1 introduction

Granular system is common in our daily life, such as silo and sand storm, which is composed of many granular entities. The understanding of such granular system is of utmost interest to a number of practical issues ranging from landslides to industrial processes [1]. Although the entities are independent, usually there exist numerous interactions between the entities due to the external field such as gravity. The behavior of the granular system is statistically determined by all the entities' behavior. Because the granular system is not a continuum, there is not a well mature theory to describe it. The numerical simulation is a good method to investigate a granular system. The discrete element method (DEM) is a useful tool to simulate the granular system [2] by solving Newton's motion equation of the particles [3], which is developed by Cundall and Stract [4], and later combined with other computational technology, the DEM achieves a new computational performance efficiency by the joint GPU hardware [5].

In the simulation of any granular system such as the sand storm, usually, an initial configuration of the granular system such as the entities' positions or packing pattern need to be known. It can be generated by free releasing a group of entities into a bottom-and-sides-closed container, and due to the gravity, the entities will be settled into the container, and the positions of the entities, usually taken as spheres (3D) or circle disks, can be obtained by using DEM [6-7]. However, it is very time-consumed process to simulate an initial configuration of a granular system, even a spherical particle system, such that it takes several hours to several days to simulate only a few seconds of the physical process running on a personal computer (PC) [5]. Fortunately, many other algorithms are developed, among of which the advanced front technology is **???**[8]. By using this algorithm, a configuration of one million disks can be generated only needs 3.77s on a PC with a 1GHz processor [8]. However, the overlap between the entities, disks or spheres, cannot be considered, or only a given value can be considered [8]. Actually, there is the universal gravitation for any entity on the Earth, therefore the overlap must be generated between two entities due to the gravity, which is different for the entity with different size and at the different position. The overlap between the entities in the initial configuration of a granular system is very important not only for achieving a high density [9], but also related to the calculation of some other parameters in the further study. Such that in the wind sand system, the charges carried on the sand particles lifting off away from the sand bed by wind is proportional to the overlap between sand particles [10].

Motivated by this, a new method is proposed in this paper to quickly generate initial circle-disk configuration considering the overlap between circle disks due to the gravity. The algorithm of this method is described in section 2 and the performance of this method in generating a 2D circle sand particle bed is shown in section 3, and finally a conclusion is drawn in section 4.

2 Algorithm

The method proposed in this paper contains two steps. the first step is to generate an particle packing pattern of a circle-disk system considering the friction between circle disks and the friction of the disk with the wall, but without considering the gravity, and second step is to calculate the circle positions considering the gravity and the overlap between the circle disks and the overlap between the circle disk and wall are also simultaneously calculated. Next we will introduce the algorithm of each step in detailed.

2.1 Advanced front approach considering friction

For a given granular system, taking the 2D circle disks (called as particles) for example, composed of N circle disks with size distribution $P(r)$, in which r is the particle radius. In order to generate a particle packing pattern in a closed container with an open upper side shown as in Fig.1(a), the advanced front approach considering friction is adopted in this paper. A rectangular coordinate system is established shown as in Fig.1(a), and x is along the bottom side and y is along the left vertical side.

First, choose any two particles named i and j from the granular system with the radius r_i and r_j, and position them closely left/right in lower corner of the container without any overlap with the left/right side and the bottom side shown as in Fig.1(a). In the advanced front approach it is important to get an advanced front.

Next we will introduce how to get the information an advance front. Assume the left side, the bottom side and the right side as L, B and R. The chain L-A_i-A_j-B-R is called as an advanced front [??], in which A_i and A_j are the centers of the particles i and j. The advanced front is renewed as the new particle is positioned into the packing pattern. If the disks cover the whole bottom side like the pattern shown as in Fig.1(b), the chain L-A_m-A_n-A_o....A_q-A_p-R is also called as the advanced front. Any advanced front begins from the left side of the container and ends to the right side of the container. Each pair of two adjacent neighbouring particles such as L-A_i, A_i-A_j, A_j-B, or B-R provides the new position for packing a new particle shown as in Fig.1(a). These positions are required to be occupied by a newly coming particle in turn. When we pick a particle for the particles left in the granular system, named as k, if the L-A_i is not occupied, we have to try to position the particle k tangentially neighbouring with the left side and particle i, else if the L-A_i is occupied shown as in Fig.1(c), we need look for the first not occupied position, and then position the particle k tangentially neighbouring particles shown as in Fig.1(d).

However, there are some accidences happened such if the particle k is too big and the particle k will overlap with the particle j such as the dash circle shown as in Fig.2(a) when it is positioned tangentially neighbouring with L and the particle i, and the position of k need to be calculated by adjacent neighbouring with L and particle j such as the solid circle shown as in Fig.2(a); if the particle k overlaps with behind particle such as the particle i' shown as in Fig. 2(b), the position of k need to be obtained by adjacent neighbouring particles i and j; if the particle k overlaps with the front particle shown as in dash square, the position of the particle k needs to recalculated, detailed in Ref. [??]. While the position of the particle k obtained by method mentioned above may not the final position. If the situations shown as in Figs.3(a)-3(b) occurs, we need to calculate a new position for the particle k. In Fig.3(a), it is clear that the particle k is unsteady because of the gravity line beyond of the support points. In addition, when the repose angle is higher than the angles of the line joining the centers two neighbouring particles to the horizontal, the dynamic friction will work on the particle k and the particle k will slide, therefore the particle k will also be unsteady, shown as the two situations I and II of the dash circles in Fig.3(b). If the first situation occurs, the particle k will fall down and finds a new position. If the second situation occurs, we will calculate the angles of the line joining the particle k center and its neibouring particles center to the horizontal, compare which with the repose angle, until the former is lower than the later shown as the situation *IK* of the solid circle in Fig.3(b). Until all particles are positioned in the container, an initial particle packing pattern is generated.

2.2 Analytical mechanics to calculate particle position

Based on the particle packing pattern generated in **section 2.1**, for any particle i (i=1,..., N), the particles contacting with the particle i are known, denoted as J_i, and the total number particles contacting with the particle i and the label are known. Thus the total energy of the granular system, elastic energy due to the compression between particles for any particle and the gravity potential, U, can be calculate by the following formula,

$$U = \sum_{i=1}^{N} \sum_{J_i} \frac{k_{i,J_i}}{2} \left[\sqrt{\left(x_i - x_{J_i}\right)^2 + \left(y_i - y_{J_i}\right)^2} - (R_i + R_{J_i}) \right]^2 + m_i g y_i \tag{1}$$

in which k_{i,J_i} is the elastic coefficient of the particles i and J_i, and it is thought as a constant when the particles are made of the same materials, as k. (x_i, y_i) and (x_{J_i}, y_{J_i}) are the coordinates of the particles i and J_i with the radius R_i and R_{J_i}. m_i is the mass of the particle i and g is the gravity acceleration, and usually g=9.8m/s^2.

According to the principle of virtual principle [11], when the particles positions, (x_i, y_i) (i=1, ..., N) are obtained in an equilibrium system, if any low arbitrary variation δx_i or δy_i of the position x_i, and y_i, the variation of the energy, δU, remains zero as

$$\delta U = 0 \tag{2}$$

and thus it will have

$$\frac{\partial U}{\partial x_i} = k\sum_{J_i}\left(x_i - x_{J_i}\right)\left[1 - \frac{R_i + R_{J_i}}{\sqrt{\left(x_i - x_{J_i}\right)^2 + \left(y_i - y_{J_i}\right)^2}}\right] = 0 \;\; (i = 1, \dots, N) \tag{3a}$$

$$\frac{\partial U}{\partial y_i} = m_i g + k\sum_{J_i}\left(y_i - y_{J_i}\right)\left[1 - \frac{R_i + R_{J_i}}{\sqrt{\left(x_i - x_{J_i}\right)^2 + \left(y_i - y_{J_i}\right)^2}}\right] = 0 \;\; (i = 1, \dots, N) \tag{3b}$$

When the particle packing with the particle i are known from the first step, the final positions of particles can be obtained by solving equation group (3a)-3(b).

3. Illustrations

Here, several examples are presented to illustrate the performance of the method mentioned above. Firstly, we check the computational time cost to simulate an initial configuration of a 2D sand bed with 1000 disks in size region (80μm, 800μm) by the method proposed in this paper, and the computational time simulated by our method, the advanced front technology and the DEM on one PC with **4GHz** processors is listed in Table 1. From Table 1, it can be found that the computational time is a little bit longer by using our method than the one by using the advanced front technology, but the overlap between particles can be not considered by using the advanced front technology. However, it can be found that the computational time is much lower by using our method than the one by using the DEM, and the former is almost 1000 times of the later one. Of course, the computational time is dependent on the size distribution of the granular system, and the dependence of the computational time on the size distribution is shown in Table 2, in which the disk number and size region are taken as the ones used in Table 1, and the sand beds with four size distributions, normal distribution, exponent distribution, Bernoulli distribution and uniform distribution, are simulated and the corresponding simulated sand beds are shown as in Fig.4. Let's see the equation group (3a)-(3b), they are nonlinear equations, so we may obtain many solutions based on the particle packing pattern generated by step one, that means we may obtain many packing sand bed in step two by solving equation group (3a)-(3b), shown as in Fig.5. We also calculate the porosity of the different packing sand bed shown in Fig5.. ???

In addition, the final configuration of a granular system is dependent on the particle packing pattern in the step one by using the advanced front technology. Thus, the artificial particle packing can be generated according to what do you want to investigate, such as the size coherent structure of the sand bed observed in field [??]. To simulate the size coherent structure of the sand bed, we can generate the particle packing pattern of the sand bed by controlling the particle size choice in the first step shown as in Fig.6a, based on which, we solve the equation group 3(a)-(3b) to obtain the positions of the particles to generate the final configuration of the sand bed shown as in Fig.6b. By using this method, any artificial granular system according to the requirement of the different size can be generated.

4 Conclusions

A new method to generate an initial configuration of a granular system, especially for the 3D spherical system or 2D circle system, is proposed. The simulation of the 2D sand bed to illustrate a well performance can be achieved.

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Figures and captions of figures

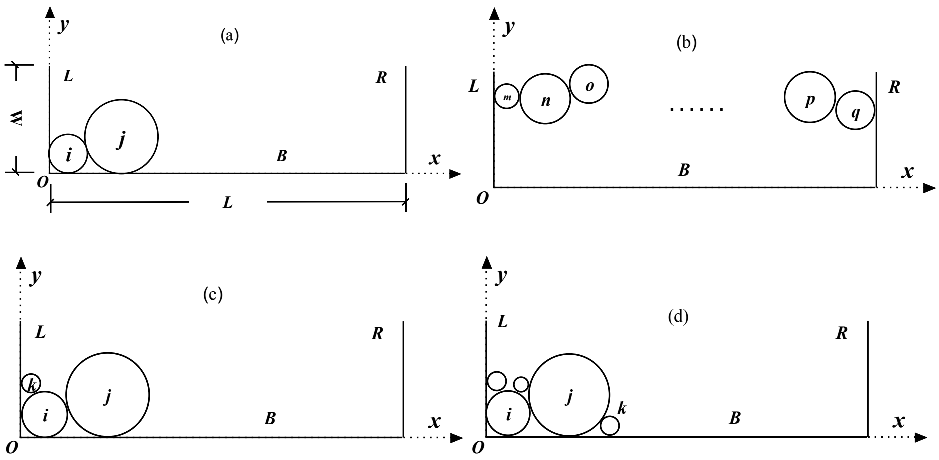

Fig.1 ???

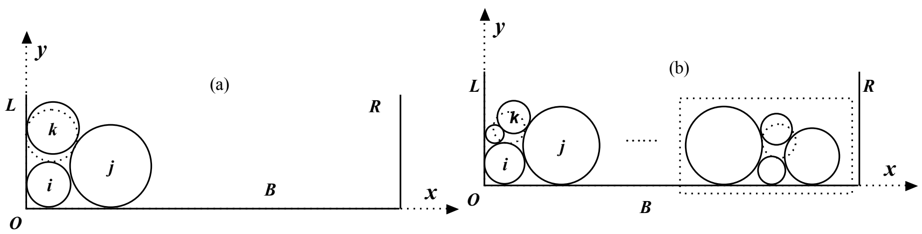

Fig.2 ???

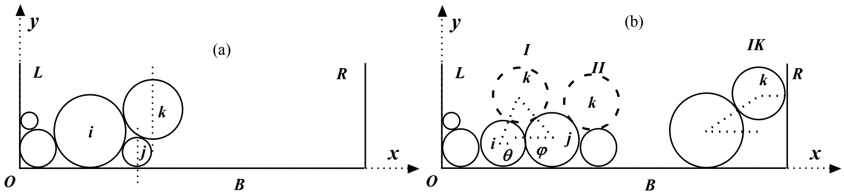

Fig.3???

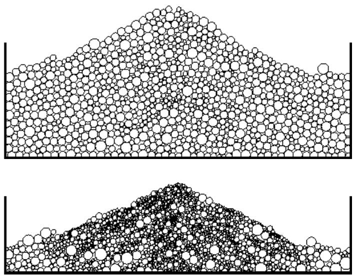

Table 1 Comparison of the performance between three methods

	Cooling	AFT	Our method
time	>3600s	0.046s	1.437s
porosity	0.815	0.801	0.825
Consider gravity	no	no	yes
时间复杂度	**O(n^2)**	**O(nlogn)**	**O(nlogn)**

Table 2 Porosity and computational time of particle packing with different size distribution

Size distribution	Porosity	Computational time
Normal	0.8254996	1.437s
Bernoulli	0.8165472	1.439s
Exponent	0.8002267	2.084s
Uniform	0.7979509	1.256s