CLUSTER SIMULATION OF COHESIVE POWDER SETTLING

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Molecular dynamics simulation of cohesive powder settling under gravity is presented. Each powder particle is modelled by a spherical cluster of computer particles. Interactions between computer particles are described by the Mie potential. In addition to the potential interactions the following forces are taken into account during the simulation: volume viscous friction, external load (gravity or gas flow), and interaction with the boundaries of the container. The presented method allows observing such phenomena as dry friction between grains and their plastic deformation and fracture due to the external loading. Various mechanisms of powder particle interactions during the settling process are investigated.

1. Introduction

The processes of powder settling in fluidized beds are of significant importance from practical and scientific points of view [1, 2]. Many works are devoted to determination of the interaction forces between powder particles [3, 4, 5, 6], but still knowledge of the necessary constitutive relations for these forces is very limited, especially in the case of the powder compression. That is why in the presented work the molecular dynamics technique is applied to model the powder settling process. Each powder particle is modelled by a cluster of computer particles interacting via the Mie potential. This type of potential is chosen because in the particular case of the Lennard-Jones potential it is proven to describe well the Van der Waals forces, which form the attraction between powder particles. The general Mie potential is similar to the the Lennard-Jones one, but it allows more flexibility in the material properties. The modelling method is conventional molecular dynamics technique, same as used in [7, 8], where the simulation is based on time integration of the equations of motion for the computer particles. During the computation the forces of interaction between the powder particles are obtained automatically as a sum of the computer particles interactions.

For the simplicity let us limit our consideration to regular spherical clusters. In Fig. 1 sequential stages of a simple computer experiment in 2D on settling 8 clusters are shown. The clusters were dropped sequentially with small time delays and small deviation in their initial positions, see Fig. 1a. Due to the attraction forces between the computer particles, the clusters stick to each other forming the shape, which is depicted in Fig. 1d. This shape is magnified in Fig. 2a. In Fig. 2b a part of the conFig. uration is shown, where the inner structure of the clusters can be observed. Each cluster contains 250 computer particles, arranged in hexagonal crystal lattice (the only closed packed lattice in 2D). The clusters in Fig. 2b are almost not deformed, preserving their initial shape. The gravity is relatively small with respect to the attraction forces, which makes it possible for the forces to hold the clusters, not allowing them to fall down. Note that the clusters at the bottom of the conFig. uration in Fig. 2a are noticeably distorted due to the weight of the upper clusters.

In the simulations the following forces are taken into account: potential interparticle force (repulsive-attractive), volume viscous friction, gravity, and interaction with the floor and walls of the container. The volume viscous friction is a small force proportional to the velocity of each particle, as if the particles are moving in a very light viscous liquid. This is necessary to remove excessive kinetic energy from the system in order to obtain equilibrium configurations. The gravity is simulated by small vertical forces equal for each particle. Let us note that the same forces can roughly model the gas flow used to compress

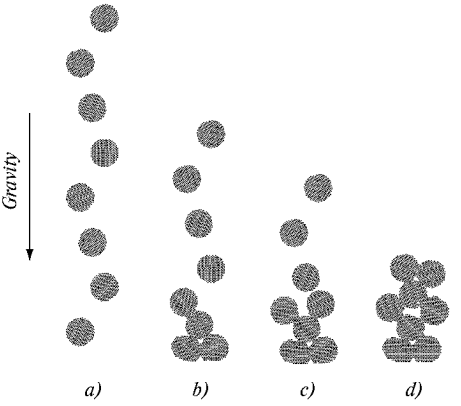

Fig. 1. Cluster settling (8 clusters, 2000 particles); frames (a)–(d) show sequential stages of the process.

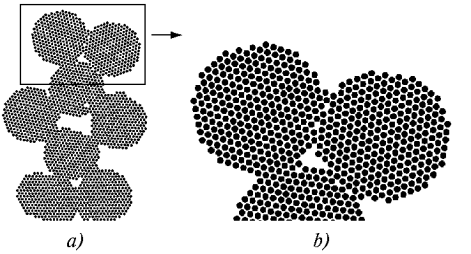

Fig. 2. The settled clusters; (a) the whole configuration, (b) zoom-up of (a).

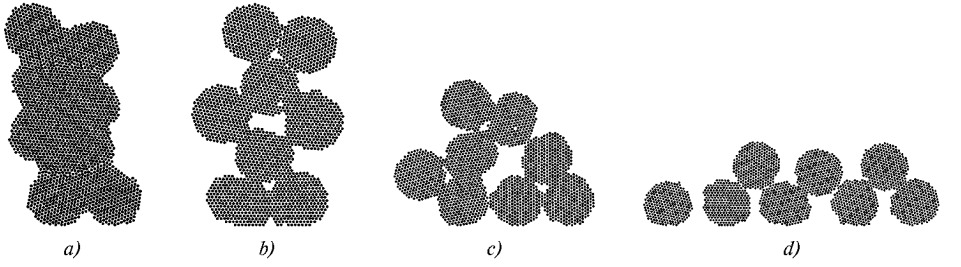

Fig. 3. Settling results for Mie potentials: (a) 4–6, (b) 6–12, (c) 10–14, (d) 14–26.

the powder. The interaction with the container is made by purely elastic repulsive forces (no friction). The interparticle forces are set by the Mie potential

$$U(r) = \frac{D}{n-m}\left[m\left(\frac{a}{r}\right)^n - n\left(\frac{a}{r}\right)^m\right], \qquad n > m; \tag{1.1}$$

where m and n are dimensionless coefficients, r is distance between interacting computer particles, D is the strength of the bond, and a is the equilibrium distance. There is no difference whether the particles belongs to the same cluster or to different ones, the potential is always the same.

For the experiment depicted in Fig. 1 it was chosen $m = 6,\ n = 12$ that results in 6–12 Mie potential, which is known better as Lennard-Jones potential. It is possible to obtain various degrees of cohesion between the clusters by varying constants $m,\ n$ in the Mie potential. This is illustrated in Fig. 3. In the first frame (Fig. 3a) Mie potential 4–6 is used, which is relatively slowly decreasing with the interparticle distance. That is why the attraction in this case is so high, that the clusters almost merge in Fig. 3a, so that it would be practically impossible to separate them from each other. In Fig. 3b the considered above Lennard-Jones potential (Mie 6–12) is used. The clusters are not merging in this case, but the attraction is high enough to prevent the clusters from falling down. Fig. 3c corresponds to Mie 10–14 potential, and Fig. 3d — to Mie 14–26 potential. The last one is so sharply decreasing with the interparticle distance, that the clusters behave almost as non-cohesive balls. But still a small friction between the clusters exists, since they are not falling on the floor completely. Note, that there is no special friction between

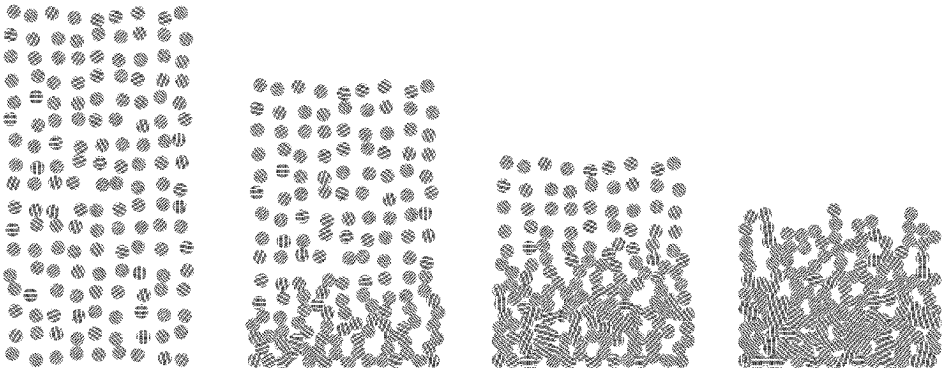

Fig. 4. Settling 153 clusters (38250 computer particles).

the clusters; the effective friction which can be observed in the computer experiments is joint result of the potential interparticle forces and energy removal by the means of the volume viscous friction. The effective friction between the clusters is a pretty complex phenomenon. It can be seen from Fig. 3d that the surface of the clusters (especially for those in the bottom) is not as smooth as it was initially. The roughness of the cluster surfaces is produced by the clusters collisions, which result into rearranging and even into interchange of the computer particles between the clusters.

In Fig. 4 computer experiment on settling the bigger system (153 clusters, 38250 computer particles) is shown. As it was in Fig. 1, the first frame (Fig. 4a) shows initial conFig. uration, where the clusters are arranged in randomly disturbed square lattice and just started to fall down. Fig. 4b–c show the settling in progress and Fig. 4d corresponds to the final stage of the experiment, when all the clusters are settled and the system has reached the equilibrium state. For this simulation Lennard-Jones potential is used, which gives relatively high cohesion between the clusters. This results in a high void ratio for the settled powder.

Let us consider in details how interaction between the clusters is performed. For this purpose Fig. 5 magnifies the lower part of Fig. 4b, where the settling process can be observed. There are several different types of the cluster interactions. In Fig. 5 the following variants of the interaction are outlined: sticking, rolling, sliding, plastic joining, and crushing. Usually interaction between two clusters contains combination of several types, but sometimes the interaction can be found in a pretty pure form. In Fig. s6-11 these types of interaction are shown in magnification and as a sequence of time frames. Sticking (Fig. 6) is the simplest type of interaction when the clusters are in equilibrium and have only small elastic deformations. Rolling (Fig. 7a–b) occurs when gravity or inertia forces are high enough to move clusters relatively to each other, but not sufficiently high to damage or separate them. The next stage of interaction is sliding (Fig. 8a–c). Usually it involves some irreversible deformation at the cluster surfaces. For example, in Fig. 8a–b it can be seen that during sliding the lower row of the particles in the upper cluster is being shifted from its original location. Plastic joining for two clusters takes place when they are subjected to additional load from other clusters, as it is shown in Fig. 9a–b. In this case two clusters merge so tightly that they hardly can be separated; and if separated, they will change their shape — see Fig. 10. The highest degree of interaction involves crushing. This happen when external load is so high that it can crumble one of the clusters, as it can be seen in Fig. 11a–c.

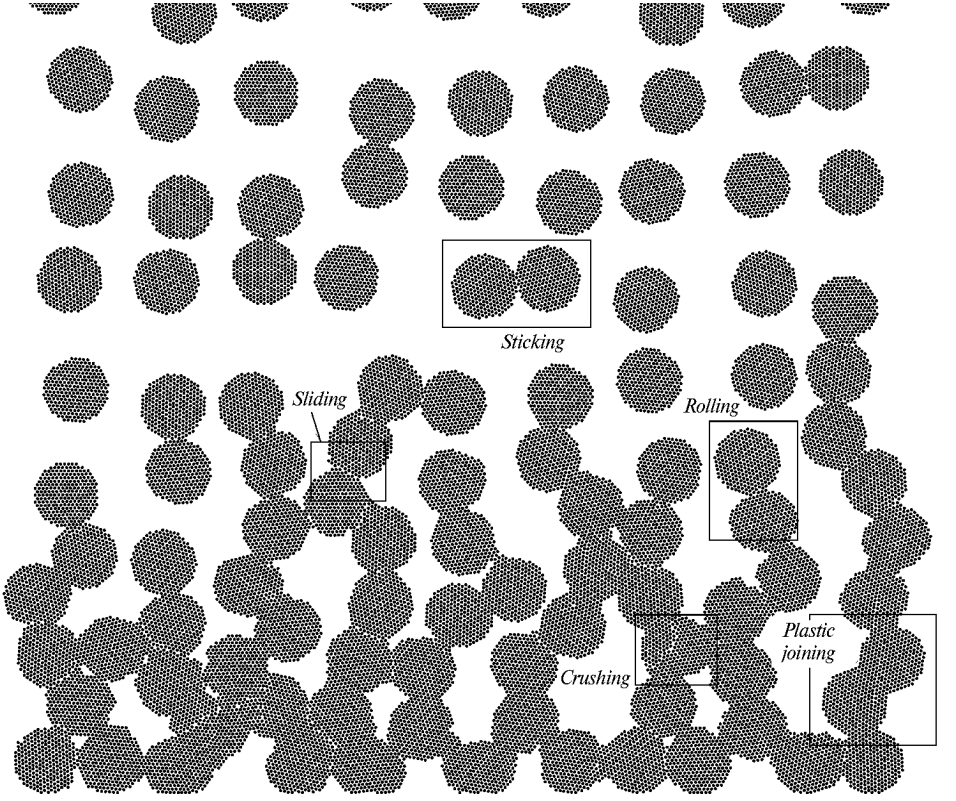

Fig. 5. Various mechanisms for cluster interaction.

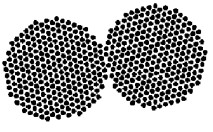

Fig. 6. Sticking.

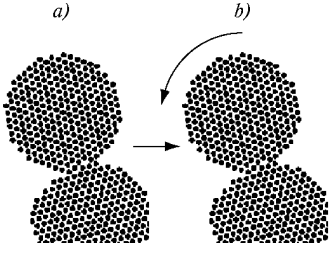

Fig. 7. Rolling.

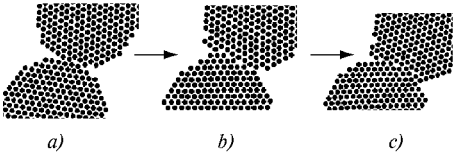

Fig. 8. Sliding.

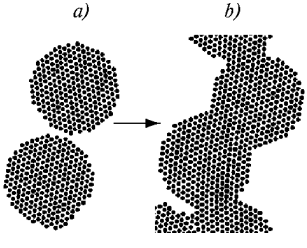

Fig. 9. Plastic joining.

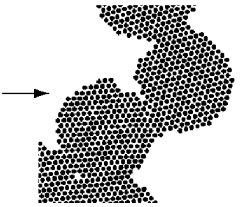

Fig. 10. Separation.

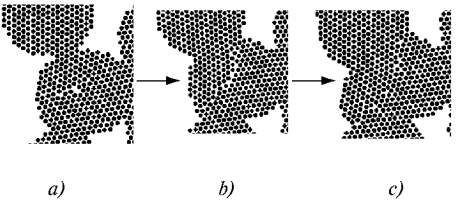

Fig. 11. Crushing.

Thus the considered method allows to describe very complicated mechanisms of cluster interaction and deforming during settling and loading. Let us remind that each cluster represents a single powder particle. The results of the computer experiments show that analytical theory of granular materials have to include description of the following features: friction (including sliding and rolling), plasticity, and fracture. The cluster computer model can help to derive constitutive equations for these types of deformation.

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