Contact detection between axially asymmetric ellipsoids in discrete element modeling

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Abstract

Particulate flow and particulate processing have received renewed interest as the driving needs of industry in understanding powder and particulate systems (e.g. in the manufacture of pharmaceuticals and the deposition of thin powder films) has met the academic development of tools, such as discrete element modeling (DEM) codes, to investigate such systems at a granular scale. The practical limit for the number of particles that can be simulated by the discrete element method depends critically on the particle shape, the data structures, and the algorithms used for contact and force generation. Simple shapes, such as spheres, though optimal in the above aspects, are not always able to reproduce phenomena of interest, and a non-spherical shape needs to be included. The focus of this paper is on representing a particle's geometry as a general ellipsoid in a computationally efficient manner via a new contact resolution algorithm. The algorithm presented here takes advantage of the properties of the normal field of the ellipsoidal geometry in combination with an efficient iterative vector-based search algorithm. Special attention is given to the software implementation of the algorithm, and a discussion of the computational efficiency of the algorithm is also provided.

Keywords: Discrete element modeling; DEM; Ellipsoids; Computational geometry

1. Introduction

The computational load of discrete particle simulations places a limit on the number of particles that can be handled by today's computers. The processing and memory resources required are determined by the number of particles, the complexity of the particles, and the algorithms and data structures used to represent them. For this reason, there is a great benefit if simple shapes such as spheres can be used. However, non-spherical particle shape has been found to be important in representing many physical processes, such as the mixing of powders and the strength of granular materials. This paper seeks to illustrate an algorithm for ellipsoids that can be competitive with sphere clusters.

The contact detection part of the pipeline is particular computationally intensive. In this paper, contact detection is split into two phases, neighbor sorting [1,2,3,4,5,6] and contact resolution. Since neighbor-sorting algorithms typically use a bounding sphere or bounding box representation of objects, the same algorithms can be adapted for use with arbitrary shapes. This paper focuses on the remaining problem of contact resolution.

Geometry can be a first-order effect in determining the behavior of many systems, as shown in discrete element modeling (DEM) simulations for angle-of-repose experiments [7]. Physical experiments also have shown that angularity and sphericity of grains are first-order effects in the angle of repose [8]. The sphere, though simple to implement, is hindered in its ability to capture key behaviors of real particle systems that contain non-spherical particles. Spheres tend to exhibit excessive rolling when subjected to small perturbations, are unable to represent the particle interlocking observed in many systems, and tend to form into regularly packed structures under dynamic loading. Though many schemes have been introduced to mitigate these drawbacks, they typically are empirically based rather than mechanically based.

The ellipsoid is the next obvious choice after a sphere as a geometric primitive to represent a particle's

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topology. It is part of the same family of quadrics as the sphere, but it offers additional favorable properties, including the capability of providing geometric interlocking, resistance to pathological rolling, and a more flexible and accurate convex hull for many particles of interest. Though several researchers have offered ellipsoid contact algorithms [9,10,11,12,13,14], the additional computational requirements required for contact resolution have persisted in being well beyond those for spheres, and the ellipsoid is rarely used in large-scale DEM models.

In this paper, we seek to take advantage of the simplicity of spheres while overcoming some of the problems inherent in the approaches just discussed. In particular, this paper provides a new contact resolution algorithm for the general ellipsoid that takes advantage of the convexity and normal field of the ellipsoidal geometry to converge quickly to a solution for the contact point.

2. Formulation

This contact resolution algorithm is structured around searching a space given a set of criteria. Therefore, it is first necessary to define the constraints on the space that is being searched. Here, the goal is to determine two independent parameters:

1. the orientation of the longitudinal cross-section of the ellipsoid that satisfies the constraint of both passing through the major axis and passing through the contact point;
2. the location along the major axis of the transverse cross-section of the ellipsoid that satisfies the constraint of both being orthogonal to the major axis and passing through the contact point.

The coordinate system that will be referred to throughout this paper is illustrated in Fig. 1.

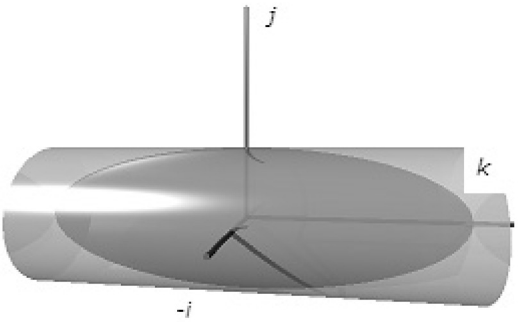

Fig. 1. Rectangular coordinate system for parameterization for the ellipsoid surface, where k is oriented along the major axis, j along the semi-minor axis, and i along the minor axis.

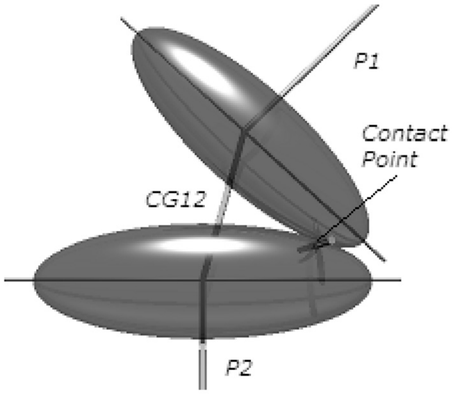

Fig. 2. Graphical representation of the result of Eq. (1) for the case of an ellipsoid pair with coplanar major axes.

2.1. Initial estimate

As with most numerical algorithms, a good initial guess can aid significantly in computational complexity. For this algorithm, the initial guess chosen is based on the vector between the centroids of the two bodies (i.e. estimating the contact condition as equivalent to that for spheres). This is shown in Fig. 2 as the segment *CG12*. The vectors *P1* and *P2* are then computed from Eq. (1) to offer the first search point:

$$\vec{P}_i = \frac{(R_i \cdot \overrightarrow{CG}_{ij} \times \hat{k}) \times \hat{k}}{\left|(R_i \cdot \overrightarrow{CG}_{ij} \times \hat{k}) \times \hat{k}\right|} \tag{1}$$

The surface is reparameterized into cylindrical coordinates, as shown in Fig. 3, and the angle θ is found by evaluating *P1* and *P2* for the respective bodies.

The contact point is determined on each body by finding the intersection of *CG12* with each body's surface. The normal to the surface is calculated on each surface and used to update the respective body's contact point estimate. This update allows two new points to be used as a new estimate: a new point along the major axis (on k from Fig. 1) and a new point on the plane containing the semi-minor and minor axes (which yields a new θ from Fig. 3).

2.2. Successive estimates

Each new θ and k position is used to produce a new candidate contact vector, which is then intersected with both surfaces to find contact point estimates. The normal is found at the contact point on each, and the procedure is repeated until it produces bounds on the location of the true contact point. Convergence is

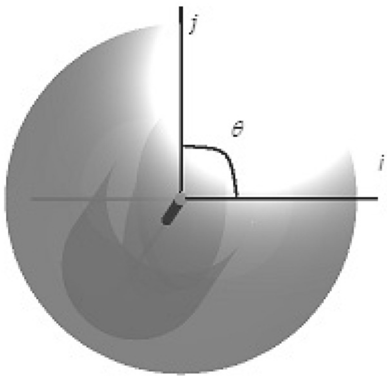

Fig. 3. Cylindrical coordinate parameterization.

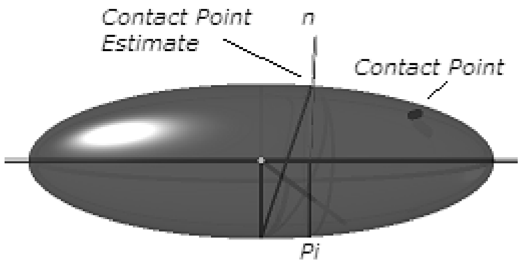

Fig. 4. Graphical representation of the contact point estimate update procedure.

determined by the skew of the surface normals at the estimated contact point on each respective body. Bounding is determined by testing whether the algorithm has 'overshot' the contact point, which is determined easily by the sign of the cross-product of the normals. The contact point update procedure is illustrated in Fig. 4.

3. Conclusions

An algorithm has been presented to offer a different approach for calculating the contact point between two generalized axially asymmetric ellipsoids (Fig. 2) using the method of equivalent spheres. The algorithm relies on the constraints imposed by the ellipsoidal geometry to reduce the surface point search from a coupled three-dimensional search space to a coupled two-dimensional search space.

Because of the almost exclusive use of vector operations, the evaluation of transcendental functions is minimized, which significantly reduces the computational requirements. In terms of theoretical floating-point operation count, the algorithm is approximately 1400 floating-point operations (flops), or approximately 1 μs per pair. Because of the methodology behind the method of equivalent spheres, extension to contact between ellipsoids and spheres or ellipsoids and triangular facets is straightforward.

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