Computer Simulation of Pouring Grains Using Stick-Slip Model

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ABSTRACT

We applied the Stick-Slip model to simulate pouring grains processes via Granular Dynamics Simulation. The dynamics mechanism and the structure formation of the 2D and 3D systems are investigated. The results show that the shape of the generated piles in the 2D and 3D systems are similar when observed superficially, but the detailed structure and the dynamic behaviour leading to that structure are very different.

Keywords: Stick-Slip model, dynamic behaviour, structure formation.

INTRODUCTION

Grains are discrete solid particles whose the particle size is larger than about one micron. They are easily observed in our daily lives. Sand, sugar, pills, potatoes, and stones are just a few examples, and anyone could easily add several items to this list (Jaeger *et al*. 1996 & De Gennes 1999). Playing with grains gave insight that the dynamics and pattern formations of dry and wet grains are very much different. The kids could easily form any kind of shapes with wet sands, but those shapes could easily damage when sands are dry. Such phenomenon is due to the difference forces acting in the grains. For dry grains, such as sand flows in an hourglass, the interstitial fluid, in this case air, plays an insignificant role in the dynamics. The flow properties of dry granular materials are largely governed by the nature of individual collisions between particles. Unlike dry grains, wet grains involve also hydrodynamic and cohesive forces. Throughout this article the simulations of pouring problems are focused on dry grains, and omit the adjective "dry" from here on.

Pouring grains onto a surface or into a container allow the grains to fall under gravity. Experimental studies (Alonso & Herrmann 1996) reported that the stable pile generated by sequentially dropping grains into a two dimensional slit between parallel plates, has an almost triangular shape, somewhat flattened near the edge. That a pile is formed at all comes from the behaviour of the individual grains when they are dropped. When they hit the grains already there, or at the bottom surface, they lose part of their kinetic energy. One reason is that the collisions are inelastic: during the deformation associated with the collision there is dissipation. A second reason is the surface roughness; the friction forces also produce dissipation. Further pile formation depends on the reaction of the existing pile to the disturbances of newly dropped grains. The grains at rest can slide before coming to rest again, leading to repeated stick-slip motion during the contact.

The exact shape of the pile structure depends on the detailed processes in the collisions and the lasting contacts between the particles and the surface or other medium. Moreover, the internal stresses within the pile are also determined by the interaction of individual grains. The problem is that the information of the detailed interaction at the level of individual grains is hardly provided by experimental studies. However, such information can be easily obtained via numerical studies. Some articles dealing with this matter have been published such as the articles written Buchholtz & Poschel (1994) and Zhou *et al*. (2001). The first article reported that angle of repose (the angle between the surface of stable pile and the horizontal surface) does depend on the surface roughness, while the second article shown that for spherical grains, the angle did also depend on the number of particles.

The goal of this study is to understand the main governing mechanisms (dynamics) and structure formations of pouring grains based on the individual grain motion, since those phenomena are crucial for direct applications, such as for mining and packaging industries.

The force model to represent the grains' motions during the deposition processes has been developed and validated by Hasan & van Opheusden (2001,2007). The force acting on particle i, $\mathbf{f}_i$, is given by

$$\mathbf{f}_i = \mathbf{f}_{ig} + \sum_{i \neq j} (\mathbf{f}_{nij} + \mathbf{f}_{tij}) \quad \ldots\ldots\ldots\ldots\ldots\ldots (1)$$

where $\mathbf{f}_{ig}$ is the gravitational force, and $\mathbf{f}_{nij}$ and $\mathbf{f}_{tij}$ are the components of contact force in the normal and tangential directions. The normal force, $\mathbf{f}_{nij}$, is modeled by a Hookean spring with damper, $\mathbf{f}_{nij} = -(k_n \boldsymbol{\delta}_{nij} + \gamma_n \mathbf{v}_{nij})$, where $\boldsymbol{\delta}_{nij}$ and $\mathbf{v}_{nij}$ represent the displacement (overlap) and relative velocity normal to the contact surface, k_n and γ_n are stiffness and damping constants. The tangential (friction) force model is basically an approximation of the Coulomb's law of friction that allows a reversible transition between static (stick) and dynamic (slip) modes. During the dynamic mode, the friction force is velocity independent, $\mathbf{f}_{tij(d)} = -\mu_d |\mathbf{f}_{nij}| \operatorname{sign}(\mathbf{v}_{tij})$, while during the static mode, the friction force is modeled by a critically damped spring, $\mathbf{f}_{tij(s)} = -(k_t \boldsymbol{\delta}_{tij} + \gamma_t \mathbf{v}_{tij})$, where μ_d is the coefficient of dynamic friction, $\boldsymbol{\delta}_{tij}$ and $\mathbf{v}_{tij}$ are the displacement and relative velocity parallel to the contact surface, k_t and γ_t are stiffness and damping constants. Each contact may undergo multiple transitions during the process. The mode changes from dynamic to static if $\mathbf{v}_{tij} < \varepsilon$ (ε is the stick velocity). If $|\mathbf{f}_{tij(s)}| > |\mathbf{f}_{smax}|$ (maximum static friction) the mode alters from static to dynamic. Hasan & van Opheusden (2001) shown that the above tangential model is more realistic to model a deposition process than the spring model (Cundall & Strack (1979), Schafer *et al.* (1996)) and model of spring with stopping criterion. The model also allows less time consumption during the simulations.

METHODS

We simulate pouring process in two and three dimensions via a Granular Dynamics (GD) method. The method traces the trajectory of each grain by solving Newton's equation of motion (1). The force equations are solved numerically using a Predictor-Corrector method, which is composed of three steps: prediction, evaluation and correction. Throughout the simulations, a fourth order Gear's Predictor-Corrector algorithm is applied. Let $\mathbf{r}_i$, $\mathbf{v}_i$, $\mathbf{a}_i$, $\mathbf{b}_i$, and $\mathbf{c}_i$ be the position of particle *i* and its first, second, third and fourth derivatives respectively. Let the superscript "P" and "C" stand for Predictor and Corrector. The Gear Predictor-Corrector algorithm of fourth order can be summarized as follows.

Prediction

Predict the particle positions and their derivatives at time $t + \Delta t$ using a fourth order Taylor series based on the particle positions and their derivatives at time *t*. This yields

$$\mathbf{r}_i^P(t+\Delta t) = \mathbf{r}_i(t) + a_1\mathbf{v}_i(t) + a_2\mathbf{a}_i(t) + a_3\mathbf{b}_i(t) + a_4\mathbf{c}_i(t) \ldots..(2a)$$

$$\mathbf{v}_i^P(t+\Delta t) = \mathbf{v}_i(t) + a_1\mathbf{a}_i(t) + a_2\mathbf{b}_i(t) + a_3\mathbf{c}_i(t) \ldots..(2b)$$

$$\mathbf{a}_i^P(t+\Delta t) = \mathbf{a}_i(t) + a_1\mathbf{b}_i(t) + a_2\mathbf{c}_i(t) \ldots\ldots..(2c)$$

$$\mathbf{b}_i^P(t+\Delta t) = \mathbf{b}_i(t) + a_1\mathbf{c}_i(t) \ldots\ldots\ldots\ldots(2d)$$

$$\mathbf{c}_i^P(t+\Delta t) = \mathbf{c}_i(t) \ldots\ldots\ldots\ldots\ldots\ldots..(2e)$$

where $a_1 = \Delta t$, $a_2 = a_1\Delta t/2$, $a_3 = a_2\Delta t/3$, and $a_4 = a_3\Delta t/4$.

Evaluation

Evaluate the force on each particle at time $t + \Delta t$ using the predicted values. This gives the corrected acceleration $\mathbf{a}_i^C(t+\Delta t)$. The corrected acceleration is compared to the predicted acceleration to estimate the size of the error in the prediction step,

$$\Delta\mathbf{a}_i(t+\Delta t) = \mathbf{a}_i^C(t+\Delta t) - \mathbf{a}_i^P(t+\Delta t) \ldots(3)$$

Correction

The difference of the acceleration is used to correct the predicted positions and their derivatives to get better results. The corrected values are given by

$$\mathbf{r}_i^C(t+\Delta t) = \mathbf{r}_i^P(t+\Delta t) + a_r\Delta\mathbf{a}_i(t+\Delta t) \ldots..(4a)$$

$$\mathbf{v}_i^C(t+\Delta t) = \mathbf{v}_i^P(t+\Delta t) + a_v\Delta\mathbf{a}_i(t+\Delta t) \ldots..(4b)$$

$$\mathbf{b}_i^C(t+\Delta t) = \mathbf{b}_i^P(t+\Delta t) + a_b\Delta\mathbf{a}_i(t+\Delta t) ..(4c)$$

$$\mathbf{c}_i^C(t+\Delta t) = \mathbf{c}_i^P(t+\Delta t) + a_c\Delta\mathbf{a}_i(t+\Delta t) ..(4d)$$

where $a_r = (19/90)a_2$, $a_v = (3/4)a_2/a_1$, $a_b = (1/2)a_2/a_3$, and $a_c = (1/12)a_2/a_4$. a_1, a_2, a_3, and a_4 have the same meaning as above.

In our simulations, the grains are spherically symmetric, but they do not rotate. They are dropped one by one from a fixed point. The surfaces/media have the same material properties as the grains. The used parameters are mass $m = 0.05$ kg, diameter $\sigma = 0.05$ m, spring constants $k_n = k_t = 10^5$ kg/s, $\gamma_n = \sqrt{(m\,k_n)}$, $\gamma_t = 2\sqrt{(m\,k_t)}$, coefficients of friction $\mu_d = 0.3$ and $\mu_s = 0.6$, and the stick velocity $\varepsilon = 10^{-3}$ m/s. The properties of pile structures for certain parameters are the average of repeated (five times) simulations with randomly initial velocities. Voronoi diagram/polygon is applied to investigate the structure of the bottom layer of the resulting piles.

RESULTS AND DISCUSSIONS

Dynamics

To study the dynamic of the system, numerical simulation data were used to produce movies, consisting of a series of consecutive snapshots of the pile configuration. Surface avalanches, where the grains slide down the pile surface, occur in both systems, but it is not the only mechanism in pile formation, and not even the most important one. It is observed that the number of particles involved in surface avalanches is relatively small.

The two-dimensional (2D) piles observed have an almost regular *hexagonally packed* structure (Figure 1a). During the pile formation, due to internal stresses, *defect lines* develop extending from the surface to the bottom of the pile, leading to a large mass transport along the crack, where a large fraction of the pile is moved horizontally, while a triangular section makes a small vertical drop. We termed this phenomenon an internal landslide.

For the smaller piles the landslides can take place at any position at the bottom. For relatively large piles the landslides mostly happen near the wings. There are several factors that may explain this observed phenomenon. When a disc is dropped and hits the pile, its energy must be dissipated before a stable pile is obtained again. For a small pile, there are only a few contact points where this dissipation can occur, and the effect of the impact on pile structure will be large.

The three-dimensional piles (3D) are very *randomly packed* (Figure 1b). Newly dropped grains hit the existing pile, bounce back and slide along the surface before settling down. In doing so they destabilise grains already in the pile, which can slide down the pile surface or destabilise their lower neighbours, causing internal rearrangements.

Internal stresses lead to movement of individual particles near *weak spots*, without changing the random nature of the pile. Weak spots develop throughout the pile. When the pile is formed in the box (Figure 1c), the dynamics are similar.

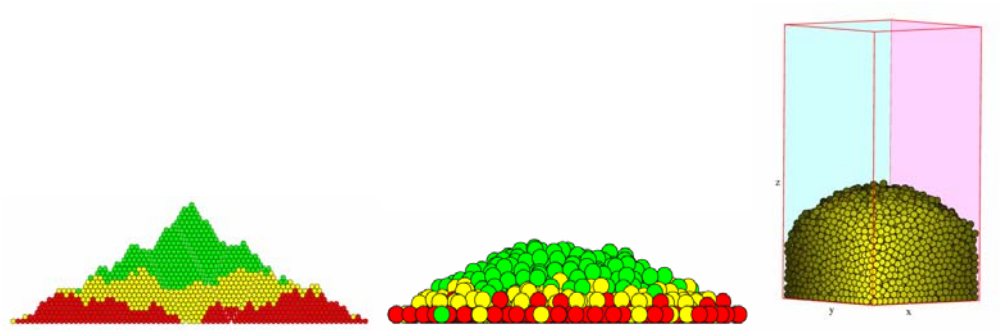
The presence of constraining walls prevents landslides, and stops the grains sliding down in the surface avalanches. Avalanches are the dominant features for the rest of the process, but only influence the upper part of the pile.

Structure

To study the history in pile formation we used different colours to indicate which particles were deposited first and which later. We observed that 2D and 3D systems on the free surface produced piles having almost *horizontally layered structures* (Figure 1a & 1b) instead of the onion-like structures that have been observed in experiments done by Alonso & Herrmann (1996). From those figures it is seen that the shape of the 2D pile is almost triangular, with a surface resembling a devils' staircase, while the 3D pile has roughly conical shape, somewhat flattened near the top, with a rather smooth surface. We calculated Voronoi polygon to determine the structure in the bottom layer of the 3D piles formed on the free surface and in the box (Figure 2). These show regions with grains having six neighbours, but not densely packed, and many fault lines with particles having a different number of nearest neighbours. The analysis can in principle be extended to Voronoi polyhedra for the full 3D structure, but it seems cumbersome. As shown in figure 2, the bottom layer structures of the two piles poured on different media do not significantly different. The effect of the walls contributes to the number of grains near having six neighbours as can be seen from Figure 2b.

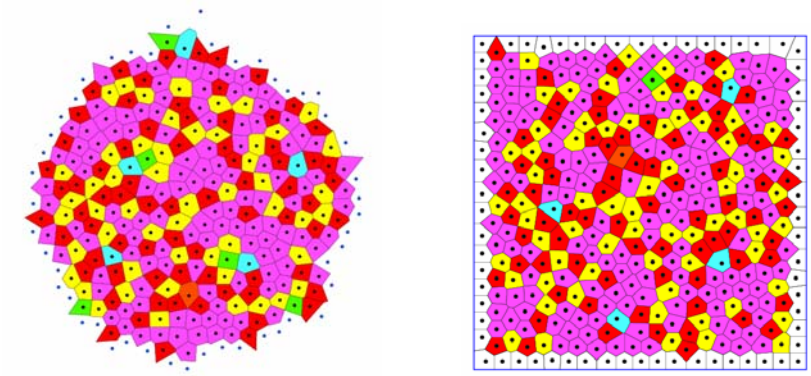
System size dependence

We also studied the effect of system size, the number of particles in the pile, while keeping all other parameters the same. The average slope and the internal density of the 2D piles appear to be relatively insensitive to system size. Larger piles have relatively fewer fault lines than smaller ones, but the effect on the structure is small. On the other hand, the results of the 3D systems indicate a dependence on system size. The slope decreases when the size increases, while the internal density increases. Indications are that continued addition of material leads to a compactification of the random structure. It is possible that very large piles, beyond the range we have studied, would have a flattened pancake like shape.



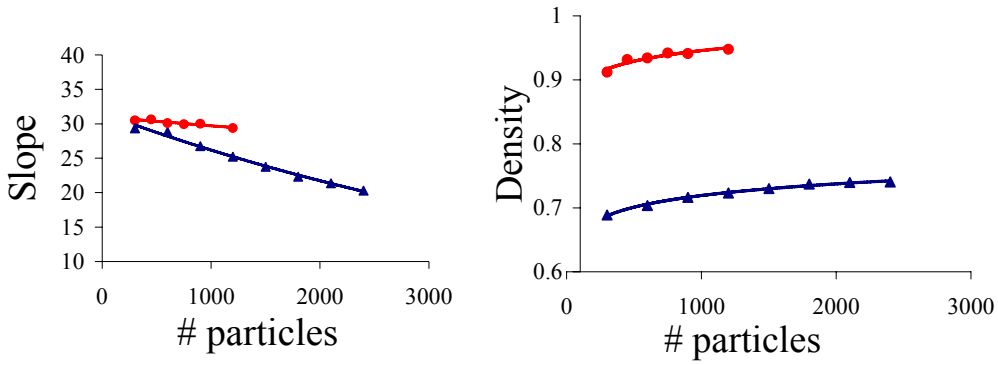
(a) (b) (c)

Figure 1. The piles of 2D (a) and 3D (b) systems formed on the free surface and in the box (c).



(a) (b)

Figure 2. Voronoi diagram of the piles formed on the free surface (a) and in the box (b)



(a) (b)

Figure 3. The effect of system size to the slope (a) and density (b) of the piles.The short graph represent for 2D system, while the longer one for 3D

CONCLUSION

Based on the results presented in the previous section, some conclusions regarding pouring grains for 2D and 3D systems numerically using Granular Dynamics simulations are drawn as the follows:

1. the dynamics for 2D consists of surface avalanches and internal landslides, while for the 3D system, beside surface avalanches, the other dynamic mechanism is internal shift;
2. the shape of the 2D pile is almost triangular, while the 3D pile is roughly conical in shape;
3. only 3D system is size dependent, the slope decreases with size and the density increases as the size increases.

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