Dynamic simulation of the formation of granular media and study of their properties

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Abstract :

A numerical model is presented which describes the evolution of a system containing a large number of deformable spherical grains based on Newton's second law. Starting from an initial state with fixed positions, velocities and grain characteristics, the system evolution is simulated by successive steps. The acceleration of each grain results from the application of an external force and from interactions with other particles. These contact forces are evaluated as functions of the grain deformations during the collisions considered as elastic. The grain bed can be deposited between vertical walls as well as with periodical conditions in the lateral directions. The properties of these packings submitted to mechanical stresses are characterized by using numerical codes which operate on unstructured tetrahedral grids on the scale of the individual grains.

Résumé :

Un modèle numérique est présenté qui permet de décrire l'évolution d'un ensemble important de grains sphériques déformables, par application de la seconde loi de Newton. A partir d'un état initial où sont spécifiées les positions, vitesses et caractéristiques des grains, on simule l'évolution du système par pas de temps successifs, pendant lesquels l'accélération de chaque grain résulte de l'application d'une force extérieure et d'éventuelles interactions avec d'autres particules. Ces forces de contacts sont évaluées en fonction de la déformation des grains lors de la collision, considérée comme élastique. Le lit peut être déposé entre des parois verticales, ou en appliquant des conditions de périodicité dans les directions horizontales. Les propriétés de ces empilements soumis à des sollicitations mécaniques sont caractérisées à l'aide de codes de calculs qui opèrent sur un maillage tétraédrique non structuré à l'échelle des grains individuels.

Key-words :

granular media ; sedimentation ; transport properties

1 Introduction

Granular materials can be found in various natural environments as well as in industrial applications and constitute a very interesting subject for scientific research due to their very complex behaviour. This study addresses the numerical simulation of the dynamic process of grain deposition and the characterization of the resulting packings through the resolution of transport equations on the local scale of the individual grains and pores, with subsequent averaging of the local fields. It is a continuation of previous works on the ballistic sequential deposition by Coelho *et al*. (1997) with an application of the numerical approach based on finite volume technique initially developped for other problems by Bogdanov *et al*. (2003).

2 Model

The formation of a granular medium is simulated as the process of deposition of spherical elastic grains in a gravitational field. Each grain is also submitted to contact forces during the

collisions with other grains or with the bottom plane, and an artificial viscous dumping force is introduced in order to bring the system to an equilibrium state (see Cundall & Strack, 1979). No rotation or friction are taken into account at this stage, but they should be introduced in the model in the future.

The displacement of the sphere *i* is described by the Newton equation

$$m_i\ddot{\mathbf{r}}_i + C_i\dot{\mathbf{r}}_i = m_i\mathbf{g} + \mathbf{F}_i \tag{1}$$

where m_i is the mass, $\mathbf{r}_i$ the center position, $\mathbf{F}_i$ the resultant of the contact forces, g the gravity acceleration, and C_i the artificial viscosity; the dots denote time derivatives. In this study, the damping coefficient is $C_i = \alpha m_i$ where α has the same value for all particles.

Two spheres are in contact when the distance between their centers is smaller than the sum of their radii

$$d_{ij} = R_i + R_j - |\mathbf{r}_i - \mathbf{r}_j| > 0 \tag{2}$$

Then, the total contact force exerced on a grain i is calculated as the sum over all contacts

$$\mathbf{F}_i = \sum_j \mathbf{F}_{ij}, \quad \mathbf{F}_{ij} = -\mathbf{n}_{ij}\int_{t_{ij}}^{t} k_{ij}\mathrm{d}(d_{ij}) = -\mathbf{n}_{ij}k_{ij}d_{ij}(t) \tag{3}$$

where the normal force between two grains is described by an elastic law whith a normal stiffness k_{ij}; d_{ij} is the relative normal displacement, and t_{ij} is the time when the grains come into contact; $\mathbf{n}_{ij}$ is the unit vector pointing from the center of the grain *i* to that of grain *j*.

According to the solution of the Hertz problem when two elastic spheres are in contact, their relative displacement d_{ij} is determined by the force F_{ij}, the radii R_i and R_j, and the elastic properties - the Poisson ratios ν_i and ν_j, and the Young modulii E_i and E_j (Landau & Lifshitz, 1981). This solution gives the normal joint stiffness in the form

$$k_{ij} = \frac{4}{3}\sqrt{d_{ij}}\left(\frac{1}{R_i} + \frac{1}{R_j}\right)^{-1/2}\left(\frac{1-\nu_i^2}{E_i} + \frac{1-\nu_j^2}{E_j}\right)^{-1} \tag{4}$$

A simpler variant of the elastic deformation is the linear model. In this case, the stiffness is fixed and does not vary with the deformation of the grains. Due to the nonlinear chararacter of the deformation of two elastic spheres, it is impossible to relate directly the linear stiffness to the elastic constants of the material. However, one can estimate its order of magnitude by supposing that the compression of the spheres is of the same order as that produced by their own weight. Namely, for two identical grains with mass m, the linear stiffness k_{eff} is

$$k_{eff} = \left[\frac{16mgRE^2}{9(1-\nu^2)^2}\right]^{1/3} \tag{5}$$

For quartz grains, $\rho = 2.66 \cdot 10^3$kg/m^3, $E = 9.6 \cdot 10^{10}$ Pa and $\nu = 0.08$. Substituting these values in (5) for $R = 10^{-3}$m yields $k_{eff} \approx 122\,000$kg/s^2.

Two types of lateral boundary conditions are used, namely transverse periodicity and elastic plane boundaries. The bottom is an elastic plane with the same propertes as the material of the grains.

3 Numerical technique

The equations (1) are discretized by using an explicit finite difference method with self-adjustable time steps. The grain center positions as well as the forces are determined at the same instants

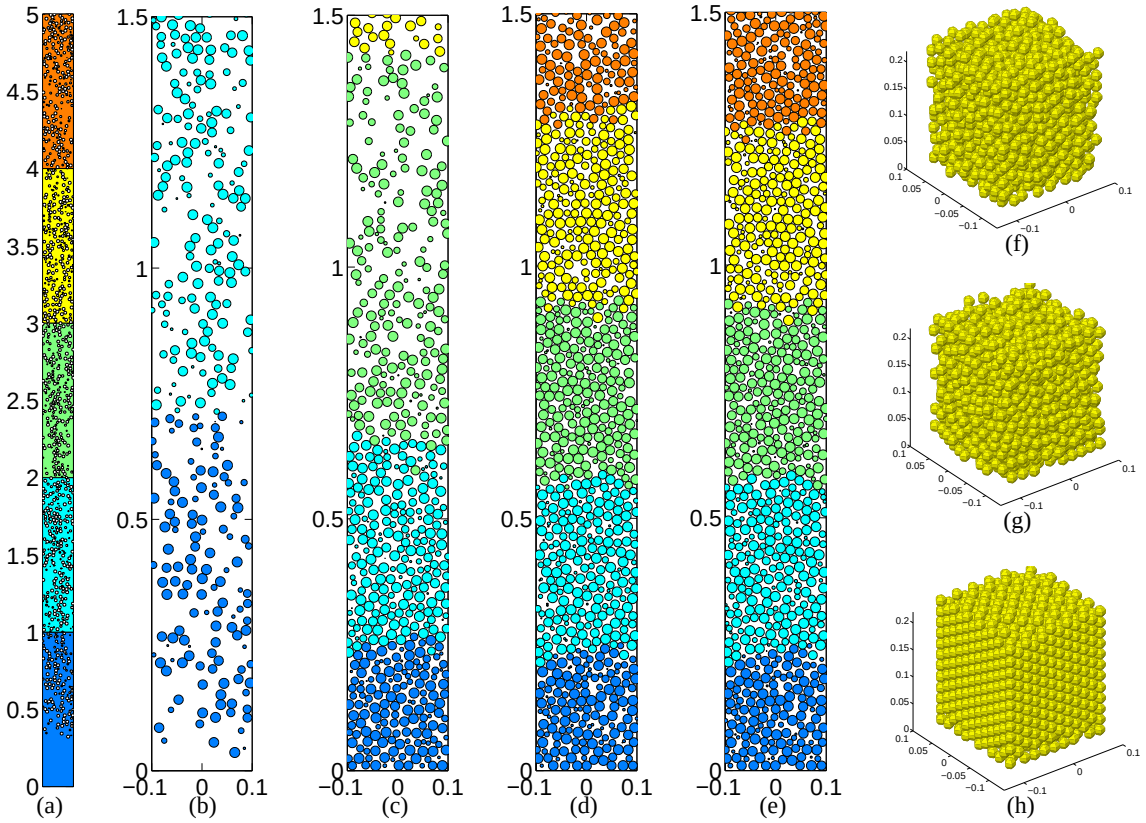


Figure 1: Deposition of 10000 spheres with the stiffness $k_i = 10^6$kg/s^2 in a periodic unit cell. Initial position (a); colors show various layers. Position of grains for $t = 0.3$s, 1s, 2s and 4s (b-e) with colors corresponding to the initial position. The data correspond to the vertical cross section at y=0. Bottom part of the packings when $k_i = 10^6$kg/s^2 (f) or 10^5kg/s^2 (g) for a periodic unit cell and $k_i = 10^5$kg/s^2 for non periodic boundary conditions (h).

while the grains velocities are calculated at intermediate times. First, given the position of all grains at the current time step, all contacts are detected according to the condition (2). Then, the contact forces are calculated from Eqs. (3). They are used in order to solve the Newton equations (1) and to find the grains velocities $\dot{\mathbf{r}}_i^+$ for the next intermediate time and to determine the new positions $\mathbf{r}_i^+$

$$\dot{\mathbf{r}}_i^+ = \frac{\dot{\mathbf{r}}_i \left(\frac{m_i}{\Delta t_{k-1/2}} - \frac{C_i}{2} \right) + m_i \mathbf{g} + \mathbf{F}_i}{\frac{m_i}{\Delta t_{k-1/2}} + \frac{C_i}{2}}, \qquad \mathbf{r}_i^+ = \mathbf{r}_i + \dot{\mathbf{r}}_i^+ \Delta t_k \tag{6}$$

The grains move freely between the collisions; hence, the time step can be easily adapted in order to follow the velocity evolution due to gravity. However, during an elastic interaction two grains form a spring with the effective stiffness (5) and joint mass $m_{ij} = (1/m_i + 1/m_j)^{-1}$. The half period of oscillation of this spring is $\tau_{cr} = \pi\sqrt{m_{ij}/k_{eff}}$ which is exactly the duration of the contact in the linear model. Due to rapid velocity changes during the collision, the time step should be a fraction of this time interval $\Delta t = \delta_t \tau_{cr}$, small enough to simulate properly these variations. This restriction imposes some limitations on the simulations because when two particles come in contact the motion of all other grains should be modelled with the same time step.

In the case of a non linear relationship between displacement and normal force during a collision, the corresponding period of oscillation τ_{cr} depends on the amplitude or, in other

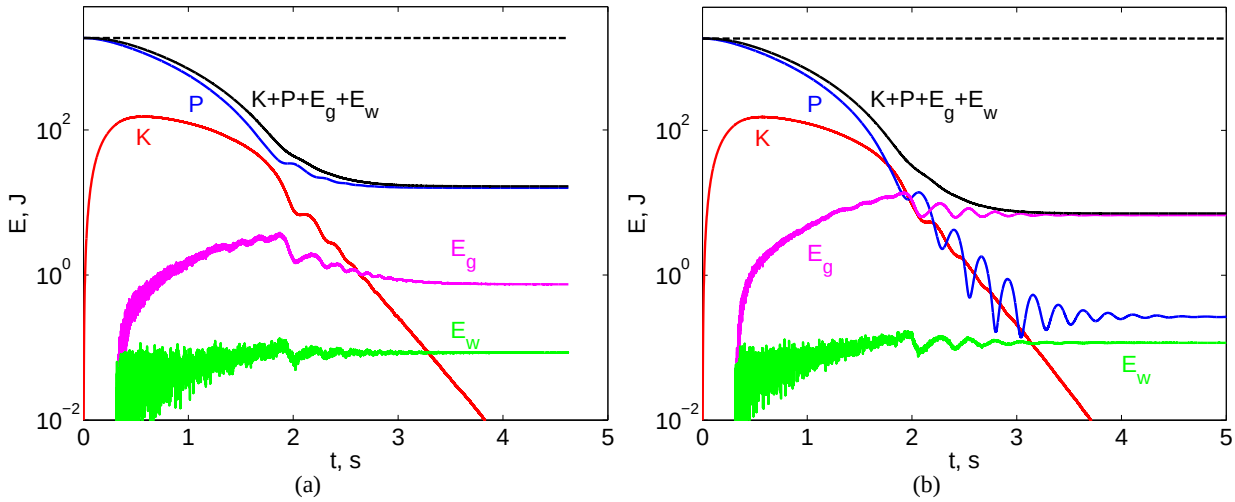


Figure 2: Energy variation in the system of 10000 grains with stiffness $k_i = 10^6$kg/s^2 (a) or 10^5kg/s^2 (b). Kinetic energy K (red), potential energy P (blue), elastic energy due to contact between grains E_g (magenta), elastic energy due to contact with the walls E_w (green), full energy (black solid lines) and full energy together with the energy lost by dissipation (black broken lines).

words, on the initial kinetic energy of the system. This situation, however, is not considered here.

In order to control the quality of the simulations, three kinds of mechanical energy are evaluated for each time step: kinetic energy K, potential energy P and energy E of elastic deformations

$$K = \sum_i \frac{m_i(\dot{\mathbf{r}}_i)^2}{2}, \quad P = \sum_i m_i g(z_i - z_b), \quad E_g = \sum_{ij} k_{ij} \frac{d_{ij}(t)^2}{2} \tag{7}$$

The elastic energy E_w accumulated during the deformation of grain during their interaction with boundary walls, can be defined in the same way as E_g.

4 Results

The simulations are performed by using a system of 10 000 spherical grains with the same radius $R = 10^{-2}$m initially randomly distributed within a cell of $0.2 \times 0.2 \times 5$m^3 at some height above the bottom plane (Fig. 1a). All particles have the same characteristics, mass $m = 10^{-2}$kg and individual linear stiffness $k_i = 10^5$ or 10^6kg/s^2 (the joint stiffness is $k_{eff} = k_i/2$). The coefficient $\alpha = 5$s^{-1} was used in all simulations.

Fig. 1b-e shows various stages of the evolution of the system in a periodic cell. One can observe that the initial vertical ordering of the particles is in general well preserved.

Fig. 1f-h shows the bottom part for thee packings. When the stiffness decreases from $k_i = 10^6$kg/s^2 to 10^5kg/s^2, the degree of overlap of the particles increases due to the decrease of the elastic resistance. The particles form a denser structure. Although the difference is not visually perceptible, the final bed thickness is 1.594m for the softer grains and 1.626m for the harder ones.

The most striking difference is due to the boundary conditions. The simulation of deposition with periodic boundary conditions does not yield any visible regularity in the final distribution of the particles (Figs. 1f,g). Conversely, when the grains fall between elastic walls, a perfectly regular structure appears (Fig. 1h). It should be noted that the lateral distance between the walls is 10 times the grain diameter, which is, perhaps, partially responsible for this phenomenon.

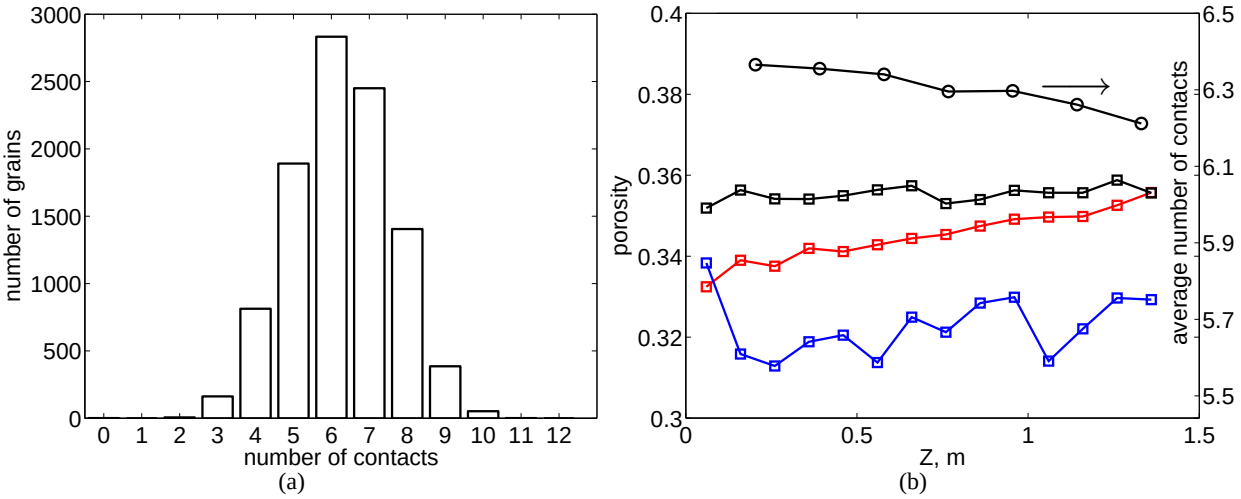


Figure 3: The distribution of the number of contacts per grain (a), the average number of contacts per grain as a function of the elevation for $k_i = 10^6$kg/s^2 (o) and the porosity (□) for various stiffnesses and boundary conditions (b): periodic systems with $k_i = 10^6$kg/s^2 (black lines) or 10^5kg/s^2 (red line) and non periodic systems with $k_i = 10^5$kg/s^2 (blue line)

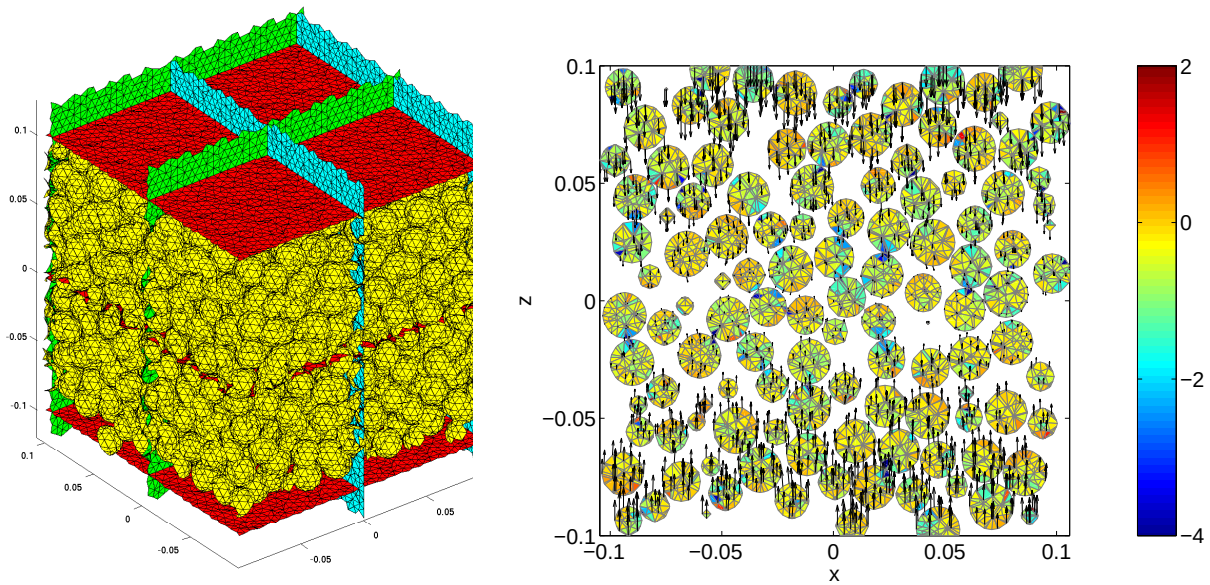
The variation of the mechanical energy of the system is shown in Fig. 2. All particles initially have a potential energy which progressively decreases when it is converted into kinetic energy. Later on, due to the dumping force, most of this energy is dissipated. However, part of it is converted into elastic energy, which progressively increases from zero to some equlibrium value. It can be noted that a larger amount of energy is stored in the final state in the form of elastic deformation for the softer grains than for the harder ones. The sum of the full mecanical energy in the system and of the losses due to energy dissipation is almost constant which confirm the robustness of the numerical technique used in this study.

The number of contacts per grain in the final state of the system varies between 4 and 9 with an average about 6 in the case of the $k_i = 10^6$kg/s^2 (see Fig. 3a). The average number slightly decreases with the elevation in the packing (Fig. 3b).

The distribution of the porosity is also presented in Fig. 3b as a function of the elevation for three types of grains packings. It is calculated per layers of thickness 0.1m from the bottom to the height 1.5m, by summing up the grain volumes and removing the overlaps due to the contacts. In the case of periodic cells, the porosity is almost uniform and slightly increases with z especially for the softer grains. In the case of non-periodic boundary conditions the distribution of the porosity is not uniform because it is strongly affected by the ordering of the grain in the bed.

The next step of the study is the analysis of the transport properties of the resulting grain packings: macroscopic thermal conductivity, permeability of the porous space and mechanical properties. These problems are solved by numerically simulating the elementary processes on the microscopic scale, with subsequent averaging on the scale of a large number of grains. This approach is presented by Adler (1992).This part is under development and only preliminary results concerning the defomation are discussed here.

First, in order to apply the numerical technique for the resolution of the elastostatic equations on the microscopic level, the system under consideration should be discretized. Unstructured tetrahedral meshes are used here. The principle of the mesh generation tool is presented by Bogdanov *et al*. (2003). Figure 4a provides an example, where only the triangulation of the



(a) (b)

Figure 4: Unit cell with triangulated spheres and artificial planes (a). Cross section of a grain packing obtained by deposition and submitted to vertical compression (b). Colors correspond to the trace of the strain tensor and the arrows show the displacement field.

grain surfaces is shown.

Then the corresponding microscopic equations for the linear elastic deformation are solved by using a finite volume formulation, under a prescribed external load. Figure 4b shows the distribution of the trace of the strain tensor within the grains as well as the local displacement field, when the packing is submitted to a vertical compression.

5 Conclusions

A numerical model for the simulation of grain deposition has been presented. The dynamic part of the problem is simulated by using Newton laws and an elastic model for the grain contacts. Then, the transport properties of the resulting packings can be analized by solving the governing equations on the microscopic scale.

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