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Short communication

A revisit of common normal method for discrete modelling of non-spherical particles

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ABSTRACT

Discrete element method (DEM) is prominent for studying granular materials at particle scale. However, how to model non-spherical particles in DEM is still challenging. In light of the present contact detection algorithms in the literature, common normal (CN) and geometric potential (GP) are two methods used for particles with smooth surfaces. Yet it has been long believed that CN gives erroneous results while GP is more preferable since they were firstly proposed for ellipsoidal particles decades ago. A revisit of CN in this work identifies two problems in the original CN, and then a new CN is proposed which can overcome these problems. Based on the comparison to sub-particle scale finite element analyses, the new CN has been further shown to be able to predict the contact plane more accurately than the original CN and GP. Such an advantage is found for the modelling of ellipsoidal and superquadric particles. The study not only proposes an improved CN algorithm but also demonstrates that CN should receive more attentions in DEM, though GP is now much more widely used.

1. Introduction

Granular materials are familiar in different industrial applications, yet their fundamentals are still far from well understood [1], calling effective methods to investigate the underlying mechanisms of their complicated behaviors. Discrete element method (DEM) [2] is a good answer to the challenge, as it provides a promising approach to study these materials at particle scale [3–5]. Although DEM can simulate the behaviors of individual particles based on first principles, the inter-particle forces need to be accurately calculated to guarantee the simulation is comparable to reality [6]. Contact force is the major inter-particle force in most granular materials. Currently, the method for calculating contact force between spherical particles has been firmly established [3], yet those for non-spherical particles are still open due to the complicated influence of particle shape and orientation [7,8]. Different methods have been exploited to calculate the contact force between non-spherical particles, which often depend on how the particle shape is represented [8]. For the particles whose surfaces can be described by continuous function representation (CFR), the contact force between them can be obtained by finding the overlap from the simultaneous equations of their surfaces. Two methods have been widely used in the literature to calculate such overlap [8], namely, the so-called geometric potential (GP) method and common normal (CN) method [9]. GP is based on finding the deepest penetrations, whereas CN on finding the parallel tangent planes. In previous studies it was tested that CN is not favorable in terms of accuracy and efficiency than GP [9], and hence GP is more commonly used in the current DEM simulations [8–12].

In this paper, we revisit the original CN algorithm proposed for ellipsoidal particles. Interestingly, we find that the previous equations contain errors and also may be ill-posed. These problems can probably be responsible for the relative large errors in previous tests. To overcome these problems, we propose a new algorithm, which is shown to be able to give correct solutions. By comparing the results to those from sub-particle finite element analyses, we further demonstrate that this new CN is more accurate than GP in the prediction of contact plane. Finally, we show that the new CN can also be extended to other CFR non-spherical particles, such as superquadric particles, for which it is also better than GP in predicting the contact plane. Our work not only proposes an improved CN algorithm, but also demonstrates that CN should receive more attentions though GP is now much more widely used.

2. Methods and results

2.1. Original common normal algorithm and its problems

As illustrated in Fig. 1, CN method is based on finding two points respectively on the two overlapping particles, i.e., $\mathbf{p}_1$ on particle 1 and $\mathbf{p}_2$ on particle 2, for which their gradient vectors on the surfaces and the vector passing through them are aligned. Here we define $\mathbf{n}_1$ as the unit vector of the gradient of $\mathbf{p}_1$, $\mathbf{n}_2$ the unit vector of the gradient of $\mathbf{p}_2$, and $\mathbf{d}_{CN}$ the vector from $\mathbf{p}_1$ to $\mathbf{p}_2$.

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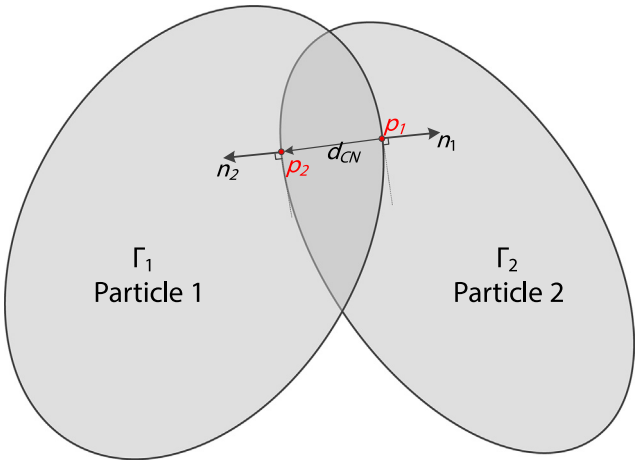

Fig. 1. 2D schematic visualization of common normal method.

The original CN algorithm was proposed by Lin and Ng [9] for ellipsoidal particles. They also presented six simultaneous equations to mathematically satisfy the geometric condition, given by:

$$\Gamma_1(x_1,y_1,z_1)=0 \tag{1}$$

$$\Gamma_2(x_2,y_2,z_2)=0 \tag{2}$$

$$\frac{\partial\Gamma_1(x_1,y_1,z_1)}{\partial x}\Big/\Delta_1+\frac{\partial\Gamma_2(x_2,y_2,z_2)}{\partial x}\Big/\Delta_2=0 \tag{3}$$

$$\frac{\partial\Gamma_1(x_1,y_1,z_1)}{\partial y}\Big/\Delta_1+\frac{\partial\Gamma_2(x_2,y_2,z_2)}{\partial y}\Big/\Delta_2=0 \tag{4}$$

$$\mathbb{R}_1=\frac{|x_2-x_1|}{\Delta}-\left|\frac{\partial\Gamma_1(x_1,y_1,z_1)}{\partial x}\right|\Big/\Delta_1=0 \tag{5}$$

$$\mathbb{R}_2=\frac{|y_2-y_1|}{\Delta}-\left|\frac{\partial\Gamma_2(x_2,y_2,z_2)}{\partial y}\right|\Big/\Delta_2=0 \tag{6}$$

where (x_1,y_1,z_1) and (x_2,y_2,z_2) are the coordinates of the points $\mathbf{p}_1$ and $\mathbf{p}_2$ on particles Γ_1 and Γ_2 respectively; $\Delta_1$and Δ_2 are the normal values of the gradient vectors of $\mathbf{p}_1$ and $\mathbf{p}_2$ respectively; Δ is the normal value of $\mathbf{d}_{CN}$; and $\mathbb{R}_1$ and $\mathbb{R}_2$ are the residues related to the solutions of Eqs. (5) and (6), respectively.

Evidently, Eqs. (3) to (6) are responsible for aligning $\mathbf{n}_1$, $\mathbf{n}_2$ and $\mathbf{d}_{CN}$. However, there are two problems in these equations. First, using absolute operator in Eqs. (5) and (6) violates the strict definition for two vectors to be in the same or opposite directions. In particular, as $\mathbf{n}_1$ should be opposite to $\mathbf{d}_{CN}$ while $\mathbf{n}_2$ parallel to $\mathbf{d}_{CN}$, Eqs. (5) and (6) should be corrected as:

$$\mathbb{R}_3=\frac{x_2-x_1}{\Delta}+\frac{\partial\Gamma_1(x_1,y_1,z_1)}{\partial x}\Big/\Delta_1=0 \tag{7}$$

$$\mathbb{R}_4=\frac{y_2-y_1}{\Delta}-\frac{\partial\Gamma_2(x_2,y_2,z_2)}{\partial y}\Big/\Delta_2=0 \tag{8}$$

where $\mathbb{R}_3$ and $\mathbb{R}_4$ are the residues related to the solutions of Eqs. (7) and (8), respectively. Secondly, these equations are focused on comparing the x and y components of the vectors, while the equality of the z component is expected to be implicitly satisfied. As these equations are solved by numerical iterations, practically there are possibilities that the solution may have very small errors on the x and y components but relatively larger errors on the z component. For example, the following equation for z dimension is expected to be satisfied besides Eqs. (5) and (6), which however is not included in the equation set:

$$\mathbb{R}_5=\frac{z_2-z_1}{\Delta}+\frac{\partial\Gamma_1(x_1,y_1,z_1)}{\partial z}\Big/\Delta_1=0 \tag{9}$$

where $\mathbb{R}_5$ is the residue related to the solution of Eq. (9).

Here we use some examples to demonstrate the aforementioned two problems. We consider two identical spheroid (axis-symmetrical ellipsoid) particles in contact. As shown in Fig. 2(a), spheroid 1 is fixed at the origin point without any rotation, while spheroid 2 with the same shape is pushed towards it through a line $\boldsymbol{L}_{12}$ defined by the zenith θ_L and azimuth angles φ_L. Spheroid 2's orientation is defined by three Euler angles (ϕ, θ, φ) in X-convention, i.e., it firstly rotates by ϕ about the Z-axis, then by θ about the new X-axis, and finally by ψ about the new Z-axis. The overlap ratio is defined as $\delta_h=\frac{h_{max}-L_{12}}{h_{max}}$, where h_{max} is the maximum distance between the centroids of two particles before they contact. Note h_{max} is dependent on the orientation of line $\boldsymbol{L}_{12}$ as well as the Euler angles. Table 1 lists all the parameters for the tested cases. For all the cases, $\varphi_L=0$ and $\varphi=0$, and the aspect ratio $\alpha=c/a$, where a, b and c are the half lengths of the particles along their three principal axes respectively, and for spheroids $a=b$. Note the cases are divided into four groups (G1 to G4). For the cases in a group, all the parameters are the same except for the overlap ratio.

Using software Mathematica [13], we have programmed scripts to solve Eqs. (1)–(6) to find (x_1, y_1, z_1) and (x_2, y_2, z_2). The solution algorithm is formulated on the basis of Line-Search Newton method [14] as detailed in the Appendix A. The solutions of the example cases are listed in Table 2. Using the solutions the angles among $\mathbf{d}_{CN}$, $\mathbf{n}_1$ and $\mathbf{n}_2$ are calculated and shown in Fig. 3(a). Evidently, for all groups, the original CN gives erroneous results as $\mathbf{d}_{CN}$ may not align with $\mathbf{n}_1$ or $\mathbf{n}_2$. To explore the reason for the misalignment, we check the residues of the equations in Table 2. From the very small values of $\mathbb{R}_1$ and $\mathbb{R}_2$ one can tell that these solutions actually satisfy Eqs. (5) and (6). However, the residues $\mathbb{R}_3$, $\mathbb{R}_4$ and $\mathbb{R}_5$ cannot all be close to zero, showing the corrected Eqs. (7) and (8), and the implicit Eq. (9) are not all satisfied. Specifically, in all these cases, $\mathbb{R}_5$ is always very large, showing that the equality of the z component cannot always be satisfied with the original CN algorithm, which may be critically responsible for the erroneous results. In addition, in some cases $\mathbb{R}_3$ and/or $\mathbb{R}_4$ are also large, showing the incorrect using of the absolute operator in Eqs. (5) and (6) also affect the results. These residues clearly demonstrate that the original equations are not properly set to guarantee the solution can satisfy CN concept due to the problems identified.

2.2. New common normal algorithm

To overcome the problems in the original CN, we propose a new algorithm in this work. Before that we should note that there are different realizations of common normal concept in the literature [15,16]. For example, Cleary et al. [15] reduced the problem from finding two points to one point by reverse the temporal evolutions of the two particles to the moment when they are just in contact at a single point, while Wellmann et al. [16] transformed the problem to the minimization of the distance between $\mathbf{p}_1$ and $\mathbf{p}_2$. Comparably Lin and Ng's algorithm is more straightforward and independent of history of particles movements. Therefore here we follow Lin and Ng's one.

Without loss of generality, two major criteria in common normal concept are rewritten as follows:

i. According to CN concept, $\mathbf{n}_1$ and $\mathbf{n}_2$ shown in Fig. 1 are anti-parallel to each other, given by:

$$\frac{\nabla\Gamma_1(x_1,y_1,z_1)}{\|\nabla\Gamma_1(x_1,y_1,z_1)\|}+\frac{\nabla\Gamma_2(x_2,y_2,z_2)}{\|\nabla\Gamma_2(x_2,y_2,z_2)\|}=0 \tag{10}$$