Dependence of the angle of repose of heaps on the particle shape (Mathematical Aspects of Pattern Formation in Complex Fluids)

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Dependence of the angle of repose of heaps on the particle shape

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Abstract
We investigate the dependence of the angle of repose for heaps of dry granular materials for heaps built from polygons which flow out of a hopper. We report the parameter dependence on inter-particle friction and particles shape. For any elongation, the angle of repose depends crucially on the coefficient of (dry/Coulomb) friction. For non-elongated particles, the angle of repose depends crucially on the number of corners of the particles.

1 Introduction
In this article we investigated the different parameters influence on the angle of repose. In both experiments and simulation via the discrete element method (DEM), the angle of repose, a fundamental quantity for the experimental classification of granular materials, depends crucially on the particles properties. Previous simulations for the angle of repose of dry granular materials used compositions of round particles and neglected friction [1, 2] (see Fig.1) or the rotational degree of freedom [3]. As a result, the slopes of the heaps were not smooth and straight, but rough and curved, which is typical for wet/cohesive, not for dry granular materials [5, 6, 7]. These simulations resorted to using rough grounds to retain a certain verisimilitude, though heaps of dry sand can be built even on mirrors, which are "microscopically" flat. The models neglect friction an rely on the interlocking of grain surfaces, so that rough grounds are necessary to obtain plausible looking results.

2 Setup of the Simulation
We simulate the sand heap in two dimensions as an aggregate of polygons. The particles have three degrees of freedom, two for the linear motion, one for the rotation. The polygons are inscribed into ellipses with varying length, for non-elongated particles into circles. The particles are simulated as "soft" particles, so that the force between neighboring particles is computed proportional to their overlap area and their Young modulus. Further components of the inter-particle-forces are the coefficient of restitution < 1 and the Coulomb friction coefficient. The forces are used for the Integration of Newton's Equations of Motion, the integration by Gear Predictor-Corrector / Backward Difference Formula (for details, see Ref. [4]).
2.1 Particle interaction

We limit our investigation to convex polygons. Though the simulation of concave polygons poses no problem in principle, a concave surface increases the number of parameters in the model, and as initial investigation, we prefer the rather overseizable parameters of friction, elongation and number of corners. The particle shape is obtained by inscribing polygons in circles/ellipses for non-elongated/elongated particles respectively. In the following, we will speak of non-elongated particles if the polygons were inscribed into circles. We will call the ratio between the longer and the shorter half axis the particles have been inscribed in their "elongation" for brevity sake. This allows to vary the corner number/ "roughness" of the particles: More corners result in a smoother rounding of the particle outline, see Fig. 2. The corners for polygons with $n$ sides are chosen by increments in $360/n \pm 10\%$ with a fixed size dispersion (see section ). The particles move according to Newton's equations of motion with interaction laws resulting from elastic interaction (Young's modulus, $10^7$ N/m for all simulations), Coulomb friction and coefficient of restitution [8]. The number of particles in the simulation was about 4900.

![Figure 2: Construction of polygons from ellipses of various elongations, non-elongated particle with six corners, elongated particle with six corners, non-elongated particle with twelve corners and elongated particles with twelve corners (from left to right).](image)

![Figure 3: Initial state (left) and end configuration (right) of a simulation for the computation of the outflow from a hopper on a non-rough ground with friction coefficient $\mu = 0.6$. The slopes are straight, as in experiments with non-spherical particles. Particles in the same layer have the same shade of gray, mixing of shades in the end configuration indicates mixing of layers.](image)

2.2 Simulation Geometry

The particle are initialized above a hopper geometry (see Fig.3) and fall down at the beginning of the simulation. During the simulation, they aggregate on the hopper surface and slide down the slopes of the hopper. The walls which limit the simulation geometry and which form the hopper have for simplicity the same simulation parameters as the particles, i.e. the same Young modulus, coefficient of restitution and friction coefficient.
2.3 Computation of the angle of repose

Because the slopes in our simulations are straight, the angle of repose can be obtained by a least-squares fit (see Fig. 4) to the center of mass of the highest particles in each segment of \( \approx 0.5 \) particle diameters length. The left and right slope of each realized heap (initial particle configurations computed from different random number sequences, i.e. the shapes of the particles, but not the size distributions, were slightly different for each run) were treated as independent configurations.

2.4 Particle size distribution

Mono-disperse particle distributions result in local ordering of particles, which are absent in most real granular materials, except e.g. mono-disperse glass beads, where the particles in a heap order like in a crystal structure. The possibility of sliding along the crystal axis reduces the stability of the heap, so we use a polydisperse particle ensemble. An example for a typical size distribution can be seen in Fig. 5.

3 Coefficient of Friction and Angle of Repose

In granular materials, particles can either move by rolling or sliding. If the coefficient of friction is over a certain threshold, the particles prefer to move by rolling, if the particles are too rough or too elongated, they do not role, but slide. Whereas for small friction
coefficients, also sliding on the ground can occur, for large coefficients of friction the buildup of the heaps takes only place via avalanches on the heap surface.

For non-elongated polygons with five corners, we computed the dependence of the angle of repose on the friction coefficient (see Fig. 7). The average angle of repose increased linearly between $\mu = 0.2$ and $\mu = 0.4$ and saturated beyond $\mu \geq 0.5$. The reason for the saturation is, that the particle rotation and friction "compete" as causes for the motion of the particles: For vanishing friction coefficients, the angle of repose can be extrapolated to 0 within error bars, consistent with the truism that materials with vanishing Coulomb friction (fluids) don't form heaps.

Figure 7: Dependence of the angle of repose on the coefficient of friction for nearly-regular pentagons.

4 Particle roughness

Though the literature of granular matter abounds with simulations of round particles, in this section we want to investigate the effect of deviation from the round shape in the absence of a particle elongation, which, in a certain way, is the roughness of the particles.
The character of sphericity or nonsphericity is crucial in the formation of the angle of repose: Whereas for polygons for five corners any rolling can be thought to be essentially suppressed, especially on the ground, for the "nearly round" particles, rolling is very likely.

4.1 Number of corners and the Angle of Repose

In this section, we explore the effect of number of corners on the angle of repose for non-elongated particles (nearly-regular polygons inscribed into a circle). The friction coefficient for the simulations with which Fig. 8 was obtained was set to $\mu = 0.6$, well in the regime where no change was observed any more in the previous section.

From five to eight corners, the angle of repose decays practically linearly, and for larger corner numbers stays essentially constant. For 10 and 15 corners the outer particles already touch the walls, so that the data are unreliable. The remarkably small angle of repose for a heap made of polygons with 25 corners, nearly round particles, can be seen in Fig. 9.

Figure 8: Dependence of the angle of repose on the number of corners of non-elongated nearly regular polygons, averages and errorbars calculated for six slopes /independent configurations, $\mu = 0.6$.

Figure 9: Final configuration of a simulation with non-elongated polygons with 25 corners and coefficient of friction $\mu = 0.6$. 
4.2 Effect of elongation 1.2

For finite elongations, the angle of repose increases for particles with many corners because the tendency to roll is suppressed in comparison to non-elongated particles. For elongation 1.2 (for a snapshot of the particles, see Fig. 10, left) the angle of repose decays linearly from 5 to 10 corners, and from 10 to 15 corners decays hardly any more. The critical angles are higher than for non-elongated particles with the same number of corners.

Figure 11: Dependence of the angle of repose for elongated particles with friction coefficient $\mu = 0.6$. (a) Dependence of the angle of repose on the number of corners for polygons with elongation 1.2, averages and error-bars calculated for six slopes /independent configurations. (b) Dependence of the angle of repose for particles on the number of corners with elongation 1.4, error-bars for up to 10 configurations.
4.3 Effect of elongation 1.4

For larger elongations (elongation 1.4 in Fig. 10, left), in contrast to elongations of 1.2 and smaller, there is no significant dependence of the critical angle on the number of corners any more (Fig. 11(b)). That means that for the elongation 1.4, the rolling is already essentially suppressed, the sliding dominates and the particle roughness does not play a crucial role in the mobilization of rolling.

![Graph showing critical angle vs number of corners]

Figure 12: Final configuration for coefficient of friction $\mu = 0.2$, particle elongation 1.4 and five corners: Most of the bulk is fluidized, but in the middle below the opening of the hopper, a heap with straight slopes is still recognizable.

4.4 Effect of a rough floor

We tried to speed up the simulation by putting particles in a layer on the ground to increase the energy dissipation, which did not work out well. In the formation of the heap on the lower layer, both sliding of the damping layer and avalanching of the particles coming from above happen simultaneously. As can be seen in Fig. 13, the slopes are not straight and the angle of repose is not well defined. As the damping layer constitutes a rough ground (albeit a moving one), this result indicates how rough bottoms in simulations may distort the results.

In Fig. 12, we used elongated particles with a very small $\mu = 0.2$ coefficient of friction. The angle of repose is not measurable from the ground: The particles touch the walls and form a nearly horizontal layers. Only on this rough layer, a heap forms in the middle under the hopper which has a measurable angle of repose, due to the rough granular layer below, not due the particle interactions with the ground.
5 Conclusion

In this work we discussed the effect of the shape of particles on the angle of repose, a paradigm on the competition between rolling and sliding in granular materials. We have shown that the angle of repose for dry granular materials depends crucially on the shape of the particles and the Coulomb friction coefficient. For non- or moderately elongated particles (i.e. up to an elongation 1.2), we found a strong dependence of the angle of repose on the particle roughness, i.e. for our polygonal particles the angle of reposed decreased with increasing number of corners. This result is in marked contrast to the results for triaxial compression, where one finds hardly any dependence of the stress-strain-diagram on the particle roughness [8]. For larger elongations, the effect of the particle roughness on the angle of repose is suppressed, because no rolling takes place anyway. In this case, the angle of repose is mostly dependent on the coefficient of friction.

Simulations which neglect even only one of these influences will not be able to reproduce neither the statics (angle of repose, stress distribution) nor the dynamics (e.g. avalanches, force networks) for realistic materials. Due to the two-dimensional simulation, the fluctuations on the data are nevertheless more pronounced than in three-dimensional experiments. The whole mechanism of formation of heaps and angle of repose is the result of the particle properties (shape and inter-particle friction) on the one hand, and of sliding on the ground and avalanches on the other hand.

References

Figure 13: Initial state (above) and end configuration (below) of a simulation for the computation of the outflow from a hopper on a rough ground with friction coefficient $\mu = 0.6$ onto a layer with particles for increased energy damping. The slopes are not straight due to the superposition of the out-flowing grains and the damping layer. Particles in the same layer have the same shade of gray, mixing of shades in the end configuration indicates mixing of layers.