The angle of repose of spherical grains in granular Hele–Shaw cells: a molecular dynamics study

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Received 16 December 2007
Accepted 9 April 2008
Published 30 April 2008

Online at stacks.iop.org/JSTAT/2008/P04026
doi:10.1088/1742-5468/2008/04/P04026

Abstract. We report the results of three-dimensional molecular dynamic simulations on the angle of repose of a sandpile formed by pouring mono-sized cohesionless spherical grains into a granular Hele–Shaw cell. In particular, we are interested in investigating the effects of those variables which may have a significant impact on the pattern formation of granular mixtures in Hele–Shaw cells. The results indicate that the frictional forces influence the formation of piles on the grain level remarkably. Furthermore, we see that increasing grain insertion rate decreases the angle of repose slightly. We also find that the cell thickness is a significant factor and the angle of repose decays when the size of the gap between the lateral walls increases. In addition to agreeing with the experimental exponential decay law, our results are in accordance with a recently proposed model which takes into account the arching effects. Using grains with different sizes reveals that the behaviour of the angle of repose when both size and cell thickness are varied is controlled by a scaled function of the ratio of these two variables.

Keywords: granular matter

ArXiv ePrint: 0711.2732
1. Introduction

The formation of a sandpile is an everyday life phenomenon which may occur in several ways, including pouring [1], discharging [2, 3], failing [4, 5], tilting and rotating [6–9]. This gravity-driven physical event is relevant to many practical applications and laboratory processes such as avalanches [10–12] and pattern formation in granular mixtures [13, 14]. It is also related to the paradigm of self-organized criticality [15] which has itself a wide realm of applicability to a diverse range of physical phenomena [16].

The angle of repose of a sandpile is a simple concept that characterizes the behaviour of granular materials on the macroscopic scale. A sandpile has an inclined free surface that does not flow. When grains are added to the sandpile the slope of this free surface increases until it exceeds a threshold value. At this point, the pile does not support new grains and releases many grains in an avalanche reducing the slope to the angle of repose, \( \theta_r \). One of the most important questions in the study of piling of grains is how to determine the relationship between the angle of repose and the relevant variables, i.e. material properties, boundary conditions, and the model interactions at the grain level. Experiments have shown that \( \theta_r \) depends on the shape, density, and size distribution of the grains, as well as humidity, formation history and geometrical boundary conditions [1]–[3].

Granular materials are ensembles of discrete particles, and as for any macroscopic system, the total number of modes is huge. What we see on the macroscopic scale, hence, is a manifestation of the collective behaviour of a large assembly of macroscopic grains that interact with each other (and perhaps with the container walls), through collisions and friction. In this regard, the molecular dynamics (MD) simulation technique provides perhaps the most realistic approach for modelling the properties of granular materials. The present work is focused on such a numerical study of the angle of repose of a heap formed by pouring dry, mono-sized spherical grains into a granular Hele–Shaw cell. Some of the experimental aspects of the phenomenon have been reported by Grasselli...
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and Herrmann [1]. However, as far as we know, there has been no three-dimensional MD study of the angle of repose in the Hele–Shaw cell, except the one by Zhuo et al [17], which studied the formation of sandpiles resulting from discharging materials by using a different model interaction. Regarding the classification made by Grasselli and Herrmann [1], what they have estimated is the outflow angle of the heap which is less than the heap angle, the subject of the current research.

In this paper, we report a detailed numerical study of the formation of a sandpile and the dependence of its angle of repose on the relevant variables. We are specifically interested in determining how $\theta_r$ changes with variables like the size of particles, the rate of mass injection, the density of grains, the thickness of the container, and wall–particle and particle–particle static friction coefficients. These are the key parameters which may impact significantly on pattern formation of granular mixtures in Hele–Shaw cells [18,19]. To answer such questions, we performed extensive MD simulations in three dimension on model systems by using a new MD scheme developed by Silbert et al [20], which is described briefly in the next section. The results of our simulations are presented in section 3, followed by the main conclusions at section 4.

2. Simulation methodology

As mentioned earlier, our simulations are based on a distinct element method (DEM) scheme, originally proposed by Silbert et al. The method has been discussed elsewhere in detail [20]. For the sake of clarity, we review the most important aspects of it here. According to this model, the spheres interact on contact through a linear spring dashpot or Hertzian interactions in the directions normal and tangential to their lines of centres. In a gravitational field $g$, the translational and rotational motions of grain $i$ in a system at time $t$, caused by its interactions with neighbouring grains or walls, can be described by Newton’s second law, in terms of the total force and torque as the following equations:

$$F_i^{\text{tot}} = m_i g + \sum (F_{n_{i,j}} + F_{t_{i,j}})$$

(1)

$$\tau_i^{\text{tot}} = -\frac{1}{2} \sum r_{i,j} \times F_{t_{i,j}}$$

(2)

where $m_i$, $r_{i,j} = r_i - r_j$ are, respectively, the mass of grain $i$ and the relative distance between grains $i$ and $j$. For two contacting grains $i, j$ at positions $r_i$, $r_j$ with velocities $v_i$, $v_j$ and angular velocities $\omega_i, \omega_j$ the force on grain $i$ is computed as follows: the normal compression $\delta_{i,j}$ is (figure 1)

$$\delta_{i,j} = d - r_{i,j}$$

(3)

and relative normal velocity $v_{n_{i,j}}$ and relative tangential velocity $v_{t_{i,j}}$ are given by

$$v_{n_{i,j}} = (v_{i,j} \cdot n_{i,j}) n_{i,j}$$

(4)

$$v_{t_{i,j}} = v_{i,j} - v_{n_{i,j}} - \frac{1}{2}(\omega_i + \omega_j)r_{i,j}$$

(5)

where $n_{i,j} = r_{i,j}/r_{i,j}$ with $r_{i,j} = |r_{i,j}|$ and $v_{i,j} = v_i - v_j$. The rate of change of the elastic tangential displacement $u_{t_{i,j}}$, set to zero at the initial of a contact, is given by [20]

$$\frac{du_{t_{i,j}}}{dt} = v_{t_{i,j}} - \frac{(u_{t_{i,j}} \cdot v_{i,j}) r_{i,j}}{r_{i,j}^2}.$$  

(6)

doi:10.1088/1742-5468/2008/04/P04026
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Figure 1. Two-dimensional illustration of two grains $i$ and $j$ in contact and position vectors $r_i$, $r_j$, respectively, with compression and overlap $\delta_{i,j}$.

The second term in equation (6) arises from the rigid body rotation around the contact point and ensures that $u_{t_{i,j}}$ always lies in the local tangent plane of contact. In equations (1) and (2), normal and tangential forces acting on grain $i$ are given by

$$F_{n_{i,j}} = f\left(\frac{\delta_{i,j}}{d}\right)\left(k_n\delta_{i,j}n_{i,j} - \gamma_n m_{\text{eff}}v_{n_{i,j}}\right)$$ \hspace{1cm} (7)

and

$$F_{t_{i,j}} = f\left(\frac{\delta_{i,j}}{d}\right)\left(k_t u_{t_{i,j}} - \gamma_t m_{\text{eff}}v_{t_{i,j}}\right)$$ \hspace{1cm} (8)

where $k_n,t$ and $\gamma_{n,t}$ are elastic and viscoelastic constants respectively and $m_{\text{eff}} = m_i m_j/(m_i + m_j)$ is the effective mass of spheres with masses $m_i$ and $m_j$. The corresponding contact force on grain $j$ is simply given by Newton’s third law, i.e., $F_{i,j} = -F_{j,i}$. For spheres of equal mass $m$, as is the case in our system, $m_{\text{eff}} = m/2$; $f(x) = \sqrt{x}$ for the linear spring dashpot (Hookean) model, and $f(x) = \sqrt{x}$ for Hertzian contacts with viscoelastic damping between spheres [20].

Static friction is implemented by keeping track of the elastic shear displacement throughout the lifetime of a contact. The static yield criterion, characterized by a local particle friction coefficient $\mu$, is modelled by truncating the magnitude of $u_{t_{i,j}}$ as necessary to satisfy $|F_{t_{i,j}}| < |\mu F_{n_{i,j}}|$. Thus the contact surfaces are treated as ‘sticking’ when $|F_{t_{i,j}}| < |\mu F_{n_{i,j}}|$, and as ‘slipping’ when the yield criterion is satisfied [21, 22].

3. Results and discussion

In this section we present the results of our extensive molecular dynamics (MD) simulations in three dimensions on model systems of $N$ mono-disperse, cohesionless and inelastic spheres of diameter $d$ and mass $m$. The system is constrained by a rectangular box with fixed rough walls and boundary conditions and free top surface, as in figure 2. A simulation was started with the random generation of spheres without overlaps from the top and left corner of the container, followed by a gravitational settling process to
form a stable heap. The results are given in non-dimensional quantities by defining the following normalization parameters: distance, time, velocity, forces, elastic constants, and stress are, respectively, measured in units of $d$, $t_0 = \sqrt{d/g}$, $v_0 = \sqrt{dg}$, $F_0 = mg$, and $k_0 = mg/d$. All data were taken after the system had reached the steady state. Because of the complexity of the model, there are a wide range of parameters that affect the results of computation. However, we usually investigate the effect of a single variable varying in a certain range while other variables are fixed at their base values as listed in table 1.

All the cases were simulated in three dimensions using a molecular dynamics code for granular materials, LAMMPS [20,23]. The equations of motion for the translational and rotational degrees of freedom are integrated with either a third-order Gear predictor–corrector scheme or a velocity Verlet scheme [24].

Table 1. Basic computational parameters.

| Parameters                              | System conditions |
|-----------------------------------------|-------------------|
| Number of particles ($N$)              | 40 000            |
| Particle size ($d$)                     | $1d_0$            |
| Particle density ($\rho$)               | $2.4(m_0/d_0^3)$  |
| Particle friction coefficient ($\mu_p$) | 0.5               |
| Wall friction coefficient ($\mu_w$)     | 0.5               |
| Particle normal stiffness coefficient ($k_n$) | $2 \times 10^3(k_0)$ |
| Particle tangential stiffness coefficient ($k_t$) | $2/7k_0$       |
| Particle normal damping coefficient ($\gamma_n$) | $50/(t_0)$ |
| Particle tangential damping coefficient ($\gamma_t$) | $0(t_0^{-1})$ |
| Wall normal stiffness coefficient ($k_n$) | $2 \times 10^3(k_0)$ |
| Wall tangential stiffness coefficient ($k_t$) | $2/7k_0$       |
| Wall normal damping coefficient ($\gamma_n$) | $50/(t_0)$ |
| Particle normal damping coefficient ($\gamma_n$) | $50/(t_0)$ |
| Time step increment                     | $2 \times 10^{-3}$ |
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Figure 3. Angle of repose (θ_r) as a function of number of grains (N) from the Hookean model for various particle–wall friction coefficients. Other parameters are fixed at their basic values as listed in table 1. The sizes of error bars (∼0.2°) are about the size of the symbol used and, therefore, omitted from the curves.

3.1. The evolution of the pile

We start from an empty vertical cell composed of two parallel plates separated by a spacer with a variable width w. A granular heap is formed in the cell by pouring mono-sized spherical grains onto the bottom plate. These grains are released from a small box located top left in the cell, as shown in figure 2. The rate of material insertion R can be varied by changing the box size. A pile with well defined shape starts to form as the number of the added grains grows. The angle of repose could then be determined from the surface profile of the heap.

The formation of a granular heap at the macroscopic level is a complicated phenomenon arising as the result of surface avalanches and also a kink mechanism [25]. At the grain level, it is a consequence of energy dissipation. In addition to frictional forces, the particle–particle inelastic collisions consume the translational and rotational energy of a falling grain. Eventually, the grain will stick to a position where its energy is less than the minimum value required to overcome the potential barrier created by frictional forces [26]. At the earlier stage of the pile formation, the numbers of grains are small. Therefore, the falling grains can move further and the angle of repose is less than that of a larger pile. On adding more grains to the pile the angle of repose grows to its asymptotic value, where the energy gain in the gravitational field is balanced by the dissipating effects. In figure 3 the evolution of the sandpile or, equivalently, the evolution of θ_r has been plotted for three values of μ_w against N, the total number of released grains. As seen from the figure, the angle of repose grows linearly for smaller values of N and then evolves quickly into a steady state, characterized by an asymptotic value of θ_r at larger values of N. For the set of parameters used in figure 3, the angle of repose is

doi:10.1088/1742-5468/2008/04/P04026
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Figure 4. Angle of repose $\theta_r$ against grain density $\rho$ from Hookean and Hertzian models. Other parameters are fixed at their basic values as listed in table 1.

almost constant for $N > 25000$. For the rest of the work we have used $N = 40000$ grains in all simulations to make sure that the angle of repose has reached its asymptotic values as shown in figure 3. The absolute value of the error in estimation of $\theta_r$ mainly arises as the result of uncertainties in the relevant lengths and is less than 0.2° for all data points. Since it is smaller than the size of the symbols used, we omit error bars from the curves.

We also note that at earlier stages of heap formation the difference between $\theta_r(N)$ values is not significant for different values of $\mu_w$, as seen in figure 3. This perhaps explains the existence of the so called dead-zone [14] in stratification of bi-dispersed mixtures. It is known that the difference between the angle of repose of two species is the key factor which together with the difference between the grain sizes determines the kinds of patterns formed in the cell [13]. If the difference between $\theta_r$ values is negligible, e.g., when the number of grains is small, the only factor that affects pattern formation is the size. As a result, for small values of $N$, the grains segregate according to their size and a dead-zone forms.

3.2. Effect of mass flow rate

A simple way of increasing the rate of mass flow into the cell is increasing the density of each grain, while its diameter is fixed. From figure 4 one can see that increasing the mass of individual grains causes a slight fluctuation, at most 0.3° around the mean values in both linear and Hertzian models. In fact, there is no hint of a dependence of $\theta_r$ on the value of the grain’s mass in our simulations in the range of parameters that we used. This conclusion is in agreement with some experimental observations [13].

A more interesting way of increasing mass flow rate is to increase $R$, the number of grains falling down on the heap at each time step. It has been found that the wavelength of the layers in granular stratification is an increasing function of this quantity [18].

doi:10.1088/1742-5468/2008/04/P04026
Moreover, above a critical flow rate $R_c$, the stratification pattern abruptly disappears [19]. Our simulations shown in figure 5 indicate that increasing the rate of grain insertion $R$ decreases the angle of repose slightly. The change in $\theta_r$ is small, about a degree, after increasing $R$ to three times its initial value. Such a slight change in the value of the angle of repose when the rate of grain insertion was varied has been reported by Grasselli and Herrmann [1].

Comparing the two ways of increasing $R$, we conclude that in the formation of a sandpile, what does really matter is not the mass itself, but the number of grains that hit the pile in a given time. This effect may be attributed to the occurrence of larger avalanches when the rate of grains falling upon top of the heap becomes larger.

### 3.3. Effect of cell thickness

The effect of cell thickness $w$ on the heap stability has been the subject of both experimental and numerical studies [1, 3, 7, 8, 17]. Careful experiments and measurements reveal that the presence of front and rear walls greatly increases the angle of repose $\theta_r$ as well as the maximal angle of movement $\theta_m$ (the maximal angle that a granular medium can reach when carefully tilted). The parameter $w$ is also a determining factor which drastically affects pattern formation of bi-dispersed granular mixtures in Hele–Shaw cells. A non-linear decrease in the wavelength of the stratification pattern with cell thickness $w$ has been reported [18]. And there is a critical cell thickness $w_c$, in some ways similar to $R_c$, above which the layered pattern abruptly vanishes [19].

To quantify the behaviour of the angle of repose when the cell thickness is varied, simulations were performed using different cell thicknesses $w$ where the rest of the parameters are fixed at their base values as listed in table 1. The results presented
Figure 6. Angle of repose $\theta_r$ against cell thickness $w$, simulated with Hookean and Hertzian models. Other parameters are fixed at their basic values as listed in table 1.

In figure 6, show that on increasing the cell thickness, the angle of repose, $\theta_r(w)$, decreases and it eventually settles down to an asymptotic value $\theta_\infty$ when the cell thickness becomes very large compared to the size of grains. Our results add to the outcomes of various experiments in different conditions, which show that pile angles $\theta_r[1,3,8,17]$ and $\theta_m[7,8]$ decrease with increasing gap width towards constant values. We can conclude that the observed phenomenon is universal and does not depend on the formation history of the pile. In fact, most authors have fitted their data with the empirical exponential law [1]

$$\theta_r(w) = \theta_\infty(1 + \alpha e^{-w/l})$$

(9)

where $\alpha$ is a constant depending on the grain properties and $l$ is a characteristic length representing the scale over which the walls affect the piling of grains. A semi-logarithmic plot of dimensionless function $g_1(\theta_r, \theta_\infty) \equiv (\theta_\infty - \theta_r(w))/\theta_\infty$ versus $w$ has been presented in figure 7, with $\theta_\infty \simeq 23.5^\circ$ and $\theta_\infty \simeq 22^\circ$ for Hookean and Hertzian models, respectively. From the slope of curve, one can estimate the characteristic number of grains defined as $n^* \equiv l/d$. The value that we obtained for $n^*$ is $\sim 5$ from both Hookean and Hertzian models, which is slightly less than the value 6 estimated by Zhuo et al for a granular heap formed by discharging materials [3,17].

Although the exponential decay of equation (9) fits all the data obtained by a number of real experiments as well as numerical simulations, no theoretical explanation has been found for it. Recently, Courrech et al [8] proposed a simple model for incorporating the lateral wall effect on piling via the Janssen effect [27], i.e. the pressure saturation that occurs with depth in confined granular media. This model introduces a new characteristic length defined as $B_r = 2K\mu_w h_{\text{freeze}}$, where $K$ is the Janssen coefficient, and $h_{\text{freeze}}$ is the flowing layer height when an induced surface avalanche is about to stop. The predicted
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Figure 7. A semi-logarithmic plot of function $g_1(\theta_r, \theta_\infty) = (\theta_r - \theta_\infty)/\theta_\infty$ versus cell thickness $w$ for the data points of figure 6.

growth of $\theta_r$ in the Courrech et al model is slower than the exponential decay and is given by

$$\frac{\sin \theta_r(w) - \sin \theta_\infty}{\cos \theta_r(w)} = 1 - \frac{w}{B_r} \left[ 1 - \exp \left( -\frac{B_r}{w} \right) \right].$$

The above equation involves trigonometric functions of $\theta$ instead of $\theta$ itself. Moreover, it contains only two fitting parameters, $\theta_\infty$ and $B_r$. In the range $w \gg B_r$ a power expansion of the right side in terms of $w^{-1}$ yields

$$g_2(\theta_r, \theta_\infty) \equiv \frac{\sin \theta_r(w) - \sin \theta_\infty}{\cos \theta_r(w)} \simeq \frac{B_r}{2} w^{-1} + O(B_r^2w^{-2}).$$

As can be seen from figure 8, our results in the range $w/d \geq 6$ fit well with a first-order approximation of $g_2$ for both Hookean (triangles) and Hertzian (squares) models. Furthermore, the estimated value of $B_r/d$ is $\sim 1.7$ for Hookean models and $\sim 1.2$ for Hertzian models, which are comparable with the value $1.8 \pm 0.4$ obtained by Courrech et al from experimental observations. In fact, the new characteristic length scale $B_r$ is about 3–4 times smaller than $l$.

There is another way to look at the phenomenon. The walls of the cell not only consume the kinetic energy of grains via friction and inelastic collisions, but also they confine them to moving in a limited space. Indeed, by changing the cell thickness, while keeping the size of grains fixed, one can even change the dimensionality of the space accessible to the grains. Investigation of the average number of contacts per grain, $\overline{z}$, in this round of simulations demonstrates the validity of this image. In figure 9 the variation of $\overline{z}$ versus $w$ has been depicted for the interior grains, i.e. grains which are not supported by the walls. The fraction of interior grains decreases with $w/d$, but even
Figure 8. A linear fit of function $g_3(\theta_r, \theta_\infty) \equiv (\sin \theta_r(w) - \sin \theta_\infty) / \cos \theta_r(w)$ versus inverse of cell thickness ($w^{-1}$) from Hookean (triangles) and Hertzian models (squares) in the range $w \geq 6d$. For comparison, the data points at $w = 4d$ have also been shown.

Figure 9. The average number of contacts for interior grains versus cell thickness $w$ from the Hookean model for the set of parameters listed in table 1.

at a small value of the cell thickness such as $w/d = 1.5$, there is still a non-negligible fraction of such grains (about 8.8% of total grains) in the cell. We also observe that for $w < 2d$, the average number of contacts becomes less than 4, which is the minimal average coordination number required to obtain a static packing of frictional spheres in
three dimensions [28, 29] indicating a crossover from a three-dimensional regime to a two-
dimensional one. At $w = 1.5d$, the mean number of contacts is 3.3, very close to the
minimal value $\overline{z} = 3$ needed for a stable packing of frictional spheres in two dimensions.
On the other hand, for large values of $w/d$, where the angle of repose saturates to its bulk
value, the value of $\overline{z}$ quickly reaches the asymptotic value $\overline{z} = 5.2$. Of course, this limiting
value depends on the microscopic parameters of the granular materials. From figure 9 it
is clear that $\overline{z}$ evolves more rapidly to its asymptotic value than $\theta_r$. However, the number
of contacts is not the only factor which determines the mechanical stability of a heap.
The strength of each contact is another important factor which can vary even when the
number of contacts remains constant. Interestingly, a rough estimate of the length scale $l_z$ which controls the behaviour of $\overline{z}$ gives us $l_z \sim 1.5$, very close to $B_m \sim 1.7$ that we
obtained previously.

3.4. Effect of particle size

Another important and interesting parameter which we expect to affect the piling of
grains is the grain diameter $d$ itself. In general, one expects the angle of repose of a
three-dimensional sandpile not to depend on the grain size, since a pile of smaller grains
transforms into a pile of larger grains via an isotropic re-scaling of the pile coordinates [18].
On the basis of this idea, we expect that in granular Hele–Shaw cells the angle of repose of
a pile will be a function of $w/d$, because the confinement of the pile between two vertical
plates removes the spatial symmetry in the perpendicular direction. As a result, in an
isotropic re-scaling of a sandpile in a Hele–Shaw cell, the gap between walls should be
re-scaled with grain size too.

In order to examine this idea, we performed a series of simulations using the base
parameter values as listed in table 1, but with different grain sizes $d$ and cell thicknesses
$w$, using a linear model. The results are sketched in figure 10, where the behaviour of $\theta_r$
has been plotted against $w/d$, for several values of grain diameters. As anticipated, all
the curves almost collapse into one curve showing that, in general, the angle of repose of a
sandpile in a Hele–Shaw cell does depend on the size of grains. In the range of parameter
values that we used here, the value of $\theta_r$ decays quickly to its asymptotic value $\theta_\infty$ for
$w/d > 20$. This is in agreement with our anticipation that in three dimensions the angle
of repose does not depend on the size of grains. The data collapse in figure 10 implies
that the parameters $\alpha$ and $\theta_\infty$ in equation (9) and $B_m$ in equation (10) do not depend on
the grain size. Furthermore, the value of the characteristic length should be proportional
to the grain size $d$. In the experiments conducted by Grasselli and Herrmann, the values
of $\theta_\infty$ and $\alpha$ turn out to be size independent too. Meanwhile, they did not find any
evidence for a linear dependence of the characteristic length on the grain diameter. In
fact, the characteristic lengths $l$ in their observations were the same for all spherical grain
sizes. This unexpected result could be due to the slight variation in size of the grains
(polydispersity of the granular materials) that they used [1]. It would also be a result of
the cohesive force between grains resulting from the capillary force for humidified grains
or from the van der Waals force for dry grains less than 100 $\mu$m [17].

On the other hand, MD simulations on heaps formed by discharging grains indicate
that $\theta_r$ depends on particle size such that, for a given $w/d$, larger grains have smaller
angles of repose [17]. This is in contrast to our results described above. But as mentioned
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Figure 10. Angle of repose as a function of cell thickness \( w \) scaled with particle size \( d \) from Hookean and Hertzian models. Other parameters are fixed at their basic values as listed in table 1.

earlier, not only the model interactions, but also the formation histories are different in these two simulations. The importance of the latter factor is a well-known experimental fact. Moreover, there are evidences that in the absence of cohesive force between grains or a size-dependent sliding coefficient [30], the size-dependent angle of repose could arise as a result of introducing the rolling friction as Zhuo et al did [17].

3.5. Effects of frictional forces

The friction between grains exhausts the translational and rotational energy of particles. It also affects significantly the mechanical stability of each contact in the sandpile. One expects, therefore, the particle–particle friction coefficient \( \mu_p \) to be one of the key parameters in determining the angle of repose of the pile. To investigate how this variable changes the behaviour of \( \theta_r \), we performed computer simulations for the spherical particles of fixed size with different \( \mu_p \) values using both Hertzian and Hookean models. The other values are as listed in table 1. The results have been presented in figure 11, showing that for both models, the angle of repose increases non-linearly with \( \mu_p \). This effect is in accordance with MD simulations of \( \theta_r \) when the pile forms from discharging materials [3,17].

We have also examined the effect of variation of the wall–particle friction coefficient \( \mu_w \) on \( \theta_r \). This is another important parameter which should affect the angle of repose, as wall friction gives a torque resistance to the rotational motion of grains. The results of simulation of the wall friction coefficient are shown in figure 12. As indicated in the figure, increasing the wall friction can significantly increase the angle of repose. Similar trends have also been observed for the grains of different sizes.
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Figure 11. Angle of repose as a function of $\mu_p$, the coefficient of friction between grains, from Hookean and Hertzian models. Other parameters are fixed at their basic values as listed in table 1.

Figure 12. Angle of repose as a function of wall–particle friction coefficient $\mu_w$ from a Hookean model. Other parameters are fixed at their basic values as listed in table 1.

4. Conclusions

We study the dependence of the angle of repose of a sandpile resulting from pouring granular materials into a Hele–Shaw cell on boundary conditions, particle characteristics, and the other parameters used in the model interaction. We saw that the most important
boundary condition is the cell thickness. The angle of repose decreases with increasing gap width towards a constant value, and the data that we obtained not only fit well with the experimental power-law decay, but also are comparable with the theoretical model of Courrech et al. The same trend has been observed in real experiments and also MD simulation of discharging materials, showing that the effect is rather universal and independent of the formation history of the pile. For cells with a large gap, the angle of repose relaxes to an asymptotic value which should correspond to the angle of repose of an isotropic three-dimensional heap.

At the grain level, the frictional forces are among the most important factors. We observed that increasing particle–particle friction and wall–particle friction coefficient increase the angle of repose non-linearly. But the most interesting microscopic characteristic of the single grains is perhaps the grain diameter \(d\). We found that for a given cell thickness, \(\theta_r\) increases with grain size, but if the wall thickness scales with grain diameter, the angle of repose remains unchanged. This also implies that the angle of repose in the three-dimensional limit does not depend on the size of grains. It should be emphasized that these observations are just valid for the case of cohesionless, mono-sized grains. Therefore, they might be at variance with the results of real experiments, where these conditions are not satisfied or the formation history is different.

Acknowledgments

We would like to thank A Amirabadizadeh, B Haghighi and S M Vaes Allaei for useful discussions. We gratefully acknowledge IASBS parallel computer centre for a generous grant of computer time.

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doi:10.1088/1742-5468/2008/04/P04026
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