Course Project of
Topics in Random Walks and Diffusion:
Modeling draining sand or draining pebble

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1 Introduction

The flow of granular media has been a field studied by many researchers. However, the theoretical approach has not achieved any notable progress, without any governing equations comparable to the Navier Stokes equation in fluid media, because of its complex dynamical behaviors such as the resistance to the sheer stress, clustering and segregation. Among others, the flow in a silo driven by gravity has particular interest from the easy experiment and confined geometry. It also has a direct application to the storage of grain.

Recently, another application of this flow has been aroused by the Nuclear engineering department, which is about the design of 'pebble bed reactor.' Unlike other reactors using rod-type of nuclear fuel, this reactor uses fuel embedded in spherical shape material. As shown in Figure 1, the core is filled with about 360,000 pebbles. To check the remaining fuel in pebbles, one pebble is discharged from the bottom of the core every 30 seconds and is replaced with new one if it is exhausted. Regardless of the replacement, a pebble is reload to the core from the top.

To prevent the case the fuel of pebble is exhausted before the checking, it is very important to make the discharge time evenly distributed over all places in the core. For this purpose, we have two factors to manipulate: the shape of core and the reloading location on top surface.

In this project, as a preliminary research of these problems, I studied a few simulation methods for describing the drainage of granular media. Void propagation model is based on directed random walk of void. Despite of its simplicity, parabolic stream lines are expected, which is also observed in experiments. By simulation I also observed the surface flow as the slide approaches to the angle of repose. A more accurate dynamics can be expected with molecular dynamics simulation. However, it seems that the force law model for the

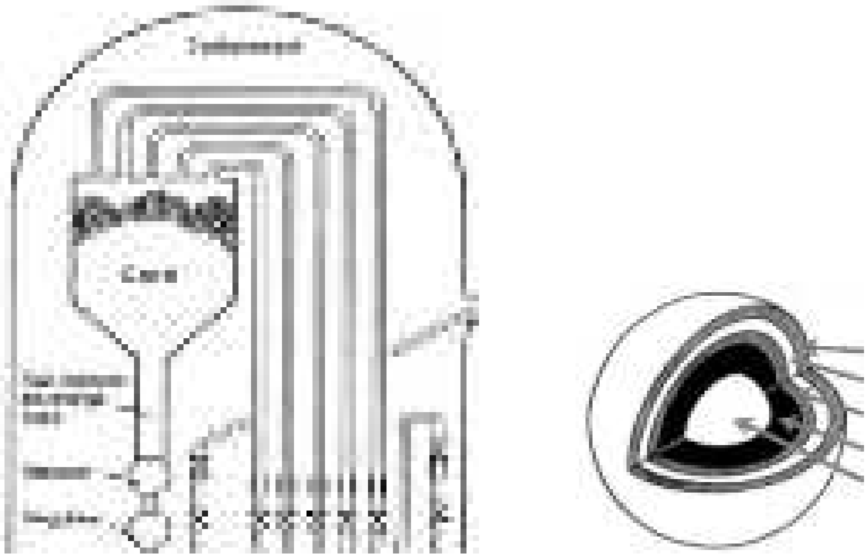

Figure 1: The core of pebble bed reactor and a pebble fuel from "http://web.mit.edu/bepple-bed/"

reactor will be different from that of sand since the flow is very slow and controlled. Cellular automata method is also applied to simulate the granular media.

2 Void propagation model and surface flow

To overcome the limitation of the continuum approach, the void propagation model was suggested [1][2]. Void diffusion model is based on the observation that the discharge of a particle and following sequences of motion filling the void can be thought to be the upward propagation of the void.

If we assume that the media is closely packed as in the Figure 2, void can go either left or right with equal probability as goes up by one layer. Thus the void density $C(x,y)$, the probability of void reaching at (x,y) has the following relation:

$$C(x, y + \triangle_y) = \frac{1}{2}C(x, y + \triangle_y) + \frac{1}{2}C(x, y + \triangle_y). \tag{1}$$

With $C(x,y)$, we can also express the velocity profile with two velocity component v_R, v_L:

$$v_R(x - \triangle_x, y + \triangle_y) = \frac{n}{2}C(x,y)$$
$$v_R(x + \triangle_x, y + \triangle_y) = \frac{n}{2}C(x,y),$$

where n is determined from the the number of void created at the bottom at hole and distance of to the nearest neighbor. The vertical and horizontal velocity can be obtained from the linear combinations of v_L and v_R.

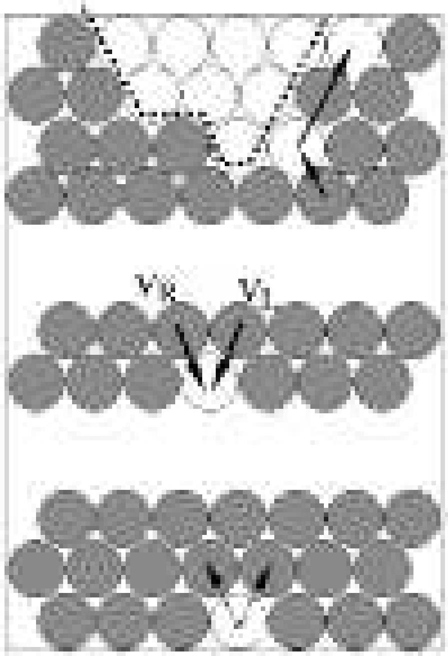

Figure 2: Void propagation model

Since the random walk of void is simple Bernoulli walk with t replaced y, we have analytic approximation of $C(x, y)$ which is valid within the central region $|x| \sim \sqrt{(}y)$.

$$C(x, y) = \frac{1}{\sqrt{\pi a y}} \exp(-\frac{x^2}{ay}), \quad a = \frac{2\triangle_x^2}{\triangle_y}$$

Since $C(x, y)$ also means the flux of flow at (x, y) from the viewpoint of particle, the stream function can be defined from $C(x, y)$ as the amount of flux passing through any line joining the origin and (x, y). If we take the path of integration as $(0, 0) - (0, y)$ and $(0, y) - (x, y)$, the first integral yields zero from the symmetry and the second integral yields the stream function:

$$\Psi(x, y) = \frac{1}{2}\mathrm{erf}(\frac{x}{\sqrt{ay}}). \tag{2}$$

From this we know the flow has parabolic stream lines, which agree with experiment [1].

Despite of the simplicity, this model can account for two phenomena which are observed in reality. One is the existence of the stagnant zone which is induced from the angle of repose in granular media. In the void propagation model, this zone corresponds to the left and right region near the bottom where voids can never reach. This stationary zone should be avoided in the design of the pebble bed reactor.

The other is formation of slide and surface flow at the slide. When the voids arrive at the top surface we can think they no longer move and they are accumulated on top. (In the

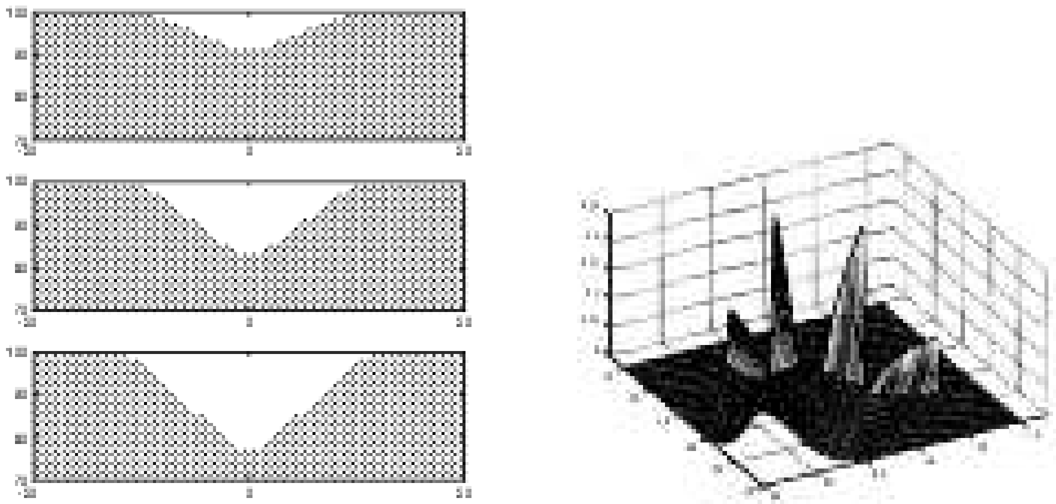

Figure 3: Surface evolution at time $t = 110, 220$ and 330 (left) and flux distribution at $t = 330$ (right)

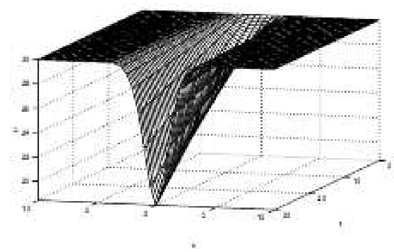

Figure 4: Surface evolution based on the stream function

viewpoint of the particle, the surface move down as particles drain.) As the accumulation glows, We can easily notice that the propagation of void no longer does the random walk when it reach beneath the accumulated void. They just flow along the slide until it is stopped by the two void above it and stay there. (Figure 2(top))

Figure 3(left) shows the evolution of the surface generated by the computer simulation. As time goes the slope of the slide approaches to the angle of repose, 45° in this case, Figure 3(right) is plot of the void density (flux) at the time of $t = 330$. The particle flux at the top layer of the slope is much higher that that of the deep layers since the flux is accumulated along the slope instead of being distributed to two above particles. The high flux implies that particles slide down along the slide and this corresponds to the 'surface flow' which is reported in the experiment[2] except that the flow region is about 10 layers deep in reality.

I tried to describe the surface evolution as continuous function, possibly in terms of PDE, but to fail. Figure 4 is the evolution of the surface in the continuum limit based on the stream function (2). Though it shows a development of the sharp peak at $x = 0$, the slope exceeds

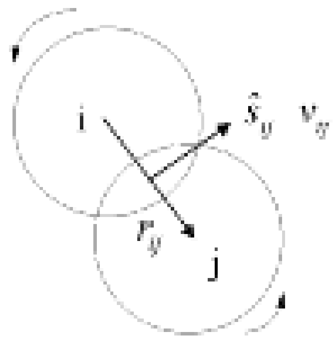

Figure 5: Overlap of two particles in the Molecular Dynamics simulation

the angle of repose as time goes.

3 Molecular dynamics simulation

The more exact and realistic method is molecular dynamics(MD) simulation which is basically the integration of Newton's equations. As the computational power increases, it has been possible to trace as many particles as used in experiment. But this method is still controversial since force laws between particles or boundary are not fully discovered. Thus most simulation results are focused verifying the force laws in comparison with experiment.

In case of hard granular media, the inter-particle force change drastically as two particle is close enough to be touched, which make numerical integration difficult. To avoid this, colliding soft sphere model is used, in which the repulsive force appears when they 'overlaps'.

One of the force law in recent use is Lennard-Jones(LJ) form, where the repulsive force between i and j particle is given as

$$f_{ij}^r = \frac{48\epsilon}{r_{ij}}[(\frac{\sigma}{r_{ij}})^{12} - \frac{1}{2}(\frac{\sigma}{r_{ij}})^6]\hat{\mathbf{r}}_{ij}.$$

The diameter of the particle is determined by $r_c = 2^{1/6}\sigma$ where the interaction cutoff occurs. Since the collision is inelastic in most cases, damping force should be also considered :

$$\begin{aligned} f_{ij}^n &= -\gamma_n \dot{\mathrm{r}}_{ij} \cdot \hat{\mathrm{r}}_{ij}, \\ f_{ij}^s &= -\mathrm{sgn}(v_{ij}^s) \min(\mu|f_{ij}^r + f_{ij}^n|, \gamma_s|v_{ij}^s|)\hat{s}_{ij} \end{aligned}$$

f_{ij}^n is normal damping, f_{ij}^s is transverse damping and v_{ij}^s is the relative tangential velocity with both translational and angular velocities taken into account. The transverse damping was bounded by the static friction force.

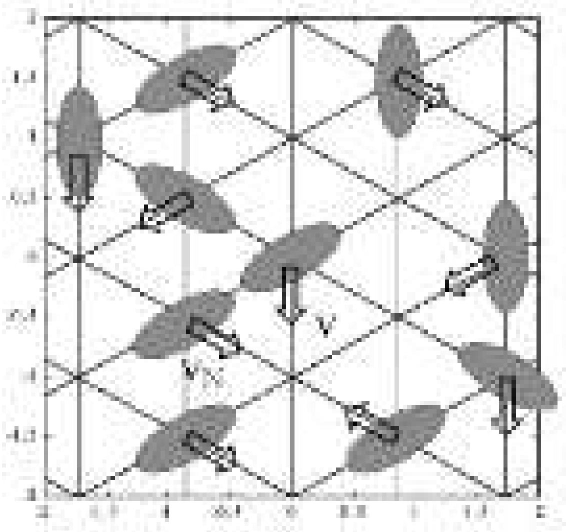

Figure 6: Cellular automata model for grass seed by G.W. Baxter and R.P. Behringer

4 Cellular automata model

Cellular automata(CA) is mainly applied to the population change of biological species by adapting a few simple rules. But it is also applied to the simulation of fluid dynamics and granular media flow. A classic application of CA to granular media was done by G.W. Baxter and R.P. Behringer[3] in 1990. They simulated the flow of seeds from a silo, which would be significantly complex in MD since the non-spherical shape increases the degree of freedom.

As shown in Figure 6, each seed occupy one site in triangular grid and has a 'state' consist of orientation and moving direction. Now one iteration is divided into two steps, namely 'interaction' and 'propagation.' In interaction step each particle choose moving direction by calculating energy states for possible moving directions and taking the lowest energy direction.

For the calculation of energy, they used a formula based on the experimental facts.

$$E = E_g + \sum_{NN} E_{in}(\text{sheer, orientation, dilation}),$$

where E_g is gravitational energy due to the decrease in height and E_{in} is interaction energy which is summed over nearest neighbors(NN) and depends on many factor. For example sheer factor can be set to be proportional the the relative moving direction.

In propagation step, they move to next sites along the determined directions. Here, their movement is made simultaneously or states are parallely updated. Because of this, two particles may compete for one site. In that case, the particle which moves to lower energy state can move and other particle stay where they were. By this simple scheme, they observed many features like long range orientation which agree with real situation.

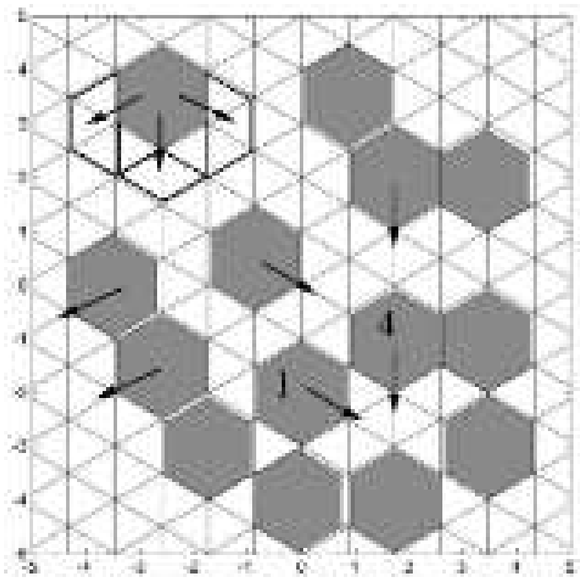

Figure 7: Hexagonal cellular automata model

I applied cellular automata to simulate the drainage of circular particles. The followings are automata rules. Also refer to Figure 7.

- Each ball is approximated as a hexagon exclusively occupying volume in the triangular grid.
- Each ball can move along three directions (down, down-left, down-right). When there are several choices of direction, 'down' is preferred since it decreases more height. Between 'down-left' and 'down-right', one is randomly chosen.
- When two ball competes for a site, lower energy movement has priority again. But in this case the priority is in relative sense that 'down' has possibility 4 times as much as 'down-left' or 'down-right'. The ratio was chosen arbitrary.
- Instead of parallel update, sequential update was used since the flow is very slow and controlled. Particles were discharged (or deleted) from hole after the movement induced by previous discharge was all settled down.

The simulation results are shown in the Figure 8. The particle traces were divided in two plots, one for those came out of the hole (right above) and did not(right below). We can also observed that much part of particle movement is due to the surface flow. The surface evolution quite looks like that of sand experiment, but that couldn't compared exactly. Nor it is certain that the discharge of pebbles will follow this pattern.

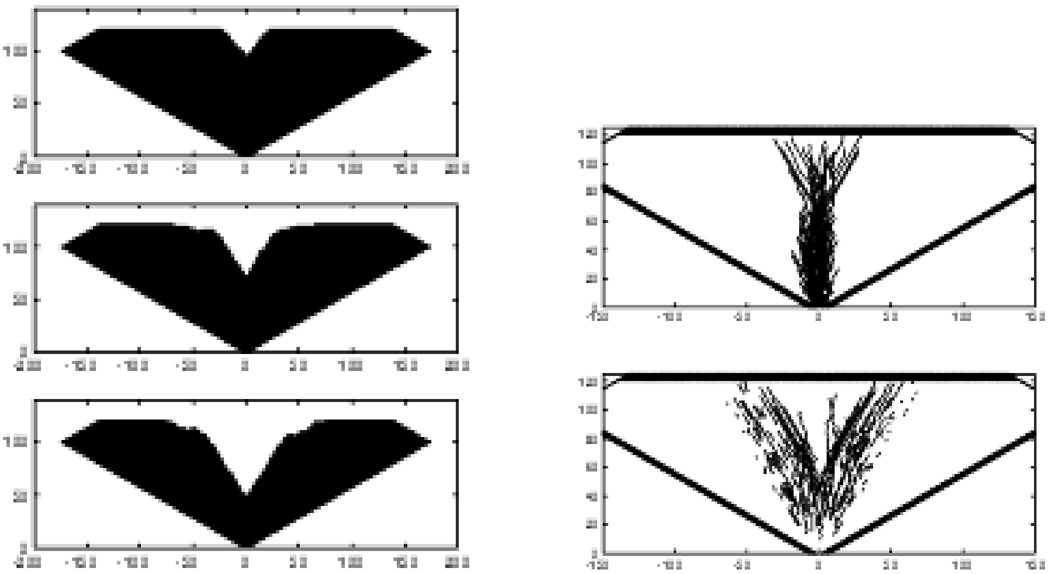

Figure 8: Simulation result of hexagonal model with 9000 particles: Surface evolution at $t = 200, 300, 1000$ (left) and traces of particles up to $t = 1000$ (right)

5 Future works

To solve the suggested questions regarding the design of the pebble bed reactor, the following is required.

- Study of pebble bed reactor:
  To simulate the dynamics of discharging process, more material properties should be known such as surface friction of both core and pebble, mass and elasticity of pebble and width of hole.

- Molecular dynamics simulation:
  Since the particle size is much bigger that usual granular media, molecular dynamics simulation is expexted to be the best model for simulation. For this purpose, developing a suitable force law is crutial. In particular it shold be one that fully implement the slow and controlled discharge process.

- Calculation of discharge time distribution:
  From the void propagation and hexagonal model, it was pointed that surface flow shares an important part of the flux to the hole. Thus it seems that surface flow should be specially treated in the calculation of discharge time of particles in a given shape of the core.

- Experiment:
  As is usual with other granular flow simulation, experiment is also suggested to compare

with the simulation result. The experiment using the marbles with similar material property will be more tractable than other sand experiments, if it is done in 2-D setting for easy particle tracking.

References

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