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A novel method based on orientation discretization for discrete element modeling of non-spherical particles

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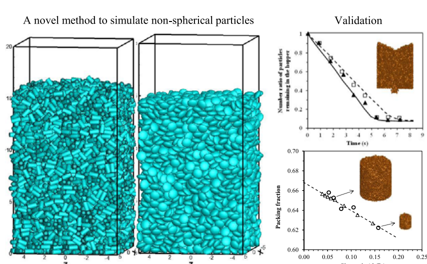
HIGHLIGHTS

- A novel method for discrete modeling of non-spherical particles is proposed.
- The method is based on a "new" concept, orientation discretization.
- The method is simple, fast and general.
- The method is comprehensively validated in a series of simulations.

GRAPHICAL ABSTRACT



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ABSTRACT

We present a novel method for discrete element modeling of non-spherical particles. The method is based on orientation discretization and pre-calculated databases and can be applied to any shaped particles in a general scheme. The method is realized in both two and three dimensions. And it is used to simulate the packing and flow of different shaped non-spherical particles. The good agreement between the simulated results and those reported in the literature, including experimental results and well established numerical results, verifies the method. The computational speed is shown to be fast and independent of particle shape. Further developments and potential applications of the method are also discussed.

1. Introduction

1.1. Discrete element method study of granular materials

Granular materials are commonly seen in nature and a broad range of industries, while they are still far from well understood (Jaeger et al., 1996; de Gennes, 1999). Previous studies on granular materials are largely at a macroscopic or global scale, the resulting information being helpful for a particulate process of particulate interest, but difficult to generate a general method for reliable scale-up, design and control/optimization. This is because the dynamic behavior of a granular material is very complicated due to the complex interactions between individual particles and their interactions with boundaries and environments. Understanding the underlying mechanisms in terms of these interactions requires particle-scale research based on the information of individual particles. However, the information, largely if not entirely, is difficult to obtain by the current experimental techniques (Aste et al., 2006; Li et al., 2006; Moreno-Atanasio et al., 2010). Computer simulation based on discrete element method (DEM) is an effective alternative (Cundall and Strack, 1979; Zhu et al., 2007). DEM uses Newton's second law to describe the motion of

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each particle without any arbitrary assumptions, and readily provides particle-scale information at each time step. Various studies of granular materials by DEM can be found in a recent review (Zhu et al., 2008).

Since the work of Cundall and Strack (1979), the algorithm for DEM has been developed continuously, from two dimensions (2D) to three dimensions (3D), from using preliminary to sophisticated force models (Langston et al., 1995; Thornton et al., 2011; Zheng et al., 2012), from handling simple and static geometries to complicated dynamic geometries (Kremmer and Favier, 2001; Dong et al., 2009b; Su et al., 2011), and from small to large scale systems (Gopalakrishnan and Tafti, 2013; Ren et al., 2013). However, in the current DEM simulations spherical particles are far more commonly used than non-spherical particles. As the overlap between two non-spherical particles is not easy to determine, neither is the contact force (Džiugys and Peters, 2001). But particle shape is a primary variable controlling the behavior of a granular material, as demonstrated in many aspects. For example, in the static systems such as particle packing, it affects packing fraction, i.e., the ratio of the volume of particles to that of the space they occupy (Zou and Yu, 1996; Donev et al., 2004; Man et al., 2005; Zhou et al., 2011); in the quasi-static systems such as a sandpile, it affects the repose angle (Matuttis et al., 2000) and the pressure dip under the pile (Zuriguel et al., 2007; Zhou et al., 2014); and in the dynamic systems such as hopper flow, it affects inter-locking between particles and hence the flow rate (Kohring et al., 1995; Matuttis et al., 2000; Cleary and Sawley, 2002; Langston et al., 2004; Liu et al., 2014).

1.2. *Current methods to model non-spherical particles*

To model different shaped particles is an evitable challenge for the development of DEM. In the literature, there are various methods to model non-spherical particles in DEM, which can be divided into several categories, as listed in Table 1. Comparing the accuracy, versatility, complexity and speed of these methods, we can see each method has advantages in one or two aspects, but always compromises the other disadvantageous aspects. Using composite particles (Favier et al., 1999; Abou-Chakra et al., 2004; Peters et al., 2009; Ferellec and McDowell, 2010), particularly clumping of spheres, the contact detection is simple, but a large number of components (spheres) will need to be used to construct a given shape, resulting in an increased computational effort. There are also different ways in selecting spheres to mimic a shape, which may bring uncertainty in the modeling (Ferellec and McDowell, 2010; Peters et al., 2009). For example, it is demonstrated that the collision behavior of such a particle strongly depends on its alignment (Kodam et al., 2010b; Kruggel-Emden et al., 2008).

Using combined surface particles can also represent any shaped particles in theory (Nezami et al., 2004; Fraige et al., 2008; Vorobiev, 2012), but practically fine meshes may need to be used to approximate a smooth curved surface (Peters et al., 2009). It also consumes relatively more computational resources considering a large amount of information for vertexes, edges and faces needed to be stored and updated during simulations, and steps required in judging every possible type of contacts between two particles, e.g., vertex-to-edge, edge-to-edge, edge-to-face, and so on. Some algorithms based on the "Common-Plane" concept have been developed, being able to avoid such tedious procedures and significantly increase the speed (Chang and Chen, 2008; Nezami et al., 2004; Vorobiev, 2012). In such an algorithm, after the identification of the "Common-Plane", the interactions between different contact types need to be handled separately, in which how to obtain the contact point deserves more attention (Boon et al., 2012). Wachs et al. (2012) recently proposed another general algorithm based on the GJK (Gilbert–Johnson–Keerthi) distance between two particles, and this method has shown to be versatile and relatively fast for shapes with a small number of components. But the method needs to assume a homothety of each particle with properly selected thickness, and the algorithm may have a loss of convergence although robust in most cases.

For a smooth and continuous surface particle, its surface can be described using a continuous function representation (CFR), thus the contact between two particles can be obtained based on the simultaneous solution of the two surface equations. Such a method can be theoretically rigorous and has been applied to modeling some regular shaped particles, e.g., ellipsoid and super-quadric particles (Lin and Ng, 1995; Cleary and Sawley, 2002; Delaney and Cleary, 2010; Hilton et al., 2010; Lu et al., 2012). But the process always involves solving higher order equations, which can only be done by time consuming numerical iterations in addition to the fact that some special treatments may also be needed to ensure the convergence in critical situations (Houlsby, 2009; Wachs et al., 2012; Xu et al., 2011). For some shapes, like ellipses or ellipsoids, various optimization methods have been proposed to improve the speed (Džiugys and Peters, 2001; Xu et al., 2011), but they cannot be generally used for other shapes. In addition, such methods cannot be directly used for particles with non-continuous surface functions, such as polyhedral particles. This problem has been tackled by using potential particles (Houlsby, 2009; Harkness, 2009; Boon et al., 2012, 2013). In this method, a continuous pseudo-potential function is constructed to approximate the surface of an angular particle, by which the

Table 1
List of typical methods for modeling of non-spherical particles in DEM.

Method	Shape definition	Contact detection	References
I. Composite particles	A particle is approximated by a combination of several spheres (or other shapes), either overlapped or not.	Detect the contacts between the sub-spheres of two particles.	(Favier et al., 1999; Abou-Chakra et al., 2004; Kruggel-Emden et al., 2008; Ferellec and McDowell, 2010; González-Montellano et al., 2011)
II. Combined surface particles	Surface of a particle is composed of a group of planar or curved surface segments, has edges and/or vertices at which the surface is not continuous, e.g., polyhedra, sphero-cylinders, cylinders.	Consider the possible contacts between different components of two particles, such as vertex-to-vertex, vertex-to-edge, edge-to-surface, etc.; "Common-Plane" algorithm; GJK-based algorithm.	(Langston et al., 2004; Nezami et al., 2004; Fraige et al., 2008; Guises et al., 2009; Vorobiev, 2012; Wachs et al., 2012)
III. Smooth and continuous surface particles	Surface of a particle can be described by a continuous equation, such as ellipsoids, super-quadrics, or pseudo-potential particles.	Find the solution for the simultaneous equations of two particles.	(Lin and Ng, 1995; Cleary and Sawley, 2002; Harkness, 2009; Houlsby, 2009; Kodam et al., 2010a, 2010b; Xu et al., 2011; Boon et al., 2012, 2013)
IV. Discretized particles	Volume or surface of a particle is represented by small voxels or points.	Based on the contacting or the overlap of the discretized voxels or points.	(Williams and O'Connor, 1999; Džiugys and Peters, 2001; Jia et al., 2007)