An efficient algorithm for granular dynamics simulations with complex-shaped objects

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Abstract

The most difficult aspect of the realistic modeling of granular materials is how to capture the real shape of the particles. Here we present a method to simulate granular materials with complex-shaped particles. The particle shape is represented by the classical concept of a Minkowski sum, which permits the representation of complex shapes without the need to define the object as a composite of spherical or convex particles. A well defined interaction force between these bodies is derived. The algorithm for identification of neighbor particles reduces force calculations to $O(N)$, where $N$ is the number of particles. The algorithm is much more efficient, accurate and easier to implement than other models. We investigate the existence of a statistical equilibrium in granular systems with circular non-spherical particles in the collisional regime. We also investigate the limit state of dissipative granular materials using biaxial test simulations. The results agree with the classical assumption of the statistical mechanics for non-dissipative systems, and the critical state theory of soils mechanics for dissipative granular materials.

Key words: Granular systems, Dynamics and kinematics of rigid bodies, Molecular dynamics methods
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1 Introduction

Rapid advances in computer simulations have led to many new developments in the modeling of particulate systems. These systems represent different real physical systems at different scales, such as the small scale of liquid crystals [1], geological scales of snow and debris flow, and the astronomical scales of planetary rings or dynamics evolution of precursors of planets [2]. Although particle shape plays an important role, most theoretical and numerical developments have been restricted to particles with spherical or circular shape. These simplification lead in some cases to unrealistic properties. In collisional
non-dissipative systems, spherical (or circular) particles can not exchange angular momentum, so that the system cannot explore all the phase space during the evolution. 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 bulk friction coefficients.

Three different approach has been presented to model the real shape of particulate materials. In the first approach the shape is represented as a scalar functions. This model allows to represent especific shapes, such as ellipses [3], ellipsoids [4] and superquadric [5]. The main drawback of those methods is that the calculations required in the contact force are much more expensive than in spherical (or circular) particles. In the second approach the non-spherical particle is represented ad aggregates or clumps of disks and spheres bonded together [6,7]. In this approach crushing and fracture of aggregates can be easily modeled. The disadvantage is that this method requires a larger number of particles.

The third approach is represent the complex shape using polygons in 2D, [8,10] or polyhedrons in 3D [11,12] The most difficult aspect for the simulations of these objects is the handling of contact interactions. Nowadays, the interaction is resolved by decomposing them in convex pieces, and applying penalty methods, impulse-based methods or dynamic constraints in the interaction between these pieces. Impulse-based methods (also called even-driven methods) allow real-time simulations, but they cannot handle permanent or lasting contacts [11]. On the other hand, constraint methods (or contact dynamics methods) can handle resting contacts with infinite stiffness, but simulations are computationally expensive and lead in some cases to indeterminacy in the solution of contact forces. This indeterminacy is removed by using penalty methods, where the bodies are allowed to interpenetrate each other and the force is calculated in terms of their overlap. However, until very recently the determination of such contact force has been heuristic and lacks physical correctness, because the interactions do not comply with energy conservation [13].

We propose a solution to this problem in 2D based in the mathematical concept of spheropolygons. These objects are generated from the Minkowski sum of a polygon with a disk, which is nothing more than the object resulting from sweeping a disk around the polygon. The 3D counterpart of these objects are the spheropolyhedrons, which were recently introduced by Pournin and Liebling for the simulations of granular media. 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. Here we introduce an efficient method to calculate dissipative and non-dissipative interaction between spheropolygons. We probe also that the model complies with the statistical mechanical principles and the physical laws of a conservative system.
Since the code can simulate particles a wide range of shapes, it can be used to investigate the effect of the aspect ratio, angularity and non-convexity of the particles on granular flow. The relevance of this investigation is demonstrated in the stress-strain response in biaxial test below, where we show that the system reach the critical state of soil mechanics, where the particle shape strongly affect the material properties of the granular media.

2 Model

Systems with different particle shapes are modeled using the concept of the Minkowski sum of a polygon (or polyline) with a disk. This mathematical operation is explained in Sub-Section 2.1. Sub-section 2.2 leads with the numerical calculation of mass properties. The interaction between the particles is obtained from the individual interaction between each vertex of one polygon and each edge of another, as explained in Sub-Section 2.3. In Sub-Section 2.4 we present a method to reduce the number of floating point operations used to calculate interaction forces is drastically reduced by using a neighbor list and a contact list for each pair of neighbor particles. In Sub-Section 2.5 we present the algorithm used in each time step of the dynamic simulation.

2.1 Minkowski sum

Given two sets of points P and Q in an Euclidean space, their Minkowski sum is given by $P + Q = \{\vec{x} + \vec{y} | \vec{x} \in P, \vec{y} \in Q\}$. This operation is geometrically equivalent to the sweeping of one set around the profile of the other without changing the relative orientation. A special case is the sum of a polygon with a disk, which is defined here as spheropolygons. Other examples of a Minkowski sum are the spherocylinder (sphere + line segment) [14], the spherosimplex (sphere+simplex) [15] and the sphero-polyhedron (sphere+polyhedron) [16], which are used in simulations of particulate systems.

The main advantage of the spheropolygons is that they allow us to represent any shape in 2D, from rounded to angular particles, and from convex to non-convex shapes. As we will see in Sub-Section 2.3 The Minkowsky sum does not need to be explicitly calculated to determine the particle interaction. The calculation of the mass properties, however, are calculated numerically, but this does not affect much the simulation time because the calculations are done only a the beginning of the simulations.
2.2 Mass properties

Before calculating the mass, center of mass and moment of inertia of the spheropolgons we need to introduce some useful concepts. Given a spheropolgon $SP = P + S$, the polygon $P$ will be called the polygon-base; and the radius $r$ of the disk $S$ spher-radius. The distance $d(\vec{X}, P)$ from a test point $\vec{X}$ to the polygon-base is defined as follows: If the point is outside the polygon, it is given by the minimum distance between the point and the edges of the polygon; If the point is inside the polygon, we let $d(\vec{X}, P) = 0$. Finally, the point $\vec{X}$ is inside of the spheropolygon when it satisfies $d(\vec{X}, P) < r$.

The point-inside-spheropolygon test combined with a basic Monte Carlo method is used to evaluate the integral expressions for mass, center of mass and the moment of inertia. The numerical integration is performed by taking a quasi-random set of points $\vec{X}_i$ uniformly distributed in a rectangular box containing the object. Then the integral over the area enclosed by the spheropolygon of any function $f(\vec{X})$ is calculated as:

$$M = \int_{SP} f(\vec{X})da \approx \frac{A_{box}}{N_p} \sum_{i=1}^{N_p} \chi(\vec{X}_i)f(\vec{X}_i).$$

(1)

$A_{box}$ is the area of the rectangular box, $\vec{X}_i$ is a quasi-random point inside $A_{box}$, and $N_p = 1.6 \times 10^4$ is the number of points. $\chi(\vec{X})$ is the characteristic function, which returns one if $\vec{X}$ is inside the spheropolygon and zero otherwise. Replacing $f(\vec{X})$ by $\sigma$, $\sigma\vec{X}$, $\sigma||\vec{X}||^2$ results in $M = m, m\vec{r}, I + m||\vec{r}||^2$ respectively, where $\sigma$ is the density, and $m$, $\vec{r}$ and $I$ are the mass, center of mass and moment of inertia.
2.3 Interaction force

To solve the interaction between spheropolygons we consider all vertex-edge
distances between the polygons base. we consider two spheropolygons $SP_i$ and
$SP_j$ 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
overlapping length between each pair of vertex-edge $(V_i, E_j)$ is defined as

$$\delta(V, E) = (r_i + r_j - d(V, E)),$$

where $d(X, E) = ||\vec{Y} - \vec{X}||$ is the Euclidean distance from the vertex $V$ to the
segment $E$. Here $\vec{X}$ is the position of the vertex $V$ and $\vec{Y}$ is its closest point on
the edge $E$. The ramp function $\langle x \rangle$ returns $x$ if $x > 0$ and zero otherwise. The
overlapping length in Eq. (2) is equivalent to the interpenetration be
tween the
disks of radii $r_i$ and $r_j$ centered on $\vec{X}$ and $\vec{Y}$.

The force $\vec{F}_{ij}$ acting on particle $i$ by the particle $j$ is defined by:

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

where $\vec{F}(V, E)$ represent the force between the vertex $V$ and the edge $E$.
if the vertex-edge pair do not overlap, $\vec{F}(V, E) = 0$. Different of vertex-edge
forces can be included in the modelL linear dashpots, non-linear Hertzian laws,
dissipative viscous forces proportional to the relative normal and tangential
velocities, sliding friction, etc The force of Eq. (3) is applied to each particle in
the middle point of the overlap region between the vertex and the edge:

$$\vec{R}(V, E) = \vec{X} + (r_i + \frac{1}{2} \delta(V, E)) \frac{\vec{X} - \vec{Y}}{||\vec{Y} - \vec{X}||},$$

so that the resulting torque on particle $i$ given by $j$ is

$$\tau_{ij} = \sum_{V_i, E_j} (\vec{R}(V_i, E_j) - \vec{r}_i) \times \vec{F}(E_i, V_j)$$
$$+ \sum_{V_j, E_i} (\vec{R}(V_j, E_i) - \vec{r}_i) \times \vec{F}(E_j, V_i),$$

where $\vec{r}_i$ is the center of mass of particle $i$.

The evolution of $\vec{r}_i$ and the orientation $\varphi_i$ of the particle is governed by the
equations of motion:

$$m_i \ddot{\vec{r}}_i = \sum_j \vec{F}_{ji} - m_i g \hat{y}, \quad I_i \ddot{\varphi}_i = \sum_j \tau_{ji}.$$
Here $m_i$ and $I_i$ are the mass and moment of inertia of the particle. The sum is over all particles interacting with this particle; $g$ is the gravity; and $\hat{y}$ is the unit vector along the vertical direction.

### 2.4 Efficient calculation of forces

The efficiency of the dynamics simulation is mainly determined by the method of contact detection. In a system of $N$ particles, each one with $M$ edges, the number of operations required to update the positions of the particle in each time step is in the order of $O(NM)$, whereas the number of calculations for contact detection is $O(N^2M^2)$. Simulations therefore become very slow when either the number of particles or the number of vertices is large.

The first step to speed up the simulations is to execute the force calculation only over neighbor particles. With this aim we introduce the neighbor list, which is the collection of pair particles whose distance between them is less than $2\delta$. (The distance between two particles is defined as the minimum of all vertex-edge distances). The parameter $\delta$ is equivalent to the Verlet distance used in simulations with spherical particles [13]. As shown in the Fig. 2, the Verlet method is equivalent to surround the particles by a skin, so that the neighbors list consists of all particles pairs whose skins overlap.

A link cell algorithm [13] is used to allow rapid calculation of this neighbor list: First, the space occupied by the particles is divided in cells of side $D+\delta$, where $D$ is the maximal diameter of the particles. Then the link cell list is defined as the list of particles hosted in each cell. Finally, the candidates of neighbors for each particle are searched only in the cell occupied by this particle, and its eight neighbor cells.

The neighbor list is calculated at the beginning of the simulation, and it is updated when the following condition is satisfied:

$$\max_{1 \leq i \leq N} \{ \Delta x_i + R_i \Delta \theta_i \} > \delta.$$  \hspace{1cm} (7)

$\Delta x_i$ and $\Delta \theta_i$ are the maximal displacement and rotation of the particle after the last neighbor list update. $R_i$ the maximal distance from the points on the particle to its center of mass. After each update $\Delta x_i$ and $\Delta \theta_i$ are set to zero. The update condition is checked in each time step. Increasing the value of $\delta$ makes updating of the list less frequent, but increases its size, and hence the memory used in the simulation. Therefore, the parameter $\delta$ must be chosen by making a compromise between the storage (size of the neighbor list) and the computer time (frequency of list updates).
Fig. 2. Method for identification of neighbor list: the space domain is divided by square cells. Then the potential neighbor of the particles are those hosted in the same cells, or in the adjacent cells. Each particle has as skin of thickness $\delta$. If the skins of two potential neighbors overlap, they are included in the neighbor list.

Neighbor list reduces the amount of calculations to $O(NM^2)$. Therefore the simulations are still very expensive when particles consist of a large number of vertices. Further reduction of the number of calculations between neighbor particles can be done by identifying which part of a particle is neighbor to the other. This idea is implemented as follows: for each element of the neighbor list, we create a contact list, which consists of those vertex-edge pairs whose distance between them is less than $r_i + r_j + 2\delta$, where $r_i$ and $r_j$ are the sphero-radii. In each time step, only these vertex-edge pairs are involved in the contact force calculations. Overall, neighborhood identification requires a neighbor list with all pair of neighbor particles, and one contact list for each pair of neighbors. These lists require little memory storage, and they reduce the amount of calculations of contact forces to $O(N)$, which is of the same
order as in simulations with spherical particles [13].

2.5 Time Integration

The equations of motion of the system are numerically solved using a four order predictor-corrector algorithm [13]. A pseudocode with the basic procedures in each time step is shown in Algorithm 1. The predicted method calculates the position (center of mass and orientation) of each particle and its derivatives using a Taylor expansion. Next the vertices of the all polygons are updated according to the predicted positions of the particles. If the neighbor update condition of Eq. 7 is satisfied, the link cell is calculated, and then it is used to update the neighbor list and the contact list of each one of its elements. Then the contact forces and torques are calculated. Finally, forces and torques are used to correct the position of the particles and their derivatives. The algorithm is basically the same as the used in polygons, except that the force is calculated using Eqs. 3. Note that the efficiency of the code is based on the simplicity of the contact force calculation, and in the fact that the Minkowski sum does not need to be calculated during the time integration.

The parameters of the simulations are a constant stiffness $k = 10^7 N/m$, gravity $g = 10 m/s^2$, density $\sigma = 1 kg/m^2$, time step $\Delta t = 10^{-5} s$ and Verlet distance $\delta = 1 m$.

**Input:** state of the particles at time $t$

**Output:** state of the particles at time $t + \Delta t$

predict position of the particles and its derivatives;

if neighbor update condition is satisfied then
  calculate link cell;
  update neighbor list;
  update contact lists;
end

update vertices of the particles;
calculate contact forces between neighbor particles;
apply contact forces to the particles;
apply gravity forces to the particles;
correct positions and its derivatives using forces and torques;

**Algorithm 1:** One time step of the time integration scheme
3 Non-dissipative granular dynamics simulations

As a first step we present here simulations results of many body conservative systems. We investigate the evolutions towards the statistical mechanical equilibrium of this simple system. Generalization to dissipative system driven by external forces will be presented in forthcoming papers.

3.1 Energy balance

The vertex-edge interaction between the particles is given by

\[ F(V, E) = k \delta(V, E) \hat{N} \]

(8)

where The material parameter \( k \) is the stiffness constant, \( \delta(V, E) \) is given by Eq. 2 and \( \hat{N} \) is the unit normal vector:

\[ \hat{N} = \frac{\vec{Y} - \vec{X}}{||\vec{Y} - \vec{X}||} \]

(9)

Here \( \vec{X} \) is the position of the vertex \( V \) and \( \vec{Y} \) is its closest point on the edge \( E \).

The question which now arises is whether the vertex-edge interaction in Eq. 8 leads to a conservative system. Let us multiply the first equation in (6) by \( \dot{\vec{r}} \) and the second one by \( \dot{\varphi} \). Next we sum both equations and then sum over all particles. After some algebra we get the energy conservation equation:

\[ E_T = \sum_{ij} E_{ij}^e + \sum_i \left( \frac{1}{2} m_i v_i^2 + \frac{1}{2} I_i \omega_i^2 \right) = cte. \]

(10)

The first term of this equation corresponds to the potential elastic energy at the contacts:

\[ E_{ij}^e = \frac{1}{2} k \left( \sum_{V_i E_j} \delta(V_i, E_j) + \sum_{V_j E_i} \delta(V_j, E_i) \right). \]

(11)

The other terms of Eq. (10) are the linear and rotational kinetic energy of the particles. We emphasized that the elastic force in Eq. (3) belongs to the potential energy defined by Eq. (11), which proves that our model is conservative. The simplicity of this force contrasts to the Pöschel’s model for interacting
Fig. 3. Systems obtained from Minkowski sum approach: (a) disks (Vertex + disk); (b) rice (segment + disk); (c) peanuts (Polyline + disk) and (d) pebbles (triangle + disk)

triangles [13], where the forces and torques associated to his potential energy lead to a much more expensive calculation.

Other important aspect of this dynamics simulation is the accuracy of the numerical solution. The numerical error in the energy calculation is evaluated by performing a series of simulations with many non-spherical particles interaction via the elastic force given by Eq. 8. Each test consists of 400 particles confined by four fixed rectangular walls. Each particle occupies an area of $1cm^2$ and the confining area is $46cm \times 46.25cm$. These dimensions lead to a volume fraction of $\Phi = 0.186$. Each sample consists of identical particles with a specific spheropolygonal shape as shown Fig. 3: disks (point+disks) rice (line+disk), peanuts (polyline+disk), and pebbles (triangle+disk).
Fig. 4. Time evolution of the total kinetic and potential energy in the non-dissipative system. As is expected from the energy conservation, the total energy keeps constants, except numerical error which are lower than 0.01% throughout all the simulations.

Initially, each particle has zero angular velocity and a linear velocity of 1 cm/s with random orientation. Due to collisions, the linear momentum of each particle changes and part of it is transferred to angular momentum. Fig 4 show the potential (a) kinetic (b) and total (c) energy of the system. Elastic energy has a negligible contribution to the energy budget, as it differs from zero only for short times during collisions. Energy conservation is numerically verified within a percentual error of 0.01%. The energy fluctuations are produced by time discretization. We shall note also that energy have a trend to grow slowly in all samples.

3.2 Statistical equilibrium

Simulations with a large number of particles show that elastic interactions allow the particles to exchange energy and momentum, whereas its contribution to the energy budget is negligible. This property leads us to investigate
the existence of a statistical equilibrium in a gas of non-spherical particles. It is expected that the system will reach the statistical equilibrium, which is characterized by an energy equipartition and a Maxwell-Boltzmann statistics for energy distribution [17]:

The energy of the system consist of rotational and translational kinetic energy. At the beginning of the simulations the rotational kinetic energy is zero, and it increases during the simulations due to collision, see left part of the Fig. ?? For all the samples, we observe the same stationary regime, where the average of rotational kinetic energy reaches the limit of 1/2 of the linear kinetic energy. This is in agreement with the theorem of equipartition of energy [17], which states that each quadratic term in the energy should contribute the same weight in the mean energy of the system. It is expected that the system reach the statistical equilibrium, which is characterized by a Maxwell-Boltzmann statistics for energy distribution [17]:

\[
\rho(E_k) dE_k = 2 \sqrt{\frac{E_k}{\pi(kT)^3}} \exp\left(-\frac{E_k}{k_B T}\right) dE_k, \tag{12}
\]

here \(E_k = \frac{1}{2}(mv_x^2 + mv_y^2 + I\omega^2)\) is the kinetic energy of the particle; \(T\) the temperature; and \(k_B\) the Boltzmann constant. The mean energy of the particles leads to \(\bar{E}_k = \int_0^\infty \rho(E_k) E_k dE_k = \frac{3}{2}k_B T\).

We also calculate the energy distribution of the particles in the stationary regime. In order to calculate the energy distribution, we take snapshots of the simulations between \(t = 1s\) and \(t = 8s\) distanced by 0.01s. In each snapshot the kinetic energy of the individual particles is measured. The histogram of the variable \(\epsilon = E_k / \bar{E}_k\) is constructed using 100 identical bins between zero and the maximal value. According to Eq. (12), the theoretical distribution of \(\epsilon\) must satisfy \(\rho(\epsilon) d\epsilon = 2 \sqrt{\beta^3} \exp(-\beta\epsilon) d\epsilon\), where \(\beta = 3/2\). An excellent agreement between this theoretical distribution and the simulations data is shown in Fig. 6. Simulations with different non-spherical shapes, which will be presented elsewhere [15], show that energy distribution for all samples collapse onto the theoretical expected value. It is also shown that the relaxation time for the statistical equilibrium is very sensitive to the degree of non-sphericity of the particle.

4 Dissipative granular dynamics simulation

Here we present biaxial tests simulations with circular and non-circular particles. Usually, the granular assemblies are compacted and loaded within a set of confining walls. These walls act as boundary conditions, and can be moved by specifying their velocity or the force applied on them. The response of the
walls can be used to calculate the global stress and strain of the assembly.

The interaction of the spheropolygons with the walls is modeled here by using a simple visco-elastic force. First, we allow the polygons to penetrate the walls. Then, for each vertex of the polygon $\alpha$ inside of the walls we include a force

Confining walls can be used to generate samples with different void ratios. Starting from a very loose packing, the sample is compacted by applying a centripetal gravitational field to the particles and on the walls, oriented to the center of mass of the assembly. Then the sample is subjected to an isotropic compression until the desired confining pressure is reached. In order to generate dense samples, the interparticle friction is set to zero during the construction. The loose samples are created taking damping coefficients 100 times greater than those used in the test stage. Samples with void ratio ranged from 0.128 to 0.271 can be achieved with this method [19].

We have investigated shear deformation of granular samples with different initial void ratios [19]. Shear bands are observed in dense samples, whereas they seem to be absent in loose ones. They share some common properties of
the shear bands in real granular materials, such as their characteristic reflection when they reach the boundary wall. Shear band orientation lies between the Roscoe angle and Mohr-Coulomb solution, as in most of the experimental data.

For large shear deformations all samples reaches the critical state, which is independent on their initial density. Once the samples reaches this state, they deform at constant void ratio and coordination number \cite{19}. The evolution of the deviatoric stress exhibits fluctuations around the residual strength. Abrupt reduction of the stress results from the collapse of force chains, as shown the Fig. 6. collapse of force chains makes the sample to approach and retreats unstable stages. A similar behavior is observed in glass bead samples \cite{20} and packings of glass spheres \cite{21}. Experimental biaxial tests show evidence of dynamic instabilities at the critical state \cite{22}. Erratic slip-stick motion at the critical state is interesting, owing to its potential analogy with earthquake dynamics \cite{23}.

Fig. 6. energy distribution $N(\epsilon)$ for the particles, where $\epsilon = E_k / \bar{E}_k$. The line corresponds to the best fit $n(\epsilon) = 2\beta \sqrt{\epsilon \beta / \pi} \exp(-\beta \epsilon)$, with $\beta = 1.5$. 
Lastly, we compare the efficiency of the many-body simulations of systems consisting of disks, spheropolygons and clumps of spheres. Each spheropolygons correspond to a particle with complex shape, and it consist on 62 vertices. The clump of spheres represents the same complex shaped particles, and it need 726 particles. The macroparticles they are simulating by summing up the contact forces between the constituting disks, and updating all the disks of each particle according with its current position. The performance of the simulations is estimated by running different processes in a Pentium 4, 3.0GHz, and calculating the Cundall number is each one of them. This number is the amount of particle time steps executed by the processor in one second, which is calculated as \( c = N_T N / T_{CPU} \), where \( N_T \) is the number of time steps, \( N \) is the number of particles and \( T_{CPU} \) is the CPU time of the simulation.

Fig. 9 shows the Cundall number versus the number of particles for the three
cases. When the number of particles is between $N = 100$ and $N = 1000$ the Cundall number is approximately constant. This constant is around 100,000 for disks, 2,000 for spheropolygons, and 50 for clumpy particles. Therefore the simulations with spheropolygons, although slower than simulations with disks, are much faster than simulations with clumpy particles. This is because each time step needs to update the position of 62 vertices of the spheropolygons whereas it needs to update the position of the 726 disks in the case of the clumpy particles. Therefore simulations with spheropolygons are more efficient than those ones with clumps of disks, because the former ones require less elements to represent the particle shape.

6 Concluding remarks

The method presented here provide an energy balance equations and a wide range of particle shape representations, including non-convex particles and tunable grain roundness. This paper shows that modeling interacting particles using spheropolygons has several advantages with respect to other existing particle-based models: i) The possibility to model non-convex particles; ii) a realistic representation of the surface curvature of particles; iii) guaranteed
Fig. 9. Stress versus strain (a) and void ration versus strain (b) for different particles shape, in biaxial test simulations. The dotted line in (a) represents $p/k_n$, where $p$ is the applied pressure on the latteral walls.
compliance with physical and statistical mechanical laws; iv) balance between accuracy and efficiency. Benchmark tests prove energy conservation with an error below 0.0001%. Simulations with many particles verify the Maxwell-Boltzmann distribution and the principle of energy equipartition. The computational efficiency is compared to simulations with disks and clumps of disks. Simulations with disks are around 50 times faster than simulation with spheropolygons. However, the speed of the simulation is 40 times faster that simulations with clumpy particles.

The method overcomes also two main difficulties existing in previous DEM developments.

(1) The interaction between polygons using the overlapping area is difficult to generalize in 3D, because the overlap between polyhedrons is much more difficult to evaluate.

(2) The elastic force used in this work does not belong from a potential, so that this model does not provide an equation for energy balance. In the investigation of fault zones, the energy balance is required to determine the energy budget in earthquakes.

The model is still very simple, but extensions to more complex interactions and 3D simulations are achievable in the near future. Cohesive and frictional forces can be incorporated by introducing internal variables in each vertex-edge contact. These variables account for elastic deformation at the contacts and they must be updated in each time step according to the sliding conditions or breaking criterion. 3D modeling using spheropolyhedra requires elastic forces similar to Eq. (3), where the sum is over all vertex-face and edge-edge interactions. Special attention is required for the case of two parallel edges in contact. This case leads to a non-uniqueness in the selection of contact points. This need to be resolved to get a physical correctness in the torque calculation.

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