New perspectives for Discrete Element Modeling: Merging Computational Geometry and Molecular Dynamics.

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Abstract.
One of the most challenging problems in the realistic modeling of granular materials is how to capture the real shape of the particles. Here we present a method to simulate systems with complex-shaped particles. This method integrates developments in two traditionally separate research areas: computational geometry and molecular dynamics. The computational geometry involves the implementation of techniques of computer graphics to represent particle shape and collision detection. Traditional techniques from molecular dynamics are used to integrate the equations of motion and to perform an efficient calculation of contact forces. The algorithm to solve the dynamics of the system is much more efficient, accurate and easier to implement than other models. The algorithm is used to simulate quasistatic deformation of granular materials using two different models. The first model consists of non-circular particles interacting via frictional forces. The second model consists of circular particles interacting via rolling and sliding resistance. The comparison of both models help us to understand and quantify the extend to which the effects of particle shape can be captured by the introduction of artificial rolling resistance on circular particles. Biaxial test simulation show that the overall response of the system and the collapse of force chains at the critical state is qualitatively similar in both 2D and 3D simulations.

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1. INTRODUCTION

The particle-based modelling of granular materials is a very active area of research. The origin of the method can be traced back 50 years before, when Loup Verlet published the paper which gives birth to the Molecular Dynamics (MD) method [1]. MD is the paradigm of modelling complex systems as a collection of particles interacting each other. The method is very popular in computer simulations in Physics, Chemistry and Biology. Even Engineers have also recognized the potential of this method, after the pioneer work of Peter Cundall in the development of a explicit MD-like model for frictional materials. Cundall's ideas led to a new area of numerical analysis of engineering problems, which is today known as Discrete Element Method (DEM). Although particle shape plays an important role, most theoretical and numerical developments have been restricted to particles with spherical or circular shape. This simplification lead in some cases to unrealistic properties. In dissipative granular systems such as sand piles or fault gouges, disks of spheres tend to roll more easily than non spherical particles, leading to unrealistic angles of repose and very low bulk friction coefficients [2].

One way to achieve realistic description of complex shapes particles without reinventing the wheel is to learn from the fast growing advances in computer graphics. New developments in these areas are fuelled by computer games industry and special effects companies. There is therefore a natural interest to put these development to a good use of solving scientific problems. The aim of this paper is to present a new approach intending to merge the molecular dynamics approach with some concepts used in computer graphics: The Minkowski operators, computational geometry and rendering. This mix results in a new molecular dynamics method that account both particle shape and interactions, allow high quality visualization, and at the same time keep a reasonable balance between accuracy and efficiency.

In our knowledge, Liebling and Pournin were the first ones to use computational geometry in the modelling of granular materials. They proposed a new approach for 3D simulations using the mathematical concept of spheropolyhedra [3, 4]. These objects are generated from the Minkowski sum of a polyhedra with an sphere. This simple concept can be used to generate very complex shapes, including non-convex bodies, without the need to decompose them into spherical or convex parts. A new method to calculate the interactions in complex shaped particles were presented using spheropolygons [5] (i.e.

the Minkowski sum between polygon and disk). and spheropolytopes [8] (the Minkowski sum of polytopes with spheres). Such interaction model presents some advantages with respect to the original interaction model of Pournin & Liebling: 1)consistency with energy balance, 2) possibility to handle multiple contacts in non-convex particles, 3)more simplicity, because forces are calculated from distances, and not from overlaps and 4) more efficiency, achieved by an extension of the Verlet list to detect neighborhood.

Here we present a summarized description of this method in 2D and 3D. In Section 2 we describe the basic components of the numerical model. In Section 3 we use the model to investigate in which extent the 2D modelling of circular particles with rolling resistance can capture the realistic behavior of granular materials. Some conclusions and perspectives of this method are presented in Section 4.

2. THE MODEL

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 $P \oplus Q = \{\vec{x}+\vec{y} \mid \vec{x} \in P,\ \vec{y} \in Q\}$. This operation is geometrically equivalent to the sweeping of one set around the profile of the other without changing the relative orientation (Fig 1). Examples of Minkowski sums are the spheropolygons (sphere $\oplus$ polygons) [5], spherocylinder (sphere $\oplus$ line segment) [7], the spherosimplex (sphere $\oplus$ simplex) [3] and the spheropolyhedron (sphere $\oplus$ polyhedron) [4], All these objects can be enclosed in the generic shape of spheropolytopes, which consists of a set of vertices V_i, edges E_i, polygonal faces F_i and the radius r of the sweeping sphere which will be called sphero-radius. The advantage of the Minkowski sum is that uses less geometrical elements than other methods to represent complex particle shape. It is also shown that the calculation of the multicontact forces between the objects are very efficient, easy to implement and it complies with the physical laws [5, 6, 8, 9].

First we introduce the interaction force between spheropolygons in 2D. We consider all vertex-edge distances between the polygons base. we consider two spheropolygons $W_i = P_i \oplus B_{r_i}$ and $W_j = P_j \oplus B_{r_j}$ with their respective polygons base P_i and P_j and sphero-radii R_i and R_j. Each polygon is defined by the set of vertices $\{V_i\}$ and edges $\{E_j\}$. The force $\vec{F}_{ij}$ acting on the spheropolygon i by the spheropolygon j is defined by:

$$\vec{F}_{ij} = \sum_{V_i E_j} \vec{F}(V_i, E_j) + \sum_{V_j E_i} \vec{F}(V_j, E_i), \qquad (1)$$

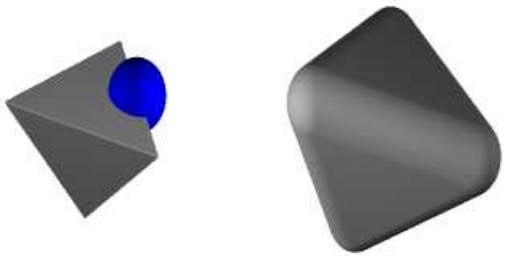

FIGURE 1. The spherotetrahedron (right) is obtained by sweeping an sphere into a tetrahedron (left).

where $F(V,E)$ is force between the vertex V and the edge E.

In the 3D case, 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,

$$\vec{F}_{ij} = \sum_{E_i,E_j} \vec{F}(E_i,E_j) + \sum_{V_i,F_j} \vec{F}(V_i,F_j) + \sum_{V_j,F_i} \vec{F}(V_j,F_i). \quad (2)$$

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 δ between them

$$\delta(G_i,G_j) = R_i + R_j - d(G_i,G_j), \qquad (3)$$

with $d(G_i,G_j)$ the distance between the features of the spheropolytopes R_i the spheroradius of the i-th spheropolytope. The point of contact between the two features is calculated as follows: First we take the spheres of radius R_i and R_j centered in the closest points $\vec{X}_i$ and $\vec{X}_j$. Then the contact point is defined as the intersection between the line from $\vec{X}_i$ to $\vec{X}_j$ and the plane containing the intersection points of the two spheres. This contact point results as

$$\vec{R}(G_i,G_j) = \vec{X}_i + \frac{R_i^2 - R_j^2 + d^2(G_i,G_j)}{2d(G_i,G_j)} \frac{\vec{X}_j - \vec{X}_i}{||\vec{X}_j - \vec{X}_i||}, \quad (4)$$

From the point of application of the contact forces we get the torque associate to each pair of features as:

$$\vec{\tau}_i(G_i,G_j) = (\vec{R}(G_i,G_j) - \vec{r}_i) \times \vec{F}(G_i,G_j) \qquad (5)$$

with $\vec{r}_i$ the center of mass of the i-particle.

Since the formulas of distance are continuous functions on the degrees of freedom of the particles, the total

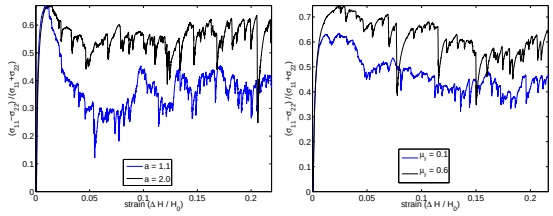

FIGURE 2. Left: stress versus strain for two values of aspect ratio. Right: stress versus strain for two different coefficients of rolling resistance. The deviatoric and volumetric components of stress are given by $\sigma_D = \sigma_{11} - \sigma_{22}$ and $\sigma_V = \sigma_{11} + \sigma_{22}$.

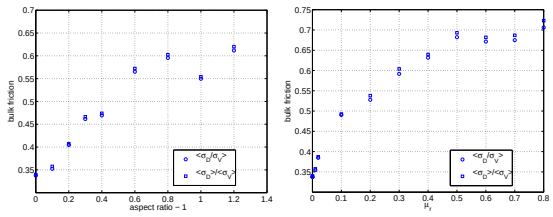

FIGURE 3. Left: mean stress ratio versus strain for different values of aspect ratio. Right: mean stress ratio versus μ_r. The averaged $< . >$ is taken for axial stress values between $\varepsilon_1 = 0.04$ and $\varepsilon_1 = 0.2$ in Fig. 2.

force is continuous too. This avoids the problems of discontinuity in time of the forces in previous models [10]. Different forces can be included in this model: for example, a force derived from a potential function of the distance leads to a conservative systems; forces depending on the relative velocity at the contact points lead to dissipative granular materials; Forces depending on the history of relative velocity at the contacts represent frictional granular systems.

The model is implemented in C++ using Object Oriented Programming. The basic classes of the simulators are Particle and Interaction. To allow high quality visualization, we use POV-Ray, which is a very popular ray traced program for image rendering.

3. BIAXIAL TEST SIMULATIONS

In this section we perform biaxial test simulations of spherical and non-spherical particles in 2D and 3D. The aim is to check whether rolling resistance on spherical particles can surrogate grain shape in granular materials. This question is essential in modeling realistic particulate materials and constructing predictive micromechanical continuum models [11]

First we compare the biaxial test simulations of two different 2D models. The first one consists of circular particles with rolling resistance. We use a isotropic model of rolling resistance, as proposed in [11]. The second model uses rice shaped particles, which are generated with spherocylinders (line segment $\oplus$ spheres) with different aspect ratios. The main results of the comparison of the two models is shown in the Fig. 2. As the aspect ratio or the particles increases, the stress in the limit of large strain increases (Fig. 2 left). A similar behavior is observed in circular particle when the coefficient of rolling resistance is increased (Fig. 2 right).

We also compare the bulk friction (averaged stress ratio) for both models of circular and non circular particles (Fig. 3. For large values of aspect ratio the bulk friction reaches a constant value around $= 0.6$. Similar behavior is observed in circular particles with rolling resistance, with a the constant value is around 0.7. This probe that the effect of rolling resistance on the strength of the materials is similar than the effect of the aspect ratio.

The buckling of force chains and its effect on stress fluctuations are very similar for both kind of simulations. Stress-drop events are more scarce as the aspect-ratio/rolling-resistance increases. These correlations allow us to understand the extend of the validity of the models of spherical (circular) particles with rolling resistance. Typically all stress drops are associated to short time events where the dissipated energy peaks. For low aspect ratios dissipation occurs mainly with buckling of force chains. However, for aspect ratios above 2.2 some stress drops may appear without force chain buckling. Such stress drops without bucking are observed in force chains of particles which are aligned each other. Since particles cannot rotate along these chains, the sliding is the preferred mechanism of collapse of force chain. Therefore the mechanism of building and collapse of force chain is governed by buckling of force chains for particles with low anisotropy, but new modes of collapse can be observed for elongated partices.

We also want to prove whether the stress collapses during shear remain in 3D simulations, we perform biaxial test simulations with spherocylinders in 3D. We attain a similar behavior than in 2D: for low shear deformation the sample compacts while the stiffness decreases. Then the sample start to dilate, the deviatoric stress peaks. In the limit state both stress ratio and density reaches a critical state with some stress fluctuation. The fluctuation comes from the collapse of force chains in the highly heterogeneous contact networks, as shown in the Fig. 4. We therefore conclude that 2D simulations behaves similar in 3D for biaxial test. However, 3D models can be used to perform more sophisticated loading program by simulating true triaxial test apparatus.

4. CONCLUDING REMARKS

The aim of this paper was to show the importance of computational geometry on the realistic modeling of

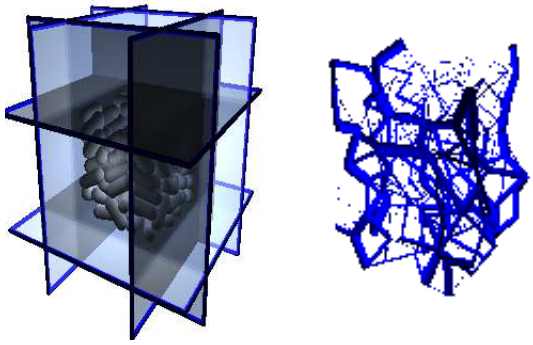

FIGURE 4. Right: Biaxial test apparatus with rice like particles. Left: contact network represented by cylinder. Each cylinder correspond to a contact, and its width encodes intensity of normal force.

granular materials. We presented the Minkowski sum approach as an attractive alternative to model 3D granular materials with arbitrary particle shape. We used the method to simulate biaxial test simulation with circular particles and rice shaped particles in 2D and 3D. Circular particles with rolling resistance allows to capture some effects of particle shape, but some modes of collapse of force chains in highly anisotropic particles cannot be captured with the model. Qualitatively the biaxial test simulations in 2D are similar than 3D. Interestingly, the broad distribution of contact forces are observed in 2D and 3D, and the stress drops seems to obey to the same mechanism in both cases: the building and collapse of force chains.

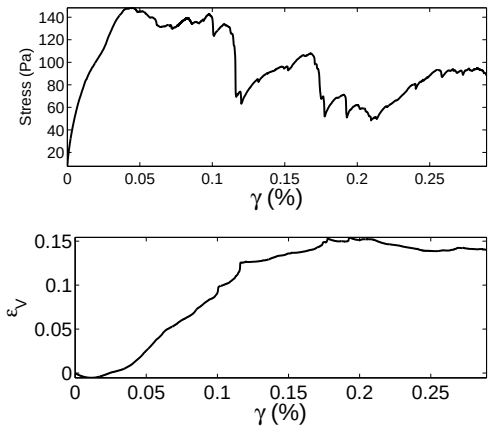

FIGURE 5. Stress versus axial strain (above) and volumetric strain versus axial strain (bellow) in 3D biaxial test simulations with rice. The void ratio is the volume of the void space divided by the volume of the particles.

We are performing the first steps in 3D simulations, and several improvements are planned for the near future: The generation of packings of particles in 3D will require the extension of the Voronoi-Minkowski diagrams introduced in [6]; The speed up of the simulation needs an extension of the Verlet list, as is proposed in [5]. A user & developer -friendly platform in C++ is under development, using the philosophy of Object Oriented Programming and the concepts of encapsulated containers [9]. The main challenges are to understand how non-convexity of the particle shape affect granular flow and global stiffness, and to determine the role of pore pressure and grain crushing in the dynamics of shear zones as observed in landslides, earthquakes and industrial particulate processes.

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REFERENCES

1. L. Verlet, *Phys. Rev* **159**, 98–103 (1967).
2. F. Alonso-Marroquin, I. Vardoulakis, H. J. Herrmann, D. Weatherley, and P. Mora, *Phys. Rev. E* **74**, 031306 (2006).
3. L. Pournin, and T. Liebling, "A generalization of distinct element method to tridimentional particles with complex shapes," in *Powders & Grains 2005*, Balkema, Leiden, 2005, pp. 1375–1478.
4. L. Pournin, *On the behavior of spherical and non-spherical grain assemblies, its modeling and numerical simulation*, Ph.D. thesis, École Polytechnique Fédérale de Lausanne (2005).
5. F. Alonso-Marroquin, *Europhysics Letters* **83**, 14001 (2008).
8. S. A. Galindo, and F. Alonso-Marroquin (2008), eprint arXiv:0811.2858, submitted to Phys. Rev. E.
7. L. Pournin, M. Weber, M. Tsukahara, J.-A. Ferrez, M. Ramaioli, and T. M. Liebling, *Granular Matter* **7**, 119–126 (2005).
6. S. A. Galindo, F. Alonso-Marroquin, and Y. Wang (2008), eprint arXiv:0811.3060, submitted to Phys. Rev. Lett.
9. F. Alonso-Marroquin, and Y. Wang, An efficient algorithm for granular dynamics simulations with complex-shaped objects (2008), arXiv:0804.0474, submitted to Granular Matter.
10. B. Mirtich, *ACM Transactions on Graphics (TOG)* **15**, 177–208 (1998).
11. A. Tordesillas, *Philosophical Magazine* **87**, 4987–5016 (2007).