Static Friction Phenomena in Granular Materials: Coulomb Law
vs. Particle Geometry

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(March 23, 2022)

Abstract

The static as well as the dynamic behaviour of granular material are determined by dynamic and static friction. There are well known methods to include static friction in molecular dynamics simulations using scarcely understood forces. We propose an Ansatz based on the geometrical shape of nonspherical particles which does not involve an explicit expression for static friction. It is shown that the simulations based on this model are close to experimental results.

PACS numbers: 05.60, 47.25, 46.10, 02.60

Typeset using REVTEX
The behaviour of fluidized dry granular material, like sand or powder, reveals a rich variety of effects, which can not be observed in other substances. Those effects have been observed and investigated by many scientists over a long period [1]–[4]. Examples for the most interesting effects are fluidization, convection cells and heap formation under vibration [2]–[4], size segregation (“Brazil–nut” effect) [10]–[12], deformation under shear force [13], shape segregation of differently shaped grains in a pipe [14] and clustering instabilities [15]. Density waves emitted from outlets [16] inside material flowing through pipes [17] and at the surface of an inclined chute [18] have been intensively investigated. Recent results gave evidence that convection cells due to walls or amplitude modulations play an important role in the process of the formation of macroscopic structures [1]. Of particular interest are the dynamic as well as the static behaviour of avalanches going down the slope of a sand pile. Theoretical as well as experimental investigations [19]–[23] led to the hypothesis that their mass and their time distributions can be described by the self organized criticality–model. There are experiments, however, that do not agree with this hypothesis [6] [24]. Recently many experimental observations have been reproduced by numerical simulations. There is a wide variety of simulation methods including Monte–Carlo simulations (e.g. [11]), molecular dynamics simulations (e.g. [4] [10] [14]), and random walk approaches [25]. These simulations gave many interesting information on the microscopic effects underlying the behaviour of macroscopic amounts of granular material. Many of the effects observed in experiments are consequences of static friction between the grains. In most of the current simulations special terms for static friction are used to mimic static behaviour of granular material e.g. [4] [26]. The aim of this paper is to show that it is possible to reproduce the experimental results by molecular dynamics simulations without introducing such a static friction force but by simulating nonspherical particles. We show that our simulations with nonspherical particles agree better with experimental results than equivalent simulations introducing static friction forces as it is usually done.

Since it is extremely complicate to calculate collisions of cubic particles we choose in two dimensions particles similar to squares but consisting of spheres. A further advantage of
this model is that we are able to vary the shape steadily from a sphere almost to a square. A related Ansatz for nonspherical grains was recently done by Gallas and Sokolowski [27], there each grain consists of two spheres rigidly glued to each other. Each of our nonspherical particles $k$ consists of four spheres with equal radii $r_i^{(k)}$, located at the edges of a square of size $L^{(k)}$, and one sphere with radius $r_m^{(k)} = L^{(k)}/\sqrt{2} - r_i^{(k)}$ in the middle of the square (fig. 1). For the case that two spheres $i$ and $j$ of the same particle $k$ or of different particles touch each other during a collision there acts the force

$$\vec{F}_{ij}^C = \left[ Y(r_i + r_j - |\vec{x}_i - \vec{x}_j|) + \gamma m_{\text{eff}} |\dot{\vec{x}}_i - \dot{\vec{x}}_j| \right] \frac{\vec{x}_i - \vec{x}_j}{|\vec{x}_i - \vec{x}_j|}$$

with $m_{\text{eff}} = \frac{m_i \cdot m_j}{m_i + m_j}$

where $Y$ is the Young modulus and $\gamma$ is the phenomenological friction coefficient. In addition to the forces between each two particles of the system, there are forces between each pair of spheres $i, j$ where $i$ and $j$ both belong to the same grain, due to a damped spring

$$\vec{F}_{ij}^S = \left[ \alpha (C^{(k)} - |\vec{x}_i - \vec{x}_j|) + \gamma_{\text{Sp}} \frac{m_i}{2} |\dot{\vec{x}}_i - \dot{\vec{x}}_j| \right] \frac{\vec{x}_i - \vec{x}_j}{|\vec{x}_i - \vec{x}_j|}$$

where $\alpha$ and $\gamma_{\text{Sp}}$ are the spring constant and the damping coefficient. If the spheres $i$ and $j$ are both located at the same edge of the square then $C^{(k)}$ equals $L^{(k)}$, if $i$ is the central sphere then $C^{(k)} = L^{(k)}/\sqrt{2}$.

The dynamics of large numbers of such nonspherical particles was investigated simulating the flow of granular material in a rotating cylinder under gravity. For the integration we used a sixth order predictor-corrector method [28]. In a cylinder of diameter $D = 260$ we simulated the flow of 1000 nonspherical particles of different size $L^{(k)}$ with Gaussian probability distribution $p(L^{(k)}) = N(3, 1)$ each consisting of five spheres. For the parameters we chose $Y = 10^4 \text{ kg/s}^2$, $\gamma = 1.5 \cdot 10^4 \text{ s}^{-1}$, $\alpha = 10^4 \text{ kg/s}^2$, $\gamma_{\text{Sp}} = 3 \cdot 10^4 \text{ s}^{-1}$ and $r_i^{(k)} = 1/4 \cdot L^{(k)}$. The cylinder consists of spheres with different radii to mimic a rough surface. The mean value of these spheres equals the mean value of the $L^{(k)}$. The cylinder was rotated clockwise with very low angular velocity $\Omega$. During the uniform rotation of the cylinder the flow of
the grains was very inhomogeneous, due to avalanches going down the inclined surface. This
behaviour is called stick–slip motion. The time evolution of the slope $\Theta$ of the surface as
well as the averaged velocity $\bar{v}$ of the particles at the surface for a fixed angular velocity
$\Omega = 0.002 \, s^{-1}$ are drawn in fig. 2 (curves $v(a), \Theta(a)$). The angle was plotted in rad, $\bar{v}$
in $50 \cdot s^{-1}$. Since the number of particles is not too large our surfaces are not smooth.
Hence we have to determine the inclination indirectly as the angle between the straight
line connecting the centre of mass point of the grains and the middle point of the rotating
cylinder and the direction of gravity. The angle and particularly the average velocity of the
surface particles fluctuate drastically and irregularly as it is typical for stick–slip motion.
This behaviour was observed experimentally before by Briscoe, Pope and Adams [29] and
by Rajchenbach [30]. The plots $v(b), \Theta(b)$ in the same figure show the equivalent data for
the simulation using spherical particles. The radii of the spheres were Gauss-distributed too
with $p(r_i) = N[1, 1]$. The spherical grains undergo the same force as the spheres of which the
nonspherical particles consist. To mimic static friction we include for the case of spherical
particles rotation as a further degree of freedom of the grains and add the force

$$\vec{F}_{sf}^{ij} = \min\{ -\gamma_s m_{eff} |\vec{v}_{rel}|, \mu |\vec{F}_{ij}^C| \} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} \vec{x}_i - \vec{x}_j \\ |\vec{x}_i - \vec{x}_j| \end{pmatrix},$$

with

$$\vec{v}_{rel} = (\vec{x}_i - \vec{x}_j) + r_i \cdot \vec{\omega}_i + r_j \cdot \vec{\omega}_j,$$

where $\vec{\omega}_i$ is the angular velocity of the $i$-th particle, $\gamma_s$ is the shear friction coefficient, and $\mu$
is the Coulomb parameter ($\gamma_s = 3 \cdot 10^4 \, s^{-1}$, $\mu = 0.5$). This Ansatz is the most popular to include
static friction between particles which roll on each other into the expressions for the forces
used in molecular dynamics simulations. It was introduced by Cundall and Strack [4] and
modified by Haff and Werner [10]. Most of the molecular dynamics simulations of granular
material base on this Ansatz. The force $\vec{F}_{sf}^{ij}$ was implemented only for the simulation of
spherical grains but not for the nonspherical.

Obviously the qualitative behaviour of the slope $\Theta$ resemble each other in both simu-
lations but quantitatively we get for nonspherical grains more than twice the mean angle
(Θ_{ns}) than for spherical (Θ_{sp}). For very low rotation velocity Ω = 2 \cdot 10^{-3} we found Θ_{sp} = 7^\circ and Θ_{ns} = 19^\circ. In the experiment [30] was measured Θ ≈ 27^\circ. The average velocity of the surface grains differs significantly too for both cases. The typical avalanches in the case of nonspherical particles cannot be observed for spheres. The curve \( \bar{v}(b) \) is much smoother. In the experiment one observes stick–slip motion [30]. Fig. 3 shows the slope Θ of the surface as a function of the angular velocity of the cylinder Ω for both nonspherical and spherical grains. In both cases the curves are close to a straight line. For much higher angular velocities than used in our simulations the grains do not move stick–slip like but continuously. In this regime was experimentally found Ω \sim (Θ − Θ_c)^m, with m = 0.5 ± 0.1 [30]. With the same Ansatz we find m ≈ 1.25 for the stick–slip regime. As shown above the simulation with nonspherical grains coincides much better with the experimental observations than equivalent simulations using spheres.

In our second simulation we investigate the evolution of a stable pile of granular material by continuously dropping particles on the top of the pile due to the experiment of Held et al. [21]. Beginning with an empty rough plane we drop the next particle when the maximum velocity vanishes, i.e. when it is smaller than a given very small threshold \( v_{max} \ll 1 \). The rough plane was simulated by a chain of fixed spheres of random radii with mean \( r_i = L^{(i)} \) where \( L^{(i)} \) is the size of the \( i \)--th nonspherical grain. The parameters of the simulation were the same as in the previous experiment.

During the simulation we noticed that the slope of a pile of nonspherical grains does not depend on the number of particles. For spherical grains, however, the heap dissolves under gravity, i.e. the slope decreases with increasing particle number. There are molecular dynamics simulations of stable piles with spherical grains, e.g. [26], but there the particles are not allowed to roll on each other, hence they can only slide, this behaviour does not correspond to experimental reality.

If the platform above which the heap is built up has a finite length \( P \) one can investigate the fluctuations of the mass \( m_h \) of a heap of definite size and the distribution of the size of
the avalanches, i.e. the mass fluctuations of the heap. In fig. 4 is drawn the time series of the mass $m_h$ for fixed $P$. The mass fluctuates irregularly due to avalanches of different size going down the surface of the heap. The size distribution of the avalanches follow a power law, fig. 5 shows the log–log–plot of the spectrum. For the exponent $h(N_A) \sim (N_A)^m$ we found $m \approx -1.4$. The experiments yield $m \approx -2.5$ [21] and $m \approx -2.134$ [22]. For the case of spherical grains we cannot find avalanches.

The ratio between the size of a grain and the radii of the spheres at the corners determines whether the grains shape is closer to a sphere or to a square. Hence we define a shape value

$$S = 1 - \frac{R_{\text{min}}^{\text{cc}}}{R_{\text{max}}^{\text{cc}}},$$

where $R_{\text{min}}^{\text{cc}}$ and $R_{\text{max}}^{\text{cc}}$ are the extremal values of the distance between the convex cover of the nonspherical grain and its central point (fig. 3). For the limit $S \to 0$ the grains have the shape of spheres. The function reaches its maximum $S_m = 0.255$ for a grain which convex cover is most similar to that of a square. To investigate the influence of the the shape $S$ of the grains on the result of the simulations we have to scale the density $\rho$ of the material the grains consist of to ensure that the total mass of each grain remains constant. Fig. 6 shows the angle of the heap as a function of the shape $S$. For grains with shape $S = S_m$, which corresponds to $(L^{(k)}/r_i^{(k)})_{S_m} = 9.66$, the inclination of the heap reaches a maximum too. The angle $\Phi \approx 23.1^\circ$ agrees with experimental data, Bretz et. al. [22] found $\Phi \approx 25^\circ$. Each other value $S$ corresponds to two different particle shapes both closer to a sphere than the $S_m$–particle. The values marked by $\odot$ are due to grains with $L^{(k)}/r_i^{(k)} \leq (L^{(k)}/r_i^{(k)})_{S_m}$, + designates the slope of the heap for particles with $L^{(k)}/r_i^{(k)} \geq (L^{(k)}/r_i^{(k)})_{S_m}$. As expected the slope $\Phi$ of the heap rises with growing $L^{(k)}/r_i^{(k)}$ up to $S$ reaches its maximum $S = S_m$. For larger ratios $L^{(k)}/r_i^{(k)} (S < S_m)$ the slope $\Phi$ decreases. The dashed line in fig. 6 displays the inclination $\Phi_{sp}$ we measured for a heap of spheres, which corresponds to $S \to 0$. The value $\Phi_{sp}$ gives a lower boundary for the slope. The observed $\Phi$ values for $S \in (0,S_m)$ lie between $\Phi_{sp}$ and $\Phi(S_m)$. The calculation for the data shown in fig. 6 are very computer time consuming. For this reason we are not able to present more data.
The simulations described above demonstrate that nonspherical grains are able to describe the static behaviour of granular materials, such as stick–slip motion in a rotated cylinder at very low angular velocity and the angle of repose of a sandpile. It is shown that equivalent simulations with spherical grains and an additional term which describes the static friction due to the Coulomb law could neither reproduce the experimental results for stick–slip motion nor for the angle of repose of a sand pile. The angle of repose reaches its extremal value for grains which shape is close to a square.

Hence we conclude that our microscopic model of nonspherical grains supplies a possible description of the static behaviour of a granular material. The results regarding non–sphericity agree well with those in [27].

The authors thank J. A. C. Gallas and H. J. Herrmann for stimulating and enlightening discussions.
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FIGURES

FIG. 1. Shape of a nonspherical particle.

FIG. 2. Time evolution of the slope $\Theta$ of the surface and the averaged velocity $\bar{v}$ of the particles at the surface of the flow for nonspherical (a) and spherical (b) grains. Due to avalanches $\bar{v}$ fluctuates significantly, while in case (b) occur only very small avalanches.

FIG. 3. The inclination $\Theta$ of the surface as a function of the angular velocity $\Omega$ of the cylinder.

FIG. 4. Total mass of a pile of nonspherical grains on a platform of finite length $P = 820$.

FIG. 5. Size distribution of the avalanches. The line displays the function $h(N_A) = (N_A)^{-1.4}$.

FIG. 6. Slope $\Phi$ of a heap over the shape value $S$ for grains with $L^{(k)}/r_i^{(k)} \leq (L^{(k)}/r_i^{(k)})_{S_m}$ (⊙) and $L^{(k)}/r_i^{(k)} \geq (L^{(k)}/r_i^{(k)})_{S_m}$ (+). The dotted line leads the eye to the function $\Phi = 130 \cdot S + \text{const}$. The dashed line displays the inclination observed in simulation with spherical particles.