Angle of Repose and Angle of Marginal Stability:
Molecular Dynamics of Granular Particles

Jysoo Lee and Hans J. Herrmann

HLRZ-KFA Jülich, Postfach 1913, W-5170 Jülich, Germany

Abstract

We present an implementation of realistic static friction in molecular dynamics (MD) simulations of granular particles. In our model, to break contacts between two particles, one has to apply a finite amount of force, determined by the Coulomb criterion. Using a two dimensional model, we show that piles generated by avalanches have a finite angle of repose $\theta_R$ (finite slopes). Furthermore, these piles are stable under tilting by an angle smaller than a non-zero tilting angle $\theta_T$, showing that $\theta_R$ is different from the angle of marginal stability $\theta_{MS}$, which is the maximum angle of stable piles. These measured angles are compared to a theoretical approximation. We also measure $\theta_{MS}$ by continuously adding particles on the top of a stable pile.

PACS numbers: 46.10+z, 62.20-x
1. Introduction

Systems of granular particles (e.g. sands) exhibit many interesting phenomena. The formation of spontaneous heap and convection cells under vibration, density waves found in the outflow through hoppers and segregation of particles are just a few examples. These phenomena are consequences of the unusual dynamical response of the system. One of the characteristic property of granular systems is that it can behave like both a solid and a fluid. One can pour (like a fluid) sand grains on a table, and they form a stable pile with finite slope (like a solid). Part of the reason why it acts like a solid is due to static friction. By static friction, we mean that one has to apply a force larger than certain threshold in order to break a contact between particles. This threshold is determined by, for example, the Coulomb criterion. Static friction is responsible for many static structures (e.g. sand pile), and have a possible implication in the dynamics of granular systems. Despite its importance, the effect of static friction has been much less studied as compared to other microscopic mechanisms. This is mainly due to the difficulty of including static friction to a theoretical framework or a simulative scheme.

In this paper, we present an implementation of static friction in a molecular dynamics (MD) simulation, which uses a scheme introduced by Cundall and Strack. Using this code, we generate piles by first filling a (two dimensional) box with grains, then removing a sidewall. The slope of the pile is finite, which is related to the finite “angle of repose ($\theta_R$).” Here, tan $\theta_R$ is defined to be the slope of the pile. This angle is strongly dependent on the friction coefficient $\mu$, and rather insensitive to other parameters of the system. Furthermore, we find that the pile obtained above is stable under tilting by an angle smaller than the finite tilting angle $\theta_T$, where $\theta_T$ is typically a few degrees. This suggests that the angle of marginal stability $\theta_{MS}$, the maximum angle of stable piles, is larger than $\theta_R$, which has been observed for real sandpile experiments. We also study the
situation of keeping on adding particles on a stable pile. The angle, at which the pile becomes unstable, can be interpreted as $\theta_{MS}$. We also propose a theoretical method to calculate $\theta_{MS}$ and $\theta_T$ from an approximate stress distribution obtained by Liffman et al.\textsuperscript{24} The theoretical values show similar dependency of the measured angles on the friction coefficient $\mu$.

2. Definition of the model

The interaction between real sand grains is too complicated to construct a model, by which all the properties of a granular system are described accurately. Instead of constructing a model to reproduce all the details from the beginning, it is often advantageous if one identifies the basic ingredients of the system, construct a model with these ingredients. It is often true that the qualitative behavior of a system is independent of the fine details of the model. Some important ingredients for a granular system are (1) repulsion between two particles in contact, (2) dissipation of energy during collision. In certain cases, the rotation of the particles could be important.\textsuperscript{25} In the previous molecular dynamics (MD) simulations of granular systems, most of these ingredients, if not all, are incorporated. For example, the repulsion and dissipation is included in most MD simulations of granular particles.\textsuperscript{10,11,16,18,22,24–27} A few of these simulations also included the rotational degree of freedom.\textsuperscript{16,18,22,24–26} Here, we will construct a model which includes the repulsion, dissipation and static friction. But, the model does not have rotational degrees of freedom.

An individual grain is modeled by a spherical particle. These particles interact with each other only if they are in contact. Consider two particles $i$ and $j$ in contact in two dimension. Let the coordinate for the center of particle $i$ ($j$) be $\vec{R}_i$ ($\vec{R}_j$), and $\vec{r} = \vec{R}_i - \vec{R}_j$. A vector $\vec{n}$ is defined to be a unit vector parallel to the line joining the centers of two particles, $\vec{r}/r$. Another vector $\vec{s}$, which is orthogonal to $\vec{n}$, is obtained by rotating $\vec{n}$ by $\pi/2$ in clockwise direction. We also define the relative velocity $\vec{v}$ to be $\vec{V}_i - \vec{V}_j$, and the
radius of particle $i$ to be $a_i$.

The force on particle $i$ exerted by particle $j$, $\vec{F}_{j\to i}$, can be written as

$$\vec{F}_{j\to i} = F_n\vec{n} + F_s\vec{s},$$

(1)

where the normal force $F_n$ is given by

$$F_n = k_n(a_i + a_j - r)^{3/2} - \gamma_n m_e (\vec{v} \cdot \vec{n}).$$

(2a)

The first term of (2a) is the three-dimensional Hertzian repulsion due to the elastic deformation, where $k_n$ is the elastic constant of the material. The second term is a velocity dependent friction term, which is introduced to dissipate energy from the system. Here, $\gamma_n$ is a constant controlling the amount of dissipation, and $m_e$ is the effective mass $m_i m_j / (m_i + m_j)$. The second term of (1), the shear force $F_s$ is

$$F_s = -\gamma_s m_e (\vec{v} \cdot \vec{s}) - \text{sign}(\delta s) \cdot \min(k_s \delta s, \mu F_n),$$

(2b)

where the first term is a velocity dependent damping term similar to the one in (2a). The second term of (2b) simulates the static friction. The basic idea is the following. When two particles start to touch each other, one puts a “virtual” spring in the shear direction. For the total shear displacement $\delta s$ during the contact, there is a restoring force, $k_s \delta s$, which is a counter-acting frictional force. The maximum value of this restoring force is given by Coulomb’s criterion—$\mu F_n$. When particles are no longer in contact with each other, we remove the spring. We want to emphasize that one has to know the total shear displacement of particles during the contact, not the instantaneous displacement to calculate the static friction. In other words, one has to remember whether a contact is new or old. The rotation of the particles is not included in the present simulation.

The particles can also interact with walls. If particle $i$ is in contact with a wall, the force exerted by the wall on the particle has exactly the same form as eqs. (2) with $a_j = 0$.
and $m_j = \infty$. Also, there is a gravitational field. The force acting on particle $i$ by the field is $-m_i g$. The total force acting on particle $i$ is the vector sum of the particle-particle interaction(s), the particle-wall interaction(s) and the gravitational force.

The trajectory of a particle is calculated by the fifth order predictor-corrector method.\textsuperscript{28} We use two Verlet tables. One is a usual table with finite skin. The other table is a list of pairs of \textit{actually} interacting particles, which is used to calculate the static friction term. For a typical situation, the CPU time needed to run 1372 particles is about 0.01 seconds per iteration on a Cray-YMP, which is comparable to the speed of the layered-link-cell implementation of a short range Lennard-Jones system.\textsuperscript{29,30}

3. Obtaining the angle of repose

As a non-trivial check whether the static friction term is working, we measure $\theta_R$ as follows. We start by randomly putting $N$ particles in a box of width $W$ and height $H$. The particles fall down due to gravity, and loose their energy due to dissipation. After a long time, they fill the box with no significant motion. We show, in Fig. 1(a), an example of the system at this stage. Here, parameters are $\mu = 0.2$, $k_n = 10^6$, $k_s = 10^4$, $\gamma_n = 5 \times 10^2$, $\gamma_s = \gamma_n / 100$, and for walls, $k_n$ is chosen to be $2 \times 10^6$. We checked the motions of the particles by monitoring the total kinetic energy of the system. The average kinetic energy per particle during the whole sequence is shown in Fig. 1(b). The kinetic energy sharply rises when the wall is removed. The pile relaxes in an oscillatory manner (see Fig. 1(b)). Next, we remove the right wall, let the particles move out of the box, and wait until the system reaches a new equilibrium. The figure 1(c) is the equilibrium reached by starting from Fig. 1(a). As shown in the figure, the new state has non-zero slope.

We try a few ways to measure $\theta_R$. We first divide the box into several vertical cells, the width of each cell is equal to the average diameter of the particles. For the center of each cell $x$, we find the maximum position $h(x)$ of the particles in the cell. The line joined
by these positions is a “surface” of the structure. Having determined \( h(x) \), we use three different ways to measure the slope: (1) By joining \( h(0) \) and \( h(W) \), (2) by fitting a straight line to \( h(x) \) using the method of least squares, and (3) by fitting a parabola to \( \sum_{i=0}^{x} h(i) \) by the least squares method. Here, if \( h(i) \) is a straight line, the sum is a parabola. In the case of \( h(x) \) being a straight line, these three methods should give identical results. In our simulation, the slopes obtained by different methods differ from each other by a few degrees. For example, we obtain (1) \( 20.14 \pm 2.15 \), (2) \( 18.90 \pm 1.49 \) and (3) \( 17.88 \pm 1.76 \) for 400 particle system with \( \mu = 0.2 \). Here the angles are averaged over 10 samples. We find, on the average, the angle by method (1) is larger than (2), and (2) is larger than (3), although they are within the error bars of each other. It is quite possible that these differences come from the finite size of the system. From now on, we use only the method 3 for calculating the slope.

4. Parameter dependences

For a fixed set of parameters which specify all the interactions, we study the dependence of \( \theta_R \) on the geometry, namely the aspect ratio \( (H/W) \) of the box and the linear size of the system. The parameters are \( k_n = 10^6, k_s = 10^4, \gamma_n = 5 \times 10^2, \gamma_s = \gamma_n/100 \). For walls, \( k_n \) is chosen to be \( 2 \times 10^6 \) to prevent particles to escape from the box. Since a system of particles with equal radii tends to form a hexagonal packing, we use particles with different sizes. The radii of the particles are drawn from a Gaussian distribution with the mean of 0.1 and width of 0.02, and the maximum (minimum) cut-off radius of a particle is 0.13 (0.07). In Fig. 2(a), we show the dependence of the angle \( \theta_R \) on the height \( H \), for values of \( \mu = 0.2 \) and the width \( W = 2.0 \). Each angle is obtained by averaging over 20 samples. The error plotted in Fig. 2(a) is the mean square sample-to-sample fluctuations. Here, we cannot see any systematic dependence on \( H \). Also for other values of \( \mu \), we find that \( \theta_R \) does not depends on the aspect ratio, as long as the ratio is sufficiently larger.
than the slope of the pile generated. We then fix the aspect ratio to be 2, and study the
dependence on the size of the system. The angle $\theta_R$ for different values of $W$ is shown in
Fig. 2(b). All angles, as well as those presented in Fig. 2(b), are averaged over 20 samples,
unless specified otherwise. For $\mu = 0.2$, these angles decrease for small sizes, and seem to
saturate starting around $W = 3.5$. For larger values of $\mu$, the angle saturates for larger
values of $W$. For example, the angle continues to decrease until $W = 4.0$ for $\mu = 0.3$. On
the other hand, for smaller $\mu$, the angle saturates for smaller $W$. For $\mu = 0.1$, there is no
obvious trend of the data, even up to the very small values of $W = 1.5$. Since we want the
angle obtained by this simulation not to suffer from a finite size effect, we will use in the
followings the values $W = 4$ and $H/W = 1$ to calculate $\theta_R$. We will also study cases of $\mu$
not larger than 0.2. The simulation for larger values of $\mu$ is limited due to the fact that
one needs a larger aspect ratio and system sizes to be free of any finite size effects.

Next, we study how $\theta_R$ depends on the various interaction parameters in the system:
$\gamma, k$ and $\mu$. In a static configuration, the damping term is absent, so ideally $\gamma$ terms do not
change $\theta_R$. However, since we prepared the sandpile by a dynamical method (by causing an
avalanche), the angle may depend on $\gamma$. Also, $k_s$ is an the elastic constant of the artificial
spring we introduced, so it should not make a difference in a static configuration, as long
as we keep the value in a reasonable range. The quantity of particular interest is the
friction coefficient $\mu$, since $\mu$ determines if contacts between particles are stable ("stick")
or unstable ("slip"). Since the stability of the whole structure (e.g. a pile) will be strongly
influenced by that of individual contacts, we expect $\theta_R$ will be strongly dependent on $\mu$.
For example, $\theta_R$ should be zero for $\mu = 0$, if the individual grains in the pile are not
moving. We first study the effect of $k_n$ and $\gamma_n$ on $\theta_R$. We will limit ourselves only to
study the general trend such as the direction and the order of magnitude of the changes.
We also fix $\mu = 0.2$. We measure the angle (inside parenthesis) for three different values
of $k_n$, $10^4$ (16.53 ± 0.73), $10^5$ (18.65 ± 0.70) and $10^6$ (17.99 ± 0.64). The difference in
angle is very small, and there seems to be no systematic dependency. For three values of
\( \gamma_n = 50, 100, 500 \), the angles are \( 16.47 \pm 0.75, 17.15 \pm 0.62, 17.99 \pm 0.64 \). The angle seems to decrease systematically, as \( \gamma_n \) is being decreased. However, the magnitude of the changes is still small (\( \sim 5\% \)).

Now, we study the effect of \( \mu \). In Fig. 3, we show \( \theta_R \) obtained for several different values of \( \mu \). In the range of \( \mu \) we studied, there seems to be a linear relation between the angle and \( \mu \). This relation can be true for small values of \( \mu \), but it cannot be true for the entire ranges of \( \mu \). The maximum \( \theta_R \) is limited to 90 degrees, while the value of \( \mu \) can be arbitrarily large. We will come back to discuss this relation later. Note that there are two friction coefficients in the system, one between particles and another between particles and walls. We will argue that, for a sufficiently large pile, the friction coefficient which determines \( \theta_R \) is that between the particles. Consider a sandpile on a table. The stress distribution near the top part of the pile would not be altered by the stress distribution at the bottom of the pile. Therefore, only the friction coefficient between particles can change \( \theta_R \) in this region. On the other hand, the stress distribution near the bottom of the pile will greatly be influenced by the particle-wall friction coefficient. So, we expect the angle be different near the bottom of the pile, if the friction coefficients are different from each other.

The piles discussed above are generated by causing avalanches. In experiments, the structure just after an avalanche (e.g. Fig. 1(c)) is not critical, but stable. In other words, one must apply an additional finite force to make the structure unstable. One way to apply the force is by tilting the box which contains the pile. The tilting angle \( \theta_T \) is defined as the rotation angle at which the pile becomes unstable. We want to emphasize that \( \theta_T \) is shown to be non-zero for real sandpile experiments. We measure the tilting angle for our model as follows. Starting from the pile like one in Fig. 1(c), we rotate clockwise the whole box with a constant rate of \( 10^{-3} \) degree/iteration. Then, we record the angle at which the pile starts to move, which is defined as the tilting angle \( \theta_T \). The tilting angle for several
values of $\mu$ is shown in Fig. 4. Here, the width of the box $W$ is 4, and the aspect ratio is 1. Indeed, one needs a finite tilting angle for the piles generated using our model, and it gives us confidence that the model studied here is reproducing the behavior of realistic static friction. The finite $\theta_T$ implies that the pile is stable (not critical), therefore $\theta_{MS}$ should be larger than $\theta_R$.

5. Pile with constant flux

In the previous section, we argued that $\theta_R$ is smaller than $\theta_{MS}$ based on the fact that the pile is stable even if it is tilted by a finite angle smaller than $\theta_T$. We now propose a method of obtaining the angle of marginal stability as well as the angle of repose. Consider an empty box without a right wall, and put one layer of particles at the bottom. We monitor the maximum velocity of the particles. If the maximum velocity is smaller than certain value $v_{cut}$, then we insert a new particle at the upper left corner of the pile. Once the particle is added, we then wait until the maximum velocity of particles is again smaller than $v_{cut}$, then add a new particle. This procedure is repeated long time for good statistics. In Fig. 5, we show the angle of the pile just before one inserts a new particle. Here, $\mu = 0.2$, $W = H = 4.0$ and $v_{cut} = 0.1$. We also simulate the system with $v_{cut} = 0.01, 0.001$, and find no essential difference. The angle is zero at the beginning, and increasing until it seems to just fluctuate for iterations larger than $4 \times 10^5$. The curve shown in the figure is quite noisy, which suggests that many configurations (or packings) are possible in the steady state. The maximum angle of the pile one can build up before avalanches is larger than the $\theta_R$ obtained before. This could be an additional evidence that our model reproduces the difference between $\theta_{MS}$ and $\theta_R$. We can estimate the difference to be of the order of distance between two dotted lines in Fig. 5. Here, the dotted lines represents the mean square fluctuations of the angle.

6. Theoretical approach
In the previous section, we measured various angles $\theta_R$, $\theta_T$ and $\theta_{MS}$ for the model sand. How can we understand these angles? In order to calculate these angles, one should know the stress field inside the pile. Liffman et al.\textsuperscript{24} suggested an approximate way of calculating the field in a packing of equal sized spheres, which is illustrated in Fig. 6. In order to calculate the stress at a point $O$, one draws two lines of slope $\sqrt{3}$ (line $OA$) and $-\sqrt{3}$ (line $OB$) starting from the point $O$. Then, the length of the lines ($l_A$ and $l_B$) within the pile (and above the point) is approximately proportional to the force exerted by the pile. For a more detailed explanation as well as for the justification of this procedure, see Ref. 26. From this stress field, we calculate $\theta_{MS}$ as follows. Consider a point at the bottom of the pile. The normal (to the bottom surface) force at that point is $(l_A + l_B) \sin(\pi/3)$, while the tangential force is $(l_A - l_B) \cos(\pi/3)$. We then apply the Coulomb criterion. If the ratio of the tangential to the normal force is larger than $\mu$, the contact is unstable. In this way, for given $\mu$, we obtain the range of angles at which the pile is stable. The largest angle at which the pile is stable is the angle of marginal stability, which is

$$\theta_{MS} = \tan^{-1}(3\mu).$$

Since $\theta_R + \theta_T$ is approximately the angle of marginal stability, we plot both measured $\theta_R + \theta_T$ and calculated $\theta_{MS}$ by the above procedure in Fig. 7(a). The difference between the two angles is either due to the fact $\theta_{MS} \neq \theta_R + \theta_T$ or the error of the approximation. In fact, the approximation (and $\pi/3$ angle) is derived from an ordered packing of the particles with same radius. It is possible that the stress field in a disordered packing is very different from that of an ordered one. In that case, one needs a new approximation scheme to calculate the stress field. We also calculate $\theta_T$ for given angle of repose $\theta_R$ and $\mu$. It is given by

$$\mu = \frac{R \cos(\pi/3 - \theta_T) - \cos(\pi/3 + \theta_T)}{R \sin(\pi/3 - \theta_T) + \sin(\pi/3 + \theta_T)},$$

where

$$R = \frac{\tan(\pi/3 + \theta_T) + \tan(\theta_R)}{\tan(\pi/3 - \theta_T) - \tan(\theta_R)} \cdot \frac{\cos(\pi/3 + \theta_T)}{\cos(\pi/3 - \theta_T)}.$$
The $\theta_T$ obtained by eq. (4) as well as the measured tilting angle are plotted in Fig. 7(b). One can also see that the difference between the two is small. Unlike the difference in Fig. 7(a), these two angles should coincide if the stress distribution is calculated correctly. The main point of presenting the theoretical approach is to show a “first” approximation for the problem, not to do quantitative comparison between the measured and calculated angle. In order to obtain more accurate numbers, one has to know a better way of calculating the stress field inside the pile. However, it is encouraging to see that even the values obtained by the first approximation are comparable to the measured ones.

Acknowledgments

We thanks for many informative discussions with G. Ristow.
References

1. S. B. Savage, Adv. Appl. Mech. 24, 289 (1984); S. B. Savage, Disorder and Granular Media ed. D. Bideau, North-Holland, Amsterdam (1992).

2. C. S. Campbell, Annu. Rev. Fluid Mech. 22, 57 (1990).

3. H. M. Jaeger and S. R. Nagel, Science 255, 1523 (1992).

4. P. Evesque and J. Rajchenbach, Phys. Rev. Lett. 62, 44 (1989).

5. C. Laroche, S. Douady and S. Fauve, J. Phys. (France) 50, 699 (1989).

6. E. Clement, J. Duran and J. Rajchenbach, preprint.

7. G. Rátkai, Powder Technol. 15, 187 (1976).

8. S. B. Savage, J. Fluid Mech. 194, 457 (1988).

9. O. Zik and J. Stavans, Europhys. Lett. 16, 255 (1991).

10. J. A. C. Gallas, H. J. Herrmann and S. Sokolowski, Phys. Rev. Lett., in press.

11. Y-h. Taguchi, preprint.

12. J. O. Cutress and R. F. Pulfer, Powder Technol. 1, 213 (1967).

13. E. B. Pittman and D. G. Schaeffer, Comm. Pure Appl. Math. 40, 421 (1987).

14. G. W. Baxter and R. P. Behringer, T. Fagaert and G. A. Johnson, Phys. Rev. Lett. 62, 2825 (1989).

15. H. Caram and D. C. Hong, Phys. Rev. Lett. 67, 828 (1991).

16. G. Ristow, J. Physique I, 2, 649 (1992).

17. J. C. Williams, Powder Technol. 15, 245 (1976).

18. P. K. Haff and B. T. Werner, Powder Technol. 48, 239 (1986).
19. A. Rosato, K. J. Strandburg, F. Prinz and R. H. Swendsen, Phys. Rev. Lett. 49, 59 (1987).

20. P. Devillard, J. Phys. (France) 51, 369 (1990).

21. For example, it is argued that the density waves formed in Ref. 14 are due to “arching,” which is a consequence of static friction. See also, “bridge-collapsing” in shear cells [Y. M. Bashir and J. D. Goddard, J. Rheol. 35, 849 (1991)].

22. P. A. Cundall and O. D. L. Strack, Géotechnique 29, 47 (1979).

23. See, e.g., B. J. Briscoe, L. Pope and M. J. Adams, Powder Technol. 37, 169 (1984).

24. K. Liffman, D. Y. C. Chan and B. D. Hughes, preprint.

25. C. S. Campbell and C. E. Brennen, J. Fluid Mech. 151, 167 (1985).

26. P. A. Thompson and G. S. Grest, Phys. Rev. Lett. 67, 1751 (1991).

27. D. C. Hong and J. A. McLennan, preprint.

28. D. J. Tildesley and M. P. Allen, Computer Simulations of Liquids, Oxford University Press, Oxford (1987).

29. G. S. Grest, B. Dünweg and K. Kremer, Comp. Phys. Comm. 55, 269 (1989).

30. B. Dünweg, private communication.
Figure Captions

Fig. 1: (a) Box filled with $N = 1600$ particles just before the right wall is removed. The thickness of the lines between centers are proportional to the normal force. (b) Average kinetic energy per particle (in erg) during the whole sequence of simulation. The energy initially increases as particles fall down, then decays with time. When the right wall is removed (iteration = 30000), it increases again. (c) Static pile obtained after the avalanche.

Fig. 2: (a) The angle of repose $\theta_R$ vs the height $H$ with the width $W = 2$ and $\mu = 0.2$. The angle seems just fluctuate, and no systematic dependency is found. (b) The angle of repose $\theta_R$ vs $W$ for several values of $\mu$: $\mu = 0.1$ (diamond), 0.2 (box) and 0.3 (circle). Here, the aspect ratio is kept to be 2.

Fig. 3: The angle of repose $\theta_R$ vs $\mu$ with $W = H = 4$.

Fig. 4: The tilting angle $\theta_T$ vs $\mu$ with $W = H = 4$.

Fig. 5: The angle of pile measured when we add a new particle to the pile. The two dotted lines indicate the width of the fluctuation.

Fig. 6: The stress at a point inside the pile is approximately the vector sum of line $A$ and $B$.

Fig. 7: (a) The measured $\theta_R + \theta_T$ and the calculated $\theta_{MS}$ is shown for several values of $\mu$. There is a difference between the two. (b) The measured and calculated $\theta_T$ for different values of $\mu$. The difference is smaller than that of (a).