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Numerical Simulation of Random Close Packings in Particle Deformation from Spheres to Cubes *

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Variation of packing density in particle deforming from spheres to cubes is studied. A new model is presented to describe particle deformation between different particle shapes. Deformation is simulated by relative motion of component spheres in the sphere assembly model of a particle. Random close packings of particles in deformation form spheres to cubes are simulated with an improved relaxation algorithm. Packings in both 2D and 3D cases are simulated. With the simulations, we find that the packing density increases while the particle sphericity decreases in the deformation. Spheres and cubes give the minimum (0.6404) and maximum (0.7755) of packing density in the deformation respectively. In each deforming step, packings starting from a random configuration and from the final packing of last deforming step are both simulated. The packing density in the latter case is larger than the former in two dimensions, but is smaller in three dimensions. The deformation model can be applied to other particle shapes as well.

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Packings in particle deforming from spheres to polyhedra are closely related to physical phenomena such as the phase transition of liquid to solid. Sphere packing has been studied for centuries since Kepler's conjecture and the results are well known.[1] Cube packing is less studied, experimental results can be found in literature.[2,3] Remarkable distinction exists in the packing density of random close packing of spheres (0.64) and cubes (0.74). It is interesting to see the variation of packing density of particles in the deforming process form spheres to cubes, and the variation will lead to a better understanding of relative physical phenomena. Most studies on particle deformation in random packing concern only the influences of the aspect ratio of a specified particle shape,[4,5] deformations between different particle shapes are rarely studied. Zou *et al.*[2] gave a curve of porosity versus sphericity in random close packings of non-spherical particles. The curve in Fig. 2(b) of Ref. [2] was built from the interpolation of isolated experimental results of cylinders, discs, ellipsoids, spheres and cubes. In this Letter, particle deforming process between different shapes in random close packings is simulated, and a more detailed curve of packing density versus sphericity between sphere and cube is built from the numerical simulation results.

Packings of deformed particles involve non-spherical shapes and a uniform model in all deforming steps is required. In this work, the sphere assembly model[6] which represents the non-spherical particles with an assembly of component spheres is constructed. With this model, the deformation can be simulated by relative motion of the component spheres, and the non-spherical packing can be treated with sphere packing approaches. Figure 1 shows the centre locations and moving paths of the component spheres of a particle deforming from sphere to cube in both 2D and 3D cases. Centres of the component spheres are marked by small circles (2D) or spheres (3D). In the initial stage of deformation of spheral particle (step 1 in Figs. 2 and 3), equal component spheres of the particle are distributed on a circle (2D) or a sphere (3D), their centre locations can be found in Fig. 1. In the deforming process, each component sphere moves along the arrow direction, and its moving path is shown (solid lines with arrows) in Fig. 1. The deforming process is separated into n steps, the moving distance of a component sphere in each step is $l_i/(n-1)$, where l_i is the length of the moving path of ith component sphere (length of the solid lines with arrows in Fig. 1). In the final stage of deformation of cubic particle (step 11 in Figs. 2 and 3), centres of the component spheres finally arrive on a square (2D) or a cube (3D). Accordingly, particles will gradually expand during the deformation in this model.

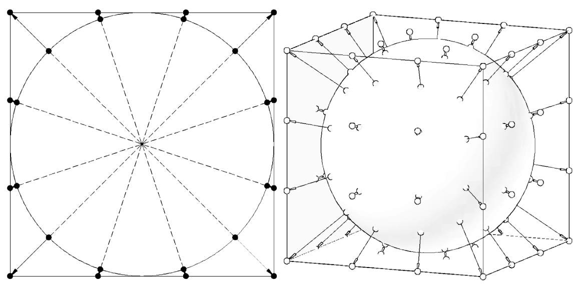

Fig. 1. Centre locations and moving paths of component spheres of a particle deforming from sphere to cube (left: 2D case, right: 3D case).

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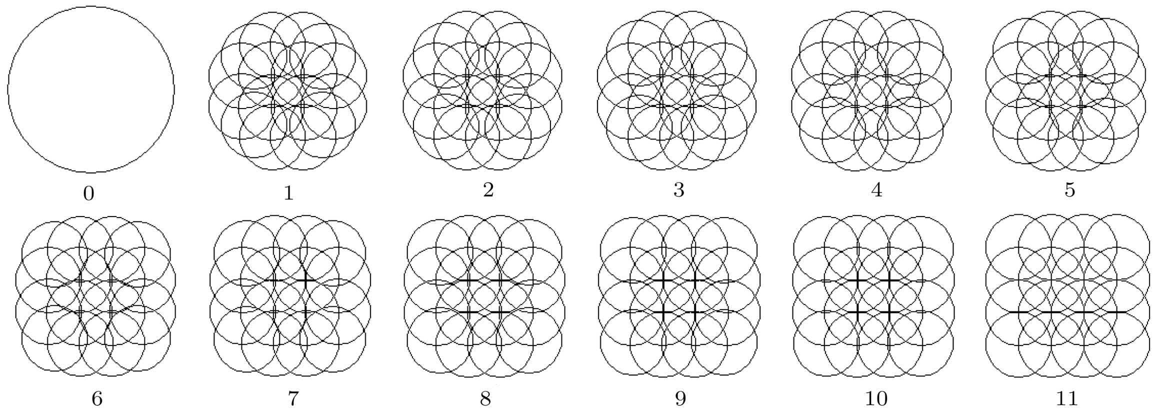

Fig. 2. Deforming steps from circle to square.

Particle deformations in both 2D and 3D cases are simulated, and the deforming process is separated into 11 steps ($n = 11$) in this work. In the 2D case, circles are transformed into squares, and the sphere assembly model of a particle is constructed with 16 overlapping component circles. Figure 2 shows the deforming steps in the 2D case. In the 3D case, spheres are transformed into cubes, and the sphere assembly model of a particle is constructed with 64 overlapping component spheres. Figure 3 shows the deforming steps in the 3D case. More component spheres will build a more accurate model but increase the CPU costs as well.

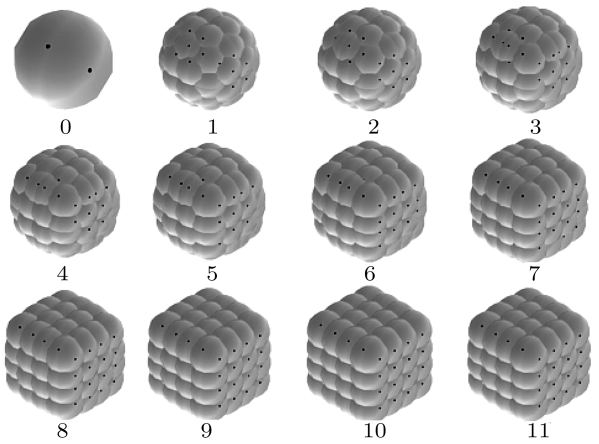

Fig. 3. Deforming steps from sphere to cube.

The shape change of a particle is evaluated by sphericity which is defined as $S_{\text{sphere}}/S_{\text{particle}}$,[2] S_{sphere} is the surface area of a sphere which has the same volume as the particle, S_{particle} is the surface area of the particle. In this work, particles are represented by overlapping spheres in their sphere assembly models. It is a burdensome task to compute the exact surface area and volume of the particles since they have rough surfaces. Fortunately, the surface area and volume of the particles in Figs. 2 and 3 can be inquired from an AutoCAD system. Figure 4 gives the variation of particle sphericity in deforming steps in both the 2D and 3D cases. The figure shows that the sphericity decreases in the deformation process in both the 2D and 3D cases.

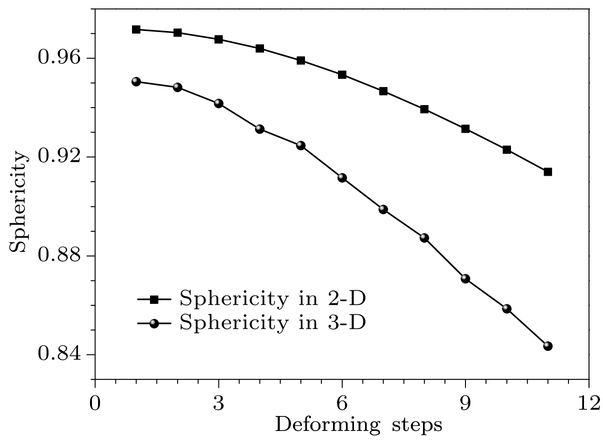

Fig. 4. Particle sphericity in deforming steps in the 2D and 3D cases.

An improved relaxation algorithm[7] is applied to generate the random close packings of particles in the deformation. The original relaxation algorithm[8] is improved by introducing the torque and rotation of sphere assembly to simulate the motion of non-spherical particles. The algorithm begins with randomly placed large overlapping configuration of particles. Afterwards, iterations of relaxation procedure are carried out to gradually reduce the overlaps of the particles. Displacement of each sphere is computed in terms of the overlaps with nearby spheres. The torque of the particle is defined as

$$\boldsymbol{M} = \frac{1}{n_a}\sum_{i=1}^{n_a}(\boldsymbol{V}_i \times \boldsymbol{P}_i), \tag{1}$$

where M is the torque vector of the particle, n_a is the number of spheres in the assembly model of the particle, $\boldsymbol{V}_i (i = 1, \ldots, n_a)$ are the vectors from the centre of the particle to the centre of each component sphere, $\boldsymbol{P}_i (i = 1, \ldots, n_a)$ are the displacement vectors of each component sphere. The rotation angle θ of the particle is computed by

$$\theta = \alpha \|\boldsymbol{M}\|_2, \quad (2)$$

where α is the rotational relaxation coefficient. The boundary of the packing region is enlarged at the end of each iteration. The finial packing is achieved when the maximum overlap rate of spheres is below a predefined value. The improved algorithm has been successfully applied to random close packing of tetrahedra.[9]

In each deforming step, packings starting from a random configuration (separate packing) and from the final packing of last deforming step (continuous packing) are both simulated. The separate packing is the normal way of random packing which has been widely studied. The continuous packing is less studied, but it may be employed to simulate some physical phenomena like crystal growth form liquid to solid. In the separate packing, deformed particles are randomly placed in the region with large overlaps between particles at the initial state in each deforming step. The packing configuration will be randomly redistributed at the beginning of next deforming step. In the continuous packing, the final packing configuration of particles of last deforming step will be the initial state of next deforming step, and the motion of each particle is continuous in the deforming process. With the implementation of the improved relaxation algorithm, overlaps between particles are eliminated at the end of each deforming step. Although the configurations at the end of last step and the beginning of next step are the same in the continuous packing, small overlaps between particles occur due to particle expansion at the beginning of each step. The relaxation procedure should be carried out again to remove these overlaps.

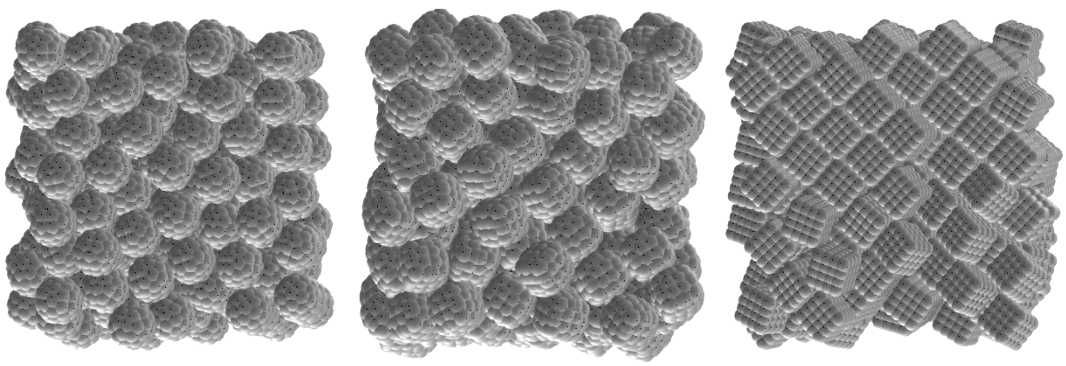

Fig. 5. Final packings of three deforming steps (left: spheres, middle: step 6 in Fig. 3, right: cubes).

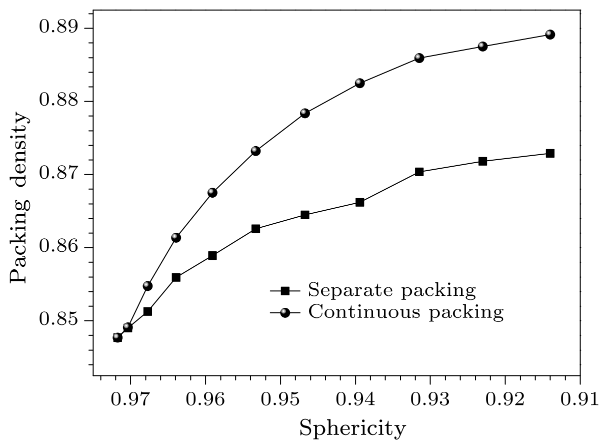

Fig. 6. Packing density vs sphericity in the 2D case.

Random close packings are simulated in this work. Cubic region and periodic boundary are applied to all the simulations. There are 500 particles deformed form circles to squares in the 2D case, and 250 particles deformed form spheres to cubs in the 3D case. Each simulation is carried out five times, and the values obtained are the averages. Figure 5 shows the final packings of three deforming steps in the 3D case. The left configuration is the final packing of spheres (step 1 in Fig. 3), the right configuration is the final packing of cubes (step 11 in Fig. 3), and the middle one is the final packing of particles at step 6 in Fig. 3.

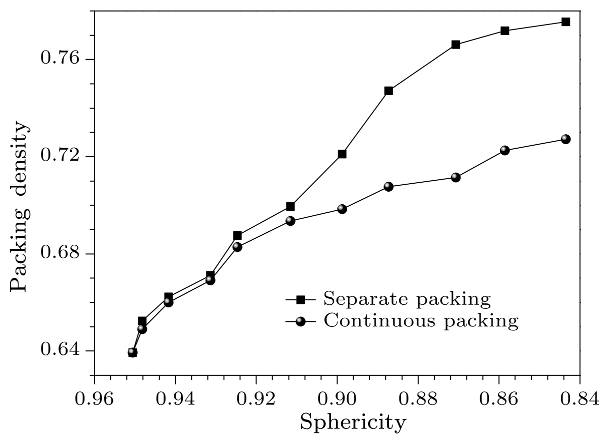

Fig. 7. Packing density vs sphericity in the 3D case.

Figure 6 shows the variation of packing density in the 2D case, and Fig. 7 shows the variation of packing density in the 3D case. Both separate and continuous packing results are given. In the separate packings, the packing density of random close packing of circles and squares in the 2D case are 0.8487 and 0.8729, respectively, while the packing density of spheres and cubes in the 3D case are 0.6404 and 0.7755. The value of spheres obtained is very close to the well-known figures (0.64).[1] The value of cubes obtained is slightly larger than the experimental results [0.75 (Ref. [2]) and 0.74 (Ref. [3])]. Note that the packing density of cubes obtained exceeds the packing density of the densest random packing [0.7421 Ref. [10])] and crystal packing [0.756 Ref. [11])] of ellipsoids. The packing density increases with the decreases of particle sphericity in both the 2D and 3D cases. The same tendency can be found in the work of Zou and Yu,[2] although their curve was obtained by interpolation with the results of other particle shapes. Spheres and cubes give the minimum and maximum of packing density in the deformation respectively. The packing densities of separate packings are larger than those of continuous packings in the 3D case (Fig. 7), whereas the opposite is true in the 2D case (Fig. 6). This result indicates that the continuous packing may give a loose configuration than the separate packing in the 3D case, while gives a denser configuration in the 2D case.

In summary, random close packings in particle deforming from sphere to cube are simulated. A spheres assembly model which describes the deformation with relative motion of component spheres is developed. Monotonic increasing of packing density in the deformation is observed in the simulations. Spheres and cubes give the minimum and maximum of packing density in the deformation respectively. The simulations also show that the continuous packing may give a loose configuration than the separate packing in the 3D case, but gives a denser configuration in the 2D case. It should be mentioned that the simulations in this work involve only geometric packing. Friction and gravity are not concerned here. The deformation model in this work can be applied to other particle shapes as well.

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