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GRAIN NON-SPHERICITY EFFECTS ON THE ANGLE OF REPOSE OF GRANULAR MATERIAL

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ABSTRACT

We use a site-site model to describe non-sphericity of particles composing a granular media. Specific effects of grain non-sphericity on the angle of repose are investigated. We report evidence indicating the possible existence of a *shape-roughness threshold* for grains: below it angles of repose are essentially the same as those obtained for spherical grains; above it there are pronounced changes on the angle of repose and it is possible to find rather large piles of grains.

Keywords: Granular Media; Non-sphericity Effects; Angle of Repose.

1. Introduction

This paper presents results of an investigation the effect of grain non-sphericity in the angle of repose of a granular material. A popular way of simulating granular media is to assume them to be made of either a monodisperse or polydisperse collection of spherical grains. Using spherical grains many interesting effects have already been discussed in the literature: see, for example, refs. 1–4 and many other references therein. Although spherical grains are quite good starting points for investigations of the properties of granular media, the phenomena that are presently attracting a lot of attention in the physics community involve granular media composed of grains which are in fact very far from spheres. For one example, think of the many recent experimental observations with sand[4]. Sand involves grains which are in fact seldom spherical. In physics, the main concern of several recent theoretical investigations has been to define models able to reproduce effects observed experimentally such as size segregation, convection, angle of repose, outflow from hoppers, from pipes, density waves, etc[4]. A fundamental common objective of all these studies is to properly address and understand the interplay of the forces, either internal or external, needed to satisfactorily explain all the effects experimentally observed. Although a great deal of progress has already been achieved, there are still many questions to answer. This is so because simulations required to answer even "simple" questions usually require extensive numerical work to generate data and to analyse them.

In this paper we want to consider the effect of non-sphericity in the dynamical behavior of granular media. To this end, rather than simple spheres, we consider grains composed of *several spheres* rigidly glued to each other.

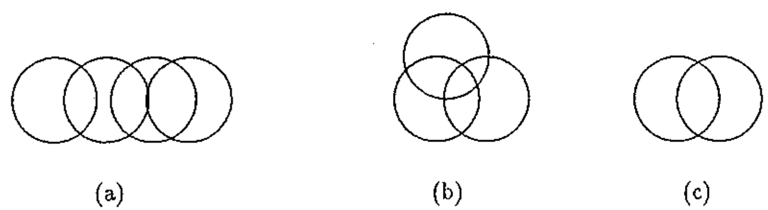

Fig. 1. Typical site-site models of non-spherical grains made of identical spheres of diameters σ. **(a)** Grain composed of four colinear centers of force; **(b)** Grain composed of three coplanar centers of force; **(c)** Schematical view of the grain used in the simulations of present paper. The two centers of force composing the grain are located at a distance e apart.

Figure 1 shows three examples of possible grain configurations. The shape of the composite grains is represented by the outer perimeter of the overlapping spheres. The individual spheres composing the grains might be chosen aligned along a line segment or not. They can be taken to be mono or polydisperse. The present paper reports results for the grain shown in Fig. 1c, made of two identical spheres of diameter σ with their centers located at a distance e apart ('eccentricity' or 'elongation' parameter). For $e = 0$ the non-spherical centers of force obviously perfectly overlap each other reproducing then the spherical limit. The introduction of these new quantities complicates but simultaneously very much enriches the model of granular media. For example, by considering grains in Fig. 1c to have diameters σ_1 and σ_2 one may roughly classify granular media into four main classes, namely,

Class A: $\sigma_1 = \sigma_2 =$ constant, e varying;
Class B: $\sigma_1 \neq \sigma_2$ but both constant, e varying;
Class C: σ_1 and σ_2 randomly distributed, $e =$ constant;
Class D: σ_1, σ_2 and e all randomly chosen from a given distribution;

Our way of dealing with non-sphericity is essentially an adaptation of site-site models widely used to study molecular fluids to granular media. In site-site models non-spherical particles are treated as composed of several sites rigidly located at fixed distances from each other. Such sites are centers of spherical potentials. In molecular liquids, the traditional way of investigating effects of non-sphericity is by using either convex molecular models or site-site models[5,6]. As is well-known, thermodynamic properties of convex molecules can be approximated very well by the properties of apropriately defined site-site systems[7]. The great advantage of using site-site models is that one deals essentially with "strings" or "blocks" of spherical particles. By properly chosing the "bond-lengths" between the individual spheres that make a particle (i.e. a *grain*) one can control the degree of non-sphericity while still generating very efficient computer codes that can be *vectorized*, allowing therefore the investigation of large assemblies of particles. The adaptation and extension of concepts and techniques familiar to describe fluids with Molecular Dynamics to simulations of macroscopic particles like those typical of granular media might perhaps be synthetized by referring simply to *Granular Dynamics*.

2. Site-site model of non-spherical grains

Following the strategy adopted in our previous studies[8], we investigate two-dimensional systems and perform Granular Dynamics simulations of inelastic particles. The present work reports results for "Class A" grains as defined above and including the following specific characteristics: as before, grains are soft, i.e. they may slightly interpenetrate each other; they dissipate energy in two ways, viz. due to normal and shear frictions. We consider a generic granular media with N non-spherical grains, each individually made of M spheres of equal size and density. For simplicity we consider first all spheres as having a constant diameter σ and to be symmetrically located at distances L_m, $m = 1, 2, \ldots M$ along a line passing through the center of mass of the grain. All grains are allowed to translate and to rotate freely in space under the action of a gravity and confined by a rectangular container. As before[8], the dynamics was studied using a predictor-corrector integrator. This means that we follow the dynamics by accurately integrating Newton's equation of motion for each individual grain. Although our program can handle grains made up of several spheres and we already did preliminary simulations with them, in the present paper we will only report results obtained by considering $M = 2$ spheres. Other results will be presented elsewhere[9].

When two spheres n and m belonging to different grains i and j overlap (i.e. when their distance is smaller than the sum of their radii) several forces act on them. The forces acting on the sphere n of the i-th grain are: 1.) an elastic restoration force

$$\vec{f}_{el}^{(i_n)} = Y m_i \{ |\vec{r}_{i_n j_m}| - \frac{1}{2}(\sigma_{i_n} + \sigma_{j_m}) \} \frac{\vec{r}_{i_n j_m}}{|\vec{r}_{i_n j_m}|}, \qquad (1a)$$

where Y is the Young modulus, m_i is the mass of grain i and $\vec{r}_{i_n j_m}$ points from sphere i_n to j_m; 2.) a dissipation due to the inelasticity of the collision

$$\vec{f}^{(i_n)}_{diss} = -\gamma m_i \{(\vec{v}_i - \vec{v}_j) \cdot \vec{r}_{i_n j_m}\} \frac{\vec{r}_{i_n j_m}}{|\vec{r}_{i_n j_m}|^2}, \tag{1b}$$

where γ is a phenomenological dissipation coefficient and $\vec{v}_i$ is the translational velocity of the grain i. To define a sliding friction we introduce now the relative tangential velocity

$$\vec{V}^{tang}_{i_n j_m} = \vec{v}_i - \vec{v}_j + \vec{\Omega}_i \times \vec{\rho}_{i_n} + \vec{\Omega}_j \times \vec{\rho}_{j_m} \tag{1c}$$

with $\vec{\Omega}_i$ being the angular velocity of the grain i; $\vec{\rho}_{i_n}$ denotes the distance from the point of contact between spheres n and m to the center of mass of the grain i. The shear friction is taken into account by two components, a sliding and a rolling friction. 3.) the sliding friction takes the form

$$\vec{f}^{slid}_{i_n j_m} = -\gamma_s m_i (V^{tang}_{i_n j_m}) \frac{\vec{t}_{i_n j_m}}{|t_{i_n j_m}|}, \tag{1d}$$

and $V^{tang}_{i_n j_m} = \vec{V}^{tang}_{i_n j_m} \cdot \vec{t}_{i_n j_m}/|t_{i_n j_m}|$. 4.) the rolling friction is

$$\vec{f}^{roll}_{i_n j_m} = -\mu[\vec{f}^{(i_n)}_{el} + \vec{f}^{(i_n)}_{diss}] \cdot \vec{t}_{i_n j_m} \frac{\vec{t}_{i_n j_m}}{|t_{i_n j_m}|^2}. \tag{1e}$$

The total shear force is therefore

$$\vec{f}^{(i_n)}_{shear} = \{f^{(i_n)}_{el} + f^{(i_n)}_{diss} + min[f^{slid}_{i_n j_m}, f^{roll}_{i_n j_m}]\} \frac{\vec{t}_{i_n j_m}}{|t_{i_n j_m}|}. \tag{1f}$$

In the expressions above γ_s is the shear friction coefficient, $\vec{t}_{i_n j_m}$ is the vector $\vec{r}_{i_n j_m}$ rotated clockwise by 90° and $\mu = 0.2$. Most of our simulations were done for $\gamma = \gamma_s = 100g$. In all cases considered we took $Y = 1000gm/\sigma$, where g is the gravity, $m = 0.001$ Kg the mass of the grains and $\sigma = 0.001$ meters. As before, we neglect *explicit* static friction terms. Note that the terms in γ and γ_s incorporate 'implicitly' effects of static friction. This is done solely for simplicity here: it is clear that such effects can be trivially taken into account as done, for example, by Cundall and Strack[10] and others since then. In principle there is no difficulty to include static friction effects in the model above if so desired. However, a major problem with static friction in our opinion is that the way in which it is presently considered in the literature seems to introduce an artificial "gluing" of the particles together. Until effects of static friction are more thoroughly investigated, rather then somewhat 'gluing' our particles together, we prefer to simply neglect static friction. When any sphere of a grain collides with a wall the same forces act on it as if it would have encountered another sphere of diameter d_0 at the collision point. In the present simulations the diameter of the spheres composing the walls were taken to be $d_0 = \sigma/2$. One single external force acts on the system: a gravitational pull $g \approx -10$ m/s^2 acting along the axis of the container.

The initial configuration was obtained by first randomly placing grains on a certain volume above a rectangular box and then letting simultaneously *all grains* to fall freely under gravity from their high positions into the rectangular box. Grains where allowed to interact for a time long enough such that the total kinetic energy of the ensemble was a number typically of the order of 10^{-6}, i.e. practically zero. In other words, we allow grains to freely reach a stationary equilibrium configuration inside the box containing them. After that we remove the right lateral wall of the box and let grains to freely relax to a new equilibrium configuration, driven exclusively by the external gravitational field and the friction forces.

To have finite angles of repose it is obviously necessary that when released, grains do not horizontally scape to infinity. The horizontal kinetic energy must therefore be dissipated. There are two basic factors that help preventing zero angles of repose: the friction coefficients and the roughness of the bottom surface holding the grains. The dissipation of all x—components of the force (see eq. 1a) is necessary to obtain a pile of grains. The proper specification of the walls is very important since they will affect the angles of repose. In particular, note that smooth walls are unable to hold a pile, unless one 'glues' grains together and to the wall. In the present paper the container was made of spheres identical to those composing the grains. They were rigidly packed at a distance $\sigma/2$ from each other, where σ is the diameter of the individual spheres making the grains. This corresponds to a more or less 'intermediate' roughness of all the walls.

3. Results

Figure 2 shows the essential features that appear when non-sphericity is taken into account. Fig. 2a shows the $e = 0$ spherical limit while Fig. 2b corresponds to an eccentricity $e = 0.6$. In both cases there are $N = 300$ grains. As is easy to see, the compaction for pure spheres is much higher then that for non-spheres. In other words, the porosity after reaching the equilibrium is higher for non-spheres than for spheres, as might have been intuitively anticipated. Note that this effect is not only due to the obvious increase in the size of the grains but appears as a consequence of the more difficult arrangement of grains that is now needed in order to 'tile' the space inside the box so as to minimize voids.

As mentioned above, subsequent to equilibration under gravity we want to determine the angle of repose. After equilibration the grains fill the box up to a horizontal quota z_0 roughly (see Fig. 2) and the numerical experiment being reported here consists of removing the wall at the right hand side of the container thereby allowing the system to relax from z_0 to a triangular configuration as shown in Fig. 3 and then measuring the angle of repose. By suitably chosing the aspect ratio one may always ensure the existence of a triangle. (If needed, this might be also achieved by playing with the total number of grains: it is important to use enough grains to assure that the angle of repose does not artificially depends on

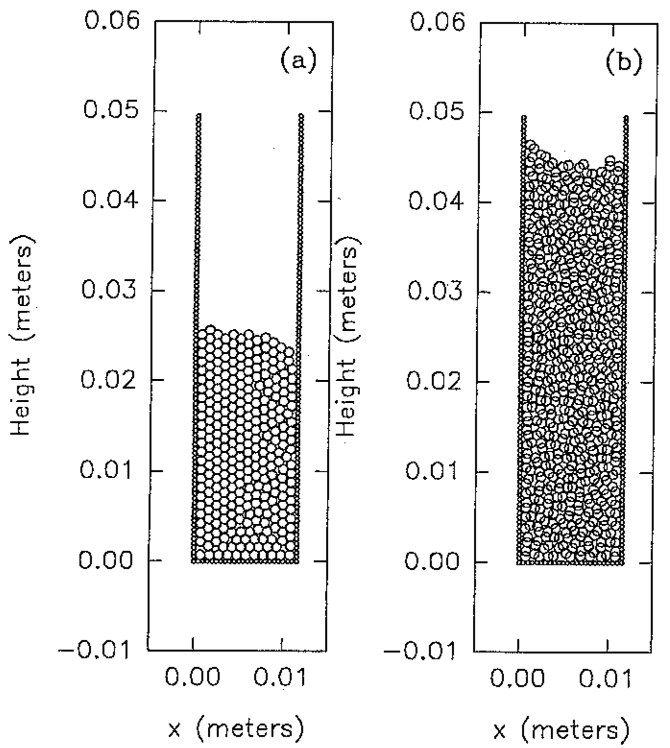

Fig. 2. Effect of non-sphericity on the packing of grains. **(a)** Packing of spherical grains ($e = 0$); **(b)** Packing of non-spherical grains with $e = 0.6$. Both containers have 300 grains.

the number of grains.) After obtaining a static (roughly triangular) pile, its basis was divided into a convenient number (of the order of 100) of identical bins and the *heights* $h(x)$ of every bin were measured as a funtion of the distance x from the vertical wall on the left. An example of results typically obtained is shown in Fig. 4, as functions of the eccentricity.

Individual angles of repose were obtained by least-square fitting straight lines to the curves shown in Fig. 4. *Final* angles of repose were then obtained by averaging the results of several runs. We also considered the rough approximation of the values α of the angle of repose by using the 'geometrical' triangle formed by the height h of the leftmost bin and the basis length b:

$$\tan \alpha = \frac{h}{b}. \tag{2}$$

These two different ways of defining the angles of repose always produced the same qualitative results. We also considered removing *simultaneously* both walls and defining *left* and *right* angles of repose. Apart from checking any eventual strong 'asymmetry' on the final piles of grains, considering both left and right angles of repose as independent quantities permited to increase the statistic of our measurements by obtaining two angles from every single run. For all parameters investigated both angles behaved always as trully independend quantities. By ploting curves of the averaged angles of repose (obtained with the two methods described above) for dif-

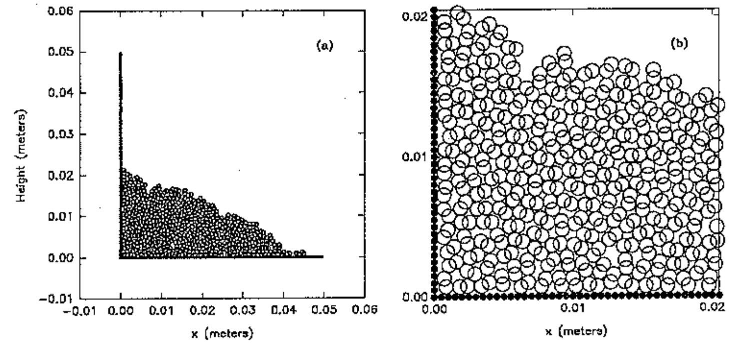

Fig. 3. Example of a ***triangular*** pile obtained after removing the rigth side wall of the container. **(a)** full pile, and **(b)** magnification of the portion on the right of the pile. Some single spheres that appear very close to the right border of the figure have another partner located outside the borders of the figure.

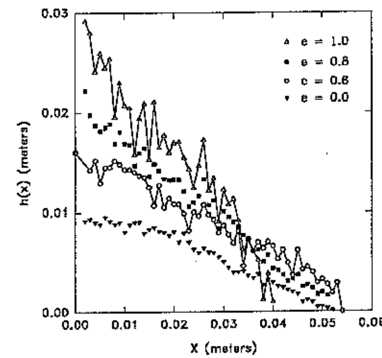

Fig. 4. Maximum height $h(x)$ of piles of grains as a function of their distance x from the vertical wall on the left. The angle of repose is obtained by approximating $h(x)$ by a least-square straight line (not shown). To guide the eye, the points belonging to the $e = 0.6$ and $e = 1.0$ curves were joined by line segments.

ferent container sizes and different number of grains one realizes that there is no noticeable dependence of the angle of repose on the aspect ratio.

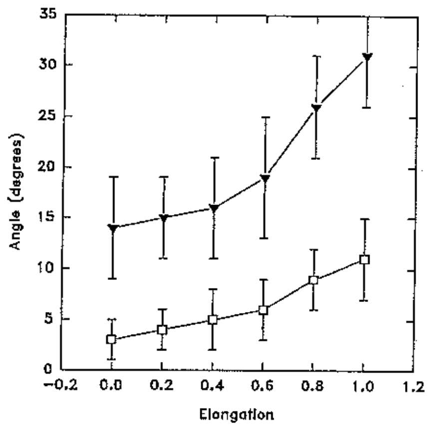

Fig. 5. Angles of repose (triangles) and tilting angles (squares) as a function of the elongation e [in units of σ] for several sets of parameters.

The upper curve in Fig. 5 shows the variation of the angle of repose as a function of the eccentricity e. As it is easy to see, for e less than about 0.5 there is relativelly small variation of the angle. However, after this *non-sphericity threshold* the angle increases quite rapidly. This shows than slight distortions from spherical shape ("eliptical grains") are not sufficient to qualitatively alter the collective behaviour of the granular powder. But stronger distortions produce quite large changes. Note that $e \geq 0.5$ are eccentricities which maximize the roughness of the grains. $e = 1.0$ corresponds to having the two centers of force making the grains to 'intersect' at one single point.

In order to see how stable the piles obtained after removing the vertical wall were with respect to perturbations, i.e. to check whether the angles of repose were critical or not in the sense that diminute perturbations could induce large modifications via avalanches[11,12], we performed an additional numerical experiment. Such experiment consisted of adiabatically raising the left corner of the horizontal wall in Fig. 3 by 'rotating' it clockwise slowly around the right (fixed) corner and measuring the 'tilting angle' for which the total kinetic energy changed by non-negligible amounts ("avalanches"). As can be see from Fig. 5, the piles obtained by removing the right wall were not critical. Further, the figure shows that angles of repose and tilting angles show basically the same qualitative behavior as functions of e. Here again it is possible to see an increase in the stability of the pile for e larger than about 0.5. We regard Fig. 5 as providing evidence that non-sphericity might be a strong factor leading to the formation of large and stable slopes as those needed to

have formation of heaps in granular media.

4. Conclusions

The present paper reported results of simulating grain non-sphericity in granular materials via site-site modeling. Specificaly, this paper considered "class A" materials, i.e. the case when grains can be assumed to be composed of two identical spheres located at a distance e apart. As a first application, our model was used to investigate the effect of non-sphericity on the angle of repose characteristic of granular media. As discussed in the previous section in details, the essential characteristic of non-sphericity is to increase the angle of repose, an increase which is quite significant after a clear threshold above which the roughness of the particles is high. Preliminary estimates seem to indicate that effects observed by considering non-sphericity are much larger than those induced by static friction. At any rate, the inclusion of non-sphericity effects seems at this point to be a step towards a more realistic model of granular media, a step perhaps less open to criticism regarding the validity of its definition than the incorporation of static friction. There is no doubt that static friction will also have to be included. A present big theoretical challenge in the field of granular media is to explain the formation of heaps in vibrated media, heaps which are extremely simple to generate experimentally but which have so far eluded numerical simulations. While assessing the relative importance of the several parameters involved as possible 'motors' for heaps we have been able to obtain heaps by 'sticking' particles together via static friction effects. However, considering the mechanisms and the duration time of collisions we tend to believe at this point that such gluing is physically unreasonable and calls for a more detailed investigation. We hope that the relatively 'more transparent' effects due to non-sphericity might decisively contribute to an explanation for the beautiful phenomena that is the formation of heaps. But this certainly remains yet to be seen.

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