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A geometric potential-based contact detection algorithm for egg-shaped particles in discrete element modeling

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ABSTRACT

This paper presents the development of an algorithm for the contact detection of egg-shaped particles in discrete element modeling and the study of the behaviors of assemblies of egg-shaped particles at macroscopic and microscopic levels. A cubic function extended from the elliptic equation (quadratic function) was used to describe the particle shape. The mass center is deviated from the origin of the cubic function. Therefore, the effect of particle asymmetry can be investigated systematically using these egg-shaped particles. Contact detection was developed based on the geometric potential method for these egg-shaped particles. The resulted optimization problem was solved by the modified Newton's method. A pre-check step was installed to improve the performance. Several anticipated numerical difficulties were circumvented. Although particle asymmetry can be examined by poly-ellipses (formed by two different semi-ellipses), the contact detection of the newly developed egg-shaped particles was found to be faster than that of two poly-ellipses. The contact detection was implemented into the program ELLIPSE2 resulted in a new program EGG2. The effect of particle asymmetry was shown through the packing properties and mechanical behaviors of assemblies of egg-shaped particles. The result demonstrated that these new particles offer the possibility to study particle shape in a wider range which cannot be accomplished by the particles of quadratic function.

1. Introduction

The discrete element method (DEM) [1] is an effective technique for numerical modeling the mechanical behavior of granular materials. Granular materials have been commonly modeled with spheres. However, nature particles shown in Fig. 1 are mostly non-spherical and asymmetric. The non-spherical effect has been examined using ellipses [2–4], ellipsoids [5,6], super-quadrics [7,8] and polygons [9–14]. In addition, numerous researchers have used clusters of spheres because of the benign contact detection between spheres. Although there are few simulations of non-regular polygons, the research focus was on the effect of different particle shapes and not on the effect of particle asymmetry [15–17]. Based on the best knowledge of the authors, there is no research on particle asymmetry. This paper should be the first of its kind.

The degree of particle asymmetry increases from circles to ellipses, and to egg-shaped particles (ESP). Normal contact force can produce a moment to the mass center when using non-spherical particles. An ESP has one axis of symmetry while an ellipse has two. Particle asymmetry can be examined by comparing the results of ESP and ellipses.

Particle asymmetry can be studied systematically by an off-center parameter, K, of the cubic function that represents the particle shape of ESP. The difference between this cubic function and the quadratic function of an ellipse is only the additional parameter (K) that relates to the deviation between the mass center and the origin of the geometric description function of particle shape. This off-center parameter K should affect the macroscopic behavior of an assembly of ESP.

This paper is organized as follows. In Section 2, a geometric description of ESP is introduced. In Section 3, the contact detection algorithm for ESP is presented together with the encountered mathematical difficulties. In Section 4, the computational cost is examined by comparing to that of elliptical particles. In Section 5, several numerical simulations were conducted using a DEM program implemented with this new contact detection algorithm. In Section 6, conclusions are presented. Appendices provide the technical details of contact detection.

2. Geometric description of egg-shaped particle

A 2-D egg-shaped particle (ESP) can be described using the following function in its local coordinate system:

$$f(x,y)=\frac{x^2}{a^2}+\frac{y^2}{b^2}\left(1+\frac{K}{a}x\right)-1=0,\ (0<K<1, x\geq -a) \quad (1)$$

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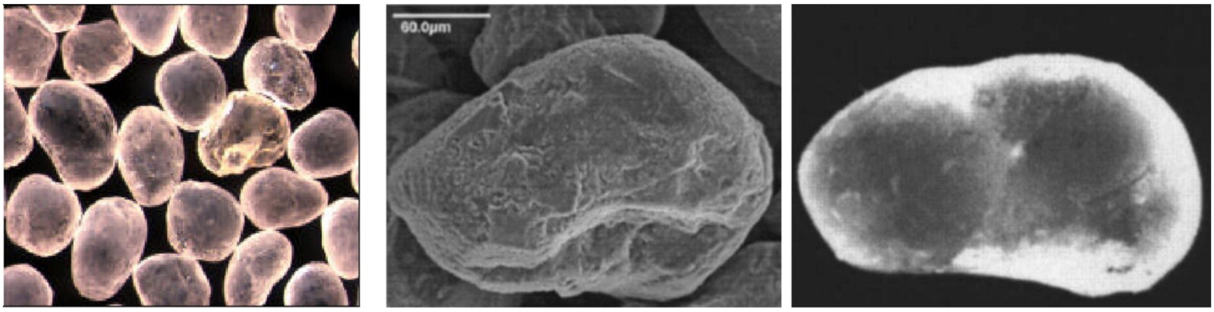

Fig. 1. Examples of asymmetric particles: Ottawa sand [18–20].

in which a and b are two radii of ESPs similar to that of an ellipse. K is defined as the off-center parameter and related to the deviation between mass center and the origin. When $K = 0$, the particle is an ellipse (or circle when $a = b$). Fig. 2 shows five ESPs with different K values ($a/b = 1.5$). As K increases, the mass center deviates more from the local center. For simplification in mathematical derivation, $K/a = k$.

Particle shape parameters (sphericity or roundness) are affected by K and a/b. The particle sphericity is computed by the ratio of the area of the particle to the area of a circle with the same perimeter [21], namely $4\pi A/p^2$. A and p are the area and perimeter of the particle respectively. Table 1 shows the sphericities of ESP of various a/b and K. For the ESP with a/b lower than 3.0, the sphericity decreases with the increase of K value. For the ESP with $a/b = 3.0$, the sphericity increases firstly and then decreases with the increase of K value. When $a/b = 4.0$, the sphericity increases slightly with K. The change of sphericity with K is very small for $a/b > 3.0$. Therefore, the influence of particle asymmetry is insignificant for the sphericity of elongated ESP.

Particle roundness is computed as the ratio of the diameter of curvature of the sharpest corner to the diameter of the largest inscribed circle [22]. Table 2 shows the particle roundness of ESP of various a/b and K. Particle roundness decreases with K for all a/b. The decrease of roundness with K is more profound for the particles with lower a/b.

Particle asymmetry can be examined using poly-ellipse (a particle formed by combining two different semi-ellipses). The advantage of using poly-ellipses is the available contact detection method. However, the contact search time can be fourfold of that of two ellipses due to the contact search of two sets of two individual ellipses.

Fig. 3 illustrates an inherent difficulty in contact detection when the contact point is near the connecting points where the two semi-ellipses meet. A jump in curvature occurs at the connecting point (solid circles) from one semi-ellipse to the other semi-ellipse.

The contact search between two poly-ellipses is decomposed into the contact search between Particle 1 and the two original ellipses Ell21 and Ell22 of Particle 2 whose semi-axis are a_{e1}, b_{e1}, a_{e2}, b_{e2} respectively (see Fig. 3). Particular points 1 and 2 were determined based on geometrical potential method (squares in Fig. 3). The particular point is a point on one ellipse which creates the smallest potential with respect to the other ellipse [2]. However, they are different from the correct particular points (open circle). Additional decision-making is needed.

3. Contact detection algorithm for two egg-shaped particles

The geometrical potential method is used to determine the contact point between two ESPs. In the geometrical potential method, the contact point is determined from the two particular points. The particular point is a point on one ellipse which creates the smallest potential with respect to the other ellipse [2]. Fig. 4 indicates the spatial distribution of the sign of the potential function (Eq. (1)) of ESP. Unlike ellipse, zones of negative potential are found away from the particle shown as the shaded areas enclosed by the dashed curves (see Fig. 4). The dashed curves and the shaded areas are called as the ghost curves and ghost zones respectively. It is an intrinsic property of Eq. (1) that will cause numerical difficulties in contact detection.

3.1. Pre-check for contact detection

Since the contact search between non-spherical particles is expensive, a pre-check for the no-contact case was always employed. For ESP, a circumscribed rectangle is used as shown in Fig. 5. The half diagonal of the rectangle, r_{max}, is used instead of r_a since the radius of the circumscribed circle can be greater than r_a (a). It is evident that the two ESPs would not be in contact when $r_{1max} + r_{2max} < d_{12}$, where d_{12} is the distance between the centers of two ESPs. The r_{max} is calculated as

$$r_{max} = \sqrt{a^2 + b_{max}^2} \tag{2}$$

in which b_{max} is expressed as

$$b_{max} = b\sqrt{\frac{1-x_m^2/a^2}{1+kx_m}} \tag{3}$$

where $k = K/a$ and $x_m = -1 + \sqrt{1-a^2k^2}/k$. Detailed deduction of b_{max} and x_m is shown in Appendix A.

3.2. Mathematical description of contact detection

When the pre-check does not indicate no-contact condition, the contact detection between two ESPs will be carried out. Local coordinate system is shown in Fig. 6. The origin is set at the center of egg2, and x-

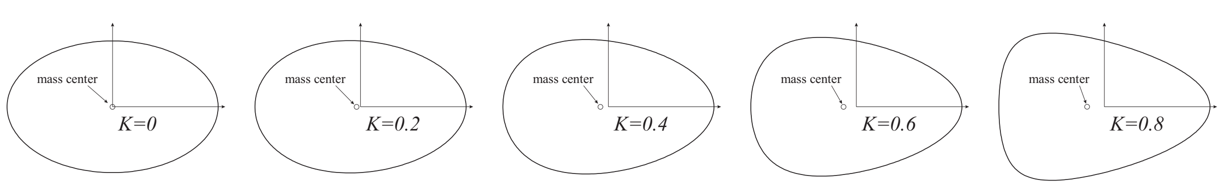

Fig. 2. ESP shape with different K values ($a/b = 1.5$).