positions of uniform point distribution within any shaped region. The distribution can be directly applied to mesh generation in finite element method [Yokoyama, Cingoski, Kaneda and Yamashita (1999)] and grid generation in meshless approaches [Atluri, Liu and Han (2006); Han, Liu, Rajendran and Atluri (2006); Liu, Han, Rajendran and Atluri (2006)].

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