

# Molecular dynamics simulation of complex particles in three dimensions and the study of friction due to nonconvexity

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We investigate the macroscopic properties of frictionless nonconvex particles using molecular dynamics. The calculations are based on a simple and efficient method to simulate complex-shaped interacting bodies. The particle shape is represented by Minkowski operators. A multicontact time-continuous interaction between bodies is derived using simple concepts of computational geometry. Three-dimensional simulations of hopper flow show that the nonconvexity of the particles strongly affects the jamming on granular flow. Also the model allows the representation of complex bodies with rough surfaces as in friction studies and the reproduction of a wide range of friction and dilatancy angles as in true triaxial tests.

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## I. INTRODUCTION

Most of our technology is still based in moving parts, and hence the development of durable and/or low friction surfaces and thin lubricating films has become an important factor in the construction of many devices. The study of the friction in these kind of surfaces is extremely important and cannot be restricted to the simple Amonton's friction law for sliding. Moreover, there is a huge complexity involved and chaotic behavior has been reported [1] making the search for simple models even more difficult. One of the features that produce macroscopic friction is microscopic roughness. Nonconvex bodies sliding against each other have multiple contact points, each of them providing a repulsive force opposing relative movement. A macroscopic model based on a continuum assumption may not be suitable for this phenomenon.

Molecular dynamics (MD) is an alternative to this problem. MD is the art of modeling complex systems as a collection of particles interacting with each other. The most typical approach for this is to solve the dynamics of interacting rigid bodies, where their real shapes are approximated by polyhedra [2]. The most difficult aspect for the simulations is to model contact interactions. Contact force methods have been proposed for two-dimensional (2D) models using polygons [3,4]. However, the extension of this method to three-dimensional (3D) simulations has proven to be extremely difficult. One reason is because the calculation of the overlap between two polyhedra is computationally very expensive. This is the main reason why most of the commercial codes for particulate systems are still based on simulations with spheres or clumps of spheres representing complex-shaped particles [5].

Recently an alternative solution to model of complex-shaped particles has been proposed [6]. The method intro-

duces the concept of spheropolygons, which is the object resulting from dilating a polygon by a sphere. The method not only guarantees energy balance but also proves to be much more efficient than previous models to represent complex particle shape [7]. In 3D models, the dilation of a polyhedra by a sphere has a precise mathematical meaning using the Minkowski operator. In our knowledge, Liebling and Pournin [8,9] were the first to introduce the Minkowski operators in particle-based simulations. In order to calculate the interactions, they assumed a single contact point between the particles [8]. This approach, however, leads to forces discontinuities in time and numerical errors such as abrupt creation of mechanical energy. Using a single contact per particle pair makes extremely difficult if not impossible to model nonconvex particles and therefore its application for fields such as tribology is limited.

In this Rapid Communication we present a solution to this problem by (i) introducing a 3D MD technique using spheropolytopes and (ii) defining a multicontact law for two bodies that solves most of the problems encountered in previous models. With it we will show the results of three sets of simulations dealing with nonconvexity friction: the hopper granular flow, the true triaxial test and the rough surface sliding.

## II. MODEL

Spheropolytopes are generated from the Minkowski addition of a polytope by a sphere, which is nothing more than the object resulting from sweeping a sphere around a polytope (see Fig. 1). A polytope is a generic mathematical concept that can refer to polygons, polyhedra, or polygonal curves in 3D. The polytope is regarded as a collection of *features* in the 3D Euclidian space: vertices, edges, and faces. The interaction between two spheropolytopes is calculated as a function of the distance between their features. The MD is implemented in a simple, efficient, and elegant algorithm based on the fact that only distances, and neither Minkowski sum nor volume overlaps need to be calculated.

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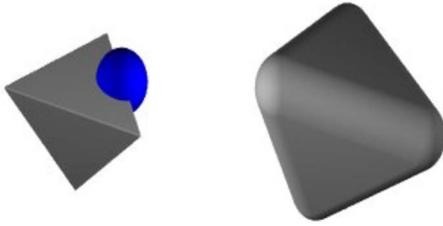


FIG. 1. (Color online) For the representation of arbitrary-shaped particles we introduce the mathematical concept of Minkowski sum. Given two sets of points  $P$  and  $Q$  in an Euclidean space, their Minkowski sum is given by  $P \oplus Q = \{\vec{x} + \vec{y} | \vec{x} \in P, \vec{y} \in Q\}$ . This operation is geometrically equivalent to the sweeping of one set around the profile of the other without changing the relative orientation (Fig. 1). The spherotetrahedron (right) is obtained by sweeping a sphere across a tetrahedron profile (left).

The algorithm has also proven to comply with the conservation laws of physics and the statistical equilibrium [6]. We believe that this model will lead to a wide range of applications of MD, as complex particle shape and realistic interactions can be captured in a unified framework using well-established concepts of MD and computational geometry.

Using the formulas of distance between the features of two spheropolytopes we calculate the interaction between them. The force  $\vec{F}_{ij}$  on the  $i$ -spheropolytope by the  $j$ -spheropolytope is taken as a superposition of the interaction between each pair of edges  $\vec{F}(E_i, E_j)$  and each pair of vertex face  $\vec{F}(V_i, F_j)$  for the spheropolytope pair,

$$\vec{F}_{ij} = \sum_{E_i, E_j} \vec{F}(E_i, E_j) + \sum_{V_i, F_j} \vec{F}(V_i, F_j) + \sum_{V_j, F_i} \vec{F}(V_j, F_i). \quad (1)$$

The force  $F(G_i, G_j)$  associated to the two features (edge-edge or vertex-face) is assumed to depend on the overlapping length  $\delta$  between them  $\delta(G_i, G_j) = R_i + R_j - d(G_i, G_j)$ , with

$d(G_i, G_j)$  being the distance between the features of the spheropolytopes and  $R_i$  being the spheroradius of the  $i$ th spheropolytope. The point of contact between the two features is calculated by taking the spheres of radius  $R_i$  and  $R_j$  centered in the closest points  $\vec{X}_i$  and  $\vec{X}_j$  and finding the intersection between the line connecting these two points and the line connecting the two intersection points of the spheres. From the point of application of the contact forces we get the torque associated to the contact force. Once all the forces and torques are calculated we integrate Newton's second law using the Verlet algorithm for the translation coordinates. The Euler equations for angular momentum is integrated using the Fincham leap frog algorithm, based on the quaternion formalism, for the orientation coordinates [10].

Since the formulas of distance are continuous functions on the degrees of freedom of the spheropolytopes, the total force is continuous too. For example, there are no jumps in the calculation of forces from a vertex changing the face that is in contact with; the interaction will smoothly change from one face to the other as the vertex start moving around the other particle. This avoids the problem of discontinuity in time of the forces in previous models [2]. Different forces can be included in this model: for example, a force derived from a potential function of the distance leads to conservative systems. Forces depending on the relative velocities at the contact points lead to dissipative granular materials. Forces depending on the history of relative velocity at the contacts represent frictional granular systems. More sophisticated forces can be used to simulate biomolecules. The electrostatic interaction between molecules can be modeled by allowing the forces to depend on the closest points between the features. In this Rapid Communication, a simple contact force between features is calculated as  $\vec{F}(G_i, G_j) = -k_n \delta(G_i, G_j) \vec{n}$ , where  $k_n$  is an elastic constant. Dissipative forces proportional to the relative velocity at the contact are also included to allow relaxation of the systems.

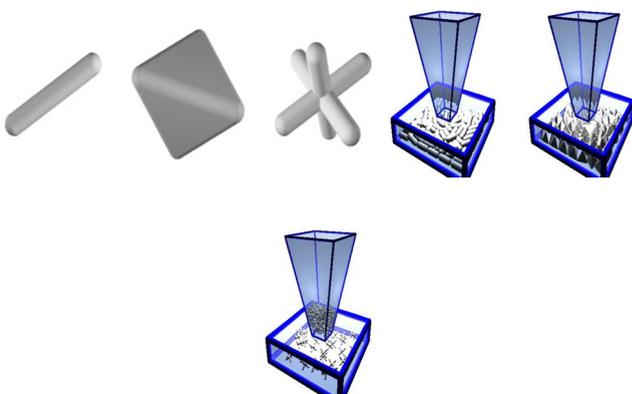


FIG. 2. (Color online) Top: spheropolytopes generated as sphere  $\oplus$  line segment (*rice*), sphere  $\oplus$  tetrahedron (*tetra*), and sphere  $\oplus$  polyline (*yermis*). Bottom: final stage of granular flow when the particles are discharged from a hopper. Simulations run without microscopic friction. Convex particles (*rice* and *tetras*) flow completely through the hopper. Nonconvex particles (*yermis*) jam, which proves the existence of macroscopic friction due to nonconvexity.

### III. HOPPER FLOW

We will start with an interesting application of this model: the study of the effect of particle shape on the jamming phe-

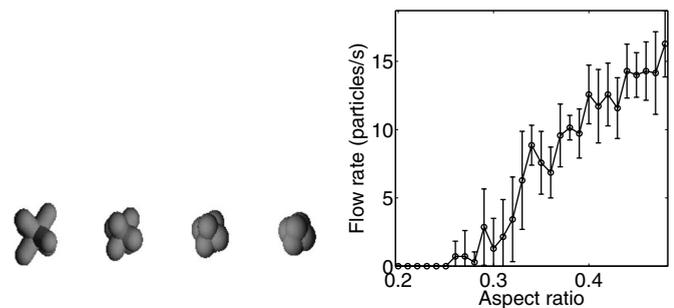


FIG. 3. Left: a yermis geometry with four different aspect ratios: 0.3, 0.4, 0.5, and 0.6. The closer is the aspect ratio to 1, the closer the particle is to a convex (spherical) shape. Right: hopper flow rates for different aspect ratios. There is a critical aspect ratio around 0.25, below which particles jam without microscopic friction.

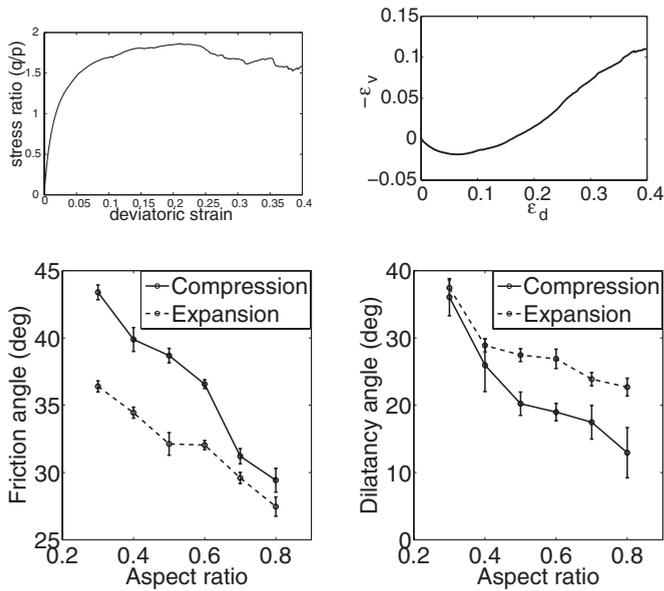


FIG. 4. Results from the true triaxial test for a sample formed of yermis grains with aspect ratio equal to 0.3. Top-left: deviatoric to pressure ratio versus deviatoric strain. Top-right: deviatoric to pressure ratio versus volumetric strain. Bottom-left: friction angle measured by the Drucker Prager criterion. The error bars are obtained by doing the experiment with different confining pressures. A small error bar indicates that the friction angle is almost independent of the chosen pressure as expected. Bottom-right: dilatancy angle measured for each one of the samples for both expansion and compression tests. Friction coefficient of 0.25 using the Cundall model [3].

nomenon of granular flow. The flow may happen when particles are discharged through a small opening, but particles may become jammed when the opening is smaller than a critical value. Modeling of gravity flow has been done using circular or spherical particles [11], but the effect of shape on flow has not been fully investigated. In particular, nonconvex particles are expected to jam more easily than convex or circular particles.

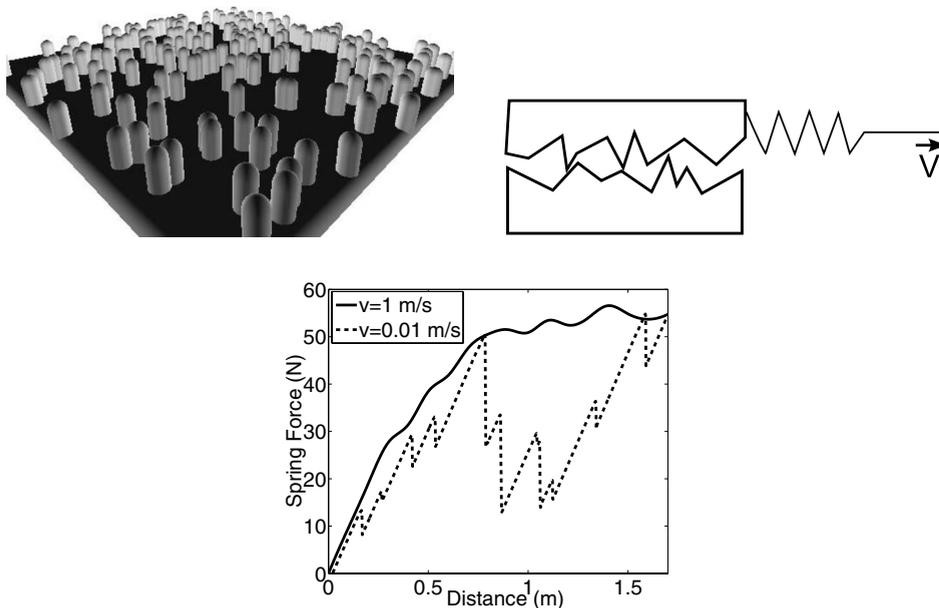


FIG. 5. Experimental setup for the study of friction due to roughness between surfaces. The spheropolytope surface is just a face with several edges pumping out of it (left). Two of these surfaces are put in contact and one of them is pulled by a spring (right). Bottom: spring force vs distance covered by the spring tip for two different spring velocities showing the stick-slip (dashed) and smooth (solid) behaviors reported in literature.

Granular flow with convex and nonconvex particles is presented using the same three particles geometries shown in Fig. 2. The simplicity of our model allows us to represent the hopper and the container as spheropolytopes. Contrary to previous findings [4] our convex-shaped particles do not become clogged in the hopper. This is because we have not introduced a static frictional force. However, as a striking result, the nonconvex particles do get stuck even though there is no static friction.

In order to quantify the effect of nonconvexity in jamming, we check the granular flow for the *yermis* geometry varying the aspect ratio (see Fig. 3) defined as  $\frac{r}{l+rr}$ , with  $r$  being the spheroradius and  $l$  the length of the cylinders conforming the particle, and keeping the volume constant. In Fig. 3 the results for several simulations of steady flow rate vs aspect ratio are shown. We can see that the higher the aspect ratio, the greater the flow rate. Therefore we can conclude that friction due to nonconvexity of the particles hinders the free flow. There is a critical aspect ratio around 0.27 that will always ensure flow through the hopper and marks the transition from the jammed state to the free state.

#### IV. TRUE TRIAXIAL TEST

Another test to check macroscopic friction produced by nonconvex shapes is the true triaxial test. This is shown in Fig. 4, where six walls (spheroplanes) enclose a sample of yermis grains. Initially we apply a confining pressure to the walls and then, after a consolidation time, we set a fixed velocity in the upper wall to ensure constant strain rate. This gives us the stress path for the common conventional drained triaxial test [12,13].

The most important results are shown in Fig. 4 for the yermis geometry with aspect ratio equal to 0.3. As can be seen, after the consolidation the sample shows a failure point after which it reaches the well-known critical state [14]. This failure is the peak in the deviatoric ( $q$ ) to pressure ( $p$ ) ratio versus deviatoric strain ( $\epsilon_d$ ). The critical state is shown

clearly in the volumetric strain  $\epsilon_v$  versus deviatoric strain  $\epsilon_d$  curve as the asymptotic state. All of these features are known to be present in drained tests on soil samples [12,13]. This reproduced behavior is part of the validation of our method.

We can apply the Drucker-Prager failure criterion [15] to find the friction angle as a function of the aspect ratio; the results are shown in Fig. 4.

As can be seen, the friction angle for both the compression and the expansion tests decreases with the aspect ratio showing one interested dependence of the macroscopic friction in the microscopic geometry. Obviously in the yermis geometry the particles are interlocked which gives the sample a higher strength.

Another important quantity is the dilatancy angle defined as the slope of the volumetric versus deviatoric strain after the minimum reached when the sample start the expansion. It is an indication of how easy is to change the volume by shear deformation. In Fig. 4 it can be seen that samples with a high aspect ratio are not so susceptible to change their volumes as samples with low (nonconvex) geometries. While with the sphere geometry we have that grains easily roll one over each other due to shearing, with a nonconvex shape, the grains should overcome the interlocking effect requiring an initial expansion before they can move freely.

## V. ROUGH SURFACE SLIDING

Following the thesis that nonconvexity causes a form of friction, the proposed model can also study the interaction between rough surfaces. In Fig. 5 a experimental setup is shown which is very easy to implement with our model: two rough surfaces sliding against each other with the upper one

being pulled by a spring moving with a certain velocity. Several experiments reported show a *stick-slip* behavior for low spring velocities and a smooth phase for high spring velocities [16,17]. The virtual experiment reproduces this phenomenon and serves as a validation for the proposed model (Fig. 5) [18,19].

## VI. CONCLUSIONS

Modeling interacting particles using spheropolytopes has several advantages with respect to other existing particle-based models: (i) the possibility to model nonconvex particles (in our case yermis, hoppers, rough surfaces, etc), (ii) a realistic representation of the surface curvature of particles, (iii) guaranteed compliance with physical laws, (iv) numerical consistency guaranteed by the continuity in the proposed contact law and (v) efficiency given by a simple model for the contact law relying only on distance calculations. This is radically different from previous approaches where the contact forces are calculated with geometric overlaps.

The most interesting aspect of this model is to provide a general framework for generic particle shape and contact interactions. Spheropolytopes is a very general shape which can be used to represent biomolecules, polymers, rocks, meteors, etc. Since it provides an easy way to model nonconvex particles due to its multicontact basis, it can be used also for the study of tribology with some examples presented in this Rapid Communication.

## ACKNOWLEDGMENT

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