An energy-based polyhedron-to-polyhedron contact model

Y.T. Feng*, K. Han, D.R.J. Owen

Civil and Computational Engineering Centre, School of Engineering, University of Wales Swansea, Singleton Park, Swansea SA2 8PP, UK

Abstract

The current work attempts to develop a non-ambiguous polyhedron/polyhedron contact algorithm within the energy-based theoretical framework, in which all of the contact characteristics, including the normal/tangential contact direction/plane and contact point are defined uniquely, thereby circumventing the numerical difficulties normally associated with the modelling of polyhedron/polyhedron contact.

Keywords: Discrete element; Normal contact model; Polyhedron/polyhedron contact; Contact energy; Contact plane; Contact point

1. Introduction

This paper is the extension of our previous work [1] on the development of an energy-based polygon/polygon contact model to three-dimensional (3D) polyhedron/polyhedron contact. The employment of polyhedra in 3D discrete element simulations is an underdeveloped area and only limited research is reported. This is not because polyhedra are too complicated geometric entities but because the procedures to establish the actual contact of two polyhedra and to further apply proper contact forces are surprisingly complex. The fundamental problem lies in the fact that a substantial number of special cases may need to be processed individually. Even worse, the contact force directions are more difficult to determine and often are not evolved in a smooth way but present a discontinuous jump when only a small relative movement occurs between the two polyhedra in contact. This numerical defect often introduces a certain amount of artificial energy into the computation, which, when accumulated and propagated, could cause severe numerical errors or result in a total simulation failure. Although it might be possible to design a scheme that could consider all possible contact scenarios [2], it is very unlikely that such a scheme will resolve completely the ambiguity of normal contact directions for all cases; furthermore, the implementation will be extremely tedious. In addition, the commonly used nodal/facet contact model in the finite element community has also proved to be inadequate to tackle general polyhedral contact situations.

A notable effort towards overcoming the above-mentioned numerical difficulties in 3D is Cundall's work [3] on the '*common plane*' model when dealing with the contact computation of two polyhedral blocks in geomechanics applications. This model presents a unified way of defining the contact plane/norm and can significantly improve the contact geometric computation. However, the 'common plane' is defined in a rather heuristic manner, and, more importantly, the model cannot guarantee a smooth evolution of the normal contact direction during the continuous relative movement of a contact pair.

The current work attempts to develop a non-ambiguous polyhedron/polyhedron contact algorithm within the energy-based theoretical framework proposed in our previous work [1], in which all the contact characteristics, including the normal/tangential contact direction/plane and contact point are defined uniquely, thereby circumventing the numerical difficulties mentioned above.

2. Contact energy-based normal contact law

Consider two rigid polyhedra I and II overlapping, at an arbitrary time instant, to form a typical polyhedron-to-polyhedron contact situation with two penetrating vertices p and q, as shown in Fig. 1. Assume that there

* Corresponding author. Tel.: +44 1792 295161; Fax: +44 1792 295676; E-mail: y.feng@swansea.ac.uk

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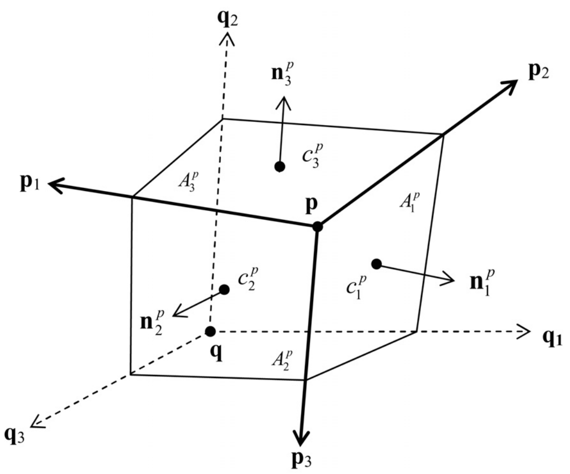

Fig. 1. A typical corner/corner contact.

are only three edges and three surfaces attached to each penetrating vertex p or q and two sets of the unit vectors of the three edges connected to p or q are $\mathbf{p}_1$, $\mathbf{p}_2$, $\mathbf{p}_3$ and $\mathbf{q}_1$, $\mathbf{q}_2$, $\mathbf{q}_3$, respectively. The two polyhedra overlap to form a six-sided polyhedron, and its volume is defined as the overlap volume V. Also assume that the normal unit vectors and the areas of the surfaces of the overlapping volume associated with bodies I and II are, respectively, $\mathbf{n}_i^p$ and A_i^p, and $\mathbf{n}_i^q$ and A_i^q (i = 1, 2, 3).

Introduce a contact energy potential $W(V)$ that is a monotone increasing function of the overlap volume V. Then the normal contact force, $\mathbf{F}_n^p$, exerted on object I at the point p is defined as

$$\mathbf{F}_n^p = -\frac{\partial W(V)}{\partial \mathbf{x}_p} = -\frac{d\,W(V)}{d\,V}\frac{\partial V}{\partial \mathbf{x}_p} = -W'(V)\nabla_{\mathbf{x}_p} V = \left\|\mathbf{F}_n^p\right\|\mathbf{n} \quad (1)$$

where

$$\mathbf{n} = -\frac{\nabla_{\mathbf{x}_p} V}{\left\|\nabla_{\mathbf{x}_p} V\right\|} \text{with} \nabla_{\mathbf{x}_p} V = \frac{\partial V}{\partial \mathbf{x}_p} \quad (2)$$

$$\left\|\mathbf{F}_n^p\right\| = W'(V)\left\|\nabla_{\mathbf{x}_p} V\right\| \quad (3)$$

and $\mathbf{n}$ defines the direction along which $\mathbf{F}_n^p$ should be applied to the object. As $\nabla x_p\ V$ is the gradient of V with respect to the translational move of p or the body I, Eq. 2 reveals the fact that, geometrically, $\mathbf{n}$ is the direction by which moving the body along reduces the overlap volume V most effectively. Physically, the normal force $\mathbf{F}_n^p$ applied in this direction can decrease the contact energy W (V) with the maximum rate.

It has been established [1] that a moment, $\mathbf{M}_\theta^p$, associated with the rotational movement about p must be present at the point p, which is defined as follows

$$\mathbf{M}_\theta^p = -\frac{\partial W(V)}{\partial \theta_p} = -\frac{d\,W(V)}{d\,V}\frac{\partial V}{\partial \theta_p} = -W'(V)\nabla_\theta^p V \quad (4)$$

where

$$\nabla_\theta^p V = \frac{\partial V}{\partial \theta_p}$$

and θ_p is an arbitrary rotational vector about the point p. ∇_θ^pV can be viewed as the gradient of V with regards to a rotational motion about the point p.

The pair of the normal contact force $\mathbf{F}_n^q$ and the moment $\mathbf{M}_\theta^q$ acting at point q on the body II also can be defined in a similar manner as

$$\mathbf{F}_n^q = -W'(V)\nabla_{\mathbf{x}_q} V, \quad \mathbf{M}_\theta^q = -W'(V)\nabla_\theta^q V \quad (5)$$

Similar to the polygon/polygon contact case, the pair $\{\mathbf{F}_n^p, \mathbf{M}_\theta^p\}$ acting at point p (or $\{\mathbf{F}_n^q, \mathbf{M}_\theta^q\}$ at q) can be equivalently replaced by a single force $\mathbf{F}_n^p$ (or $\mathbf{F}_n^q$ acting at a different position without the presence of the moment. This preferable position is again referred to as the *(reference) contact point*. In what follows, the explicit expressions of $\nabla_{\mathbf{x}_p} V$, $\nabla_\theta^p V$, $\nabla_{\mathbf{x}_q} V$ and $\nabla_\theta^q V$ are established in detail for general contact situations of two convex polyhedra.

2.1. Normal direction and normal contact forces

The three outward unit normals to the surfaces associated with object I are defined by

$$\mathbf{n}_1^p = \frac{\mathbf{p}_2 \times \mathbf{p}_3}{|\mathbf{p}_2 \times \mathbf{p}_3|}, \quad \mathbf{n}_2^p = \frac{\mathbf{p}_3 \times \mathbf{p}_1}{|\mathbf{p}_3 \times \mathbf{p}_1|}, \quad \mathbf{n}_3^p = \frac{\mathbf{p}_1 \times \mathbf{p}_2}{|\mathbf{p}_1 \times \mathbf{p}_2|}$$

Suppose that object I is moved along the direction $\mathbf{p}_1$ by a distance Δp_1, as shown in Fig. 2a. Then, the change of the overlap volume, ΔV, is

$$\Delta V = A_1^p(\mathbf{n}_1^p \cdot \mathbf{p}_1)\Delta p$$

thus

$$\frac{dV}{dp_1} = A_1^p \mathbf{n}_1^p \cdot \mathbf{p}_1$$

As

$$\frac{dV}{dp_1} = \nabla_{\mathbf{x}_p} V \cdot \mathbf{p}_1$$

it has

$$\nabla_{\mathbf{x}_p} V \cdot \mathbf{p}_1 = A_1^p \mathbf{n}_1^p \cdot \mathbf{p}_1 \quad (6)$$

Similarly,

$$\nabla_{\mathbf{x}_p} V \cdot \mathbf{p}_2 = A_2^p \mathbf{n}_2^p \cdot \mathbf{p}_2 \quad (7)$$

$$\nabla_{\mathbf{x}_p} V \cdot \mathbf{p}_3 = A_3^p \mathbf{n}_3^p \cdot \mathbf{p}_3 \quad (8)$$

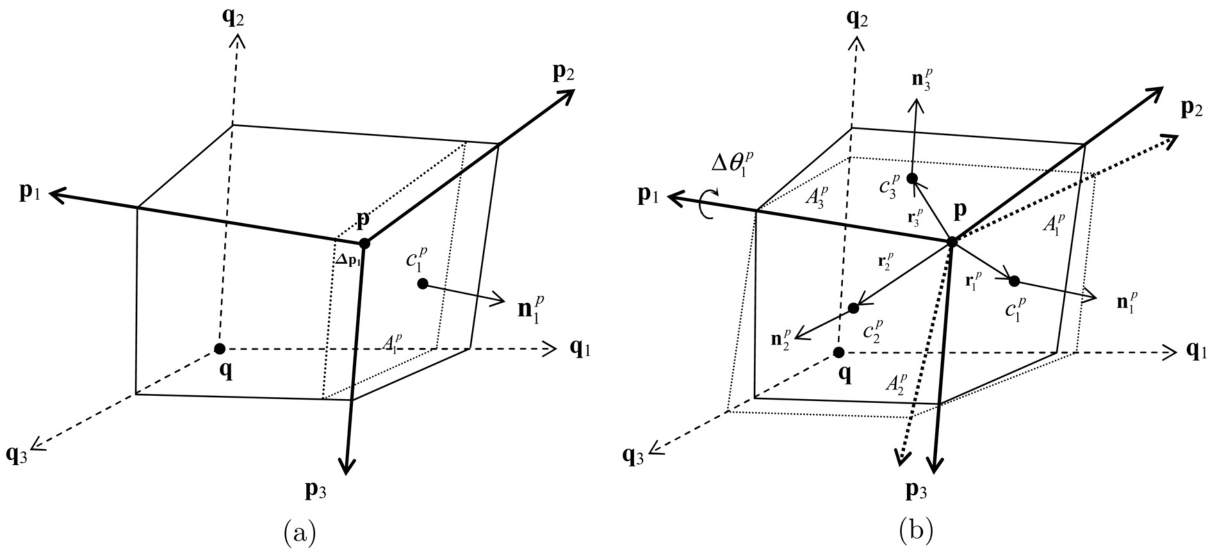

Fig. 2. Volume change due to: (a) translation along $\mathbf{p}_1$ and (b) rotation about $\mathbf{p}_1$.

It can be proved that $\nabla_{x_p} V$ should have the following form:

$$\nabla_{\mathbf{x}_p} V = A_1^p \mathbf{n}_1^p + A_2^p \mathbf{n}_2^p + A_3^p \mathbf{n}_3^p \tag{9}$$

In fact, since

$$\mathbf{n}_i^p \cdot \mathbf{p}_j = \delta_{ij} \mathbf{n}_i^p \cdot \mathbf{p}_i \quad (i, j = 1, 2, 3)$$

it follows immediately that

$$\nabla_{\mathbf{x}_p} V \cdot \mathbf{p}_i = (A_1^p \mathbf{n}_1^p + A_2^p \mathbf{n}_2^p + A_3^p \mathbf{n}_3^p) \cdot \mathbf{p}_i = A_i^p \mathbf{n}_i^p \cdot \mathbf{p}_i \quad (i = 1, 2, 3)$$

which are Eqs [6–8], and therefore Eq. [9] is proved.

The establishment of the expression in Eq. (9) provides a feasible means of commutating the normal direction $\mathbf{n}$

$$\mathbf{n} = (A_1^p \mathbf{n}_1^p + A_2^p \mathbf{n}_2^p + A_3^p) / \left\| A_1^p \mathbf{n}_1^p + A_2^p \mathbf{n}_2^p + A_3^p \right\|$$

and the force $\mathbf{F}_n^p$:

$$\mathbf{F}_n^p = -W'(V)\ (A_1^p \mathbf{n}_1^p + A_2^p \mathbf{n}_2^p + A_3^p \mathbf{n}_3^p) \tag{10}$$

Similarly, $\nabla_{x_q} V$ can be defined as

$$\nabla_{\mathbf{x}_q} V = A_1^q \mathbf{n}_1^q + A_2^q \mathbf{n}_2^q + A_3^q \mathbf{n}_3^q \tag{11}$$

and thus the normal force $\mathbf{F}_{\mathrm{n}}^{\mathrm{q}}$ is

$$\mathbf{F}_n^q = -W'(V)\ (A_1^q \mathbf{n}_1^q + A_2^q \mathbf{n}_2^q + A_3^q \mathbf{n}_3^q) \tag{12}$$

It is not difficult to prove that

$$(A_1^p \mathbf{n}_1^p + A_2^p \mathbf{n}_2^p + A_3^p \mathbf{n}_3^p) + (A_1^q \mathbf{n}_1^q + A_2^q \mathbf{n}_2^q + A_3^q \mathbf{n}_3^q) = 0$$

i.e.

$$\nabla_{\mathbf{x}_p} V + \nabla_{\mathbf{x}_q} V = 0$$

or

$$\mathbf{F}_n^p + \mathbf{F}_n^q = 0 \tag{13}$$

i.e. the normal contact forces acting on the two contacting bodies are a pair of action and reaction forces, as expected.

2.2. Contact moments

By rotating the object I around the edge $\mathbf{p}_1$ by an angle $\Delta\theta_1^p$, the volume change ΔV can be computed as (referring to Fig. 2b):

$$\Delta V = (A_1^p d_{11}^p + A_2^p d_{21}^p + A_3^p d_{31}^p) \Delta\theta_1^p$$

where $\mathrm{d}_{11}^p, \mathrm{d}_{21}^p$ and d_{31}^p are, respectively, the (signed) distances of the three surface centres, c_1^p, c_2^p and c_3^p, to the edge $\mathbf{p}_1$, which can be obtained by

$$d_{i1}^p = (\mathbf{r}_i \times \mathbf{n}_i) \cdot \mathbf{p}_1 \qquad (i = 1,\ 2,\ 3)$$

Thus,

$$\frac{dV}{d\theta_1^p} = (A_1^p \mathbf{r}_1^p \times \mathbf{n}_1^p + A_2^p \mathbf{r}_2^p \times \mathbf{n}_2^p + A_3^p \mathbf{r}_3^p \times \mathbf{n}_3^p) \cdot \mathbf{p}_1$$

As

$$\frac{dV}{d\theta_1^p} = \nabla_\theta V \cdot \mathbf{p}_1$$

it has

$$\nabla_\theta^p V \cdot \mathbf{p}_1 = \left(\sum_{j=1}^{3} \mathbf{r}_j^p \times \mathbf{n}_j^p \right) \cdot \mathbf{p}_1 \tag{14}$$

Similarly

$$\nabla_\theta^p V \cdot \mathbf{p}_2 = A_1^p d_{12}^p + A_2^p d_{22}^p + A_3^p d_{32}^p \tag{15}$$

$$\nabla_\theta^p V \cdot \mathbf{p}_3 = A_1^p d_{13}^p + A_2^p d_{23}^p + A_3^p d_{33}^p \tag{16}$$

or collectively

$$\nabla_\theta^p V \cdot \mathbf{p}_i = \sum_{j=1}^{3} A_j^p d_{ji}^p \qquad (\mathrm{i} = 1, 2, 3) \tag{17}$$

where

$$d_{ij}^p = (\mathbf{r}_j^p \times \mathbf{n}_j^p) \cdot \mathbf{p}_1$$

It is obvious that $\nabla_\theta^p V$ should be of a form

$$\nabla_\theta^p V = A_1^p \mathbf{r}_1^p \times \mathbf{n}_1^p + A_2^p \mathbf{r}_2^p \times \mathbf{n}_2^p + A_3^p \mathbf{r}_3^p \times \mathbf{n}_3^p \tag{18}$$

and thus the moment $\mathbf{M}_\theta^p$ can be determined by

$$\mathbf{M}_\theta^p = -W'(V)\ (A_1^p \mathbf{r}_1^p \times \mathbf{n}_1^p + A_2^p \mathbf{r}_2^p \times \mathbf{n}_2^p + A_3^p \mathbf{r}_3^p \times \mathbf{n}_3^p) \tag{19}$$

Similarly, $\nabla_\theta^q \mathrm{V}$ can be established as

$$\nabla_\theta^q V = A_1^q \mathbf{r}_1^q \times \mathbf{n}_1^q + A_2^q \mathbf{r}_2^q \times \mathbf{n}_2^q + A_3^q \mathbf{r}_3^q \times \mathbf{n}_3^q \tag{20}$$

and the moment $\mathbf{M}_\theta^q$ can be defined as

$$\mathbf{M}_\theta^q = -W'(V)\ (A_1^q \mathbf{r}_1^q \times \mathbf{n}_1^q + A_2^q \mathbf{r}_2^q \times \mathbf{n}_2^q + A_3^q \mathbf{r}_3^q \times \mathbf{n}_3^q) \tag{21}$$

2.3. Contact plane and (reference) contact point

With the definition of the normal contact direction, **n**, the contact (tangential) plane can be defined as the plane with **n** as its normal and passing through the mass centre of the overlap volume, c_m (with coordinates $\mathbf{x}_m$):

$$(\mathbf{x} - \mathbf{x}_m) \cdot \mathbf{n} = 0$$

Although the preceding discussion has established that the two force-moment pairs, $\{\mathbf{F}_n^p, \mathbf{M}_\theta^p\}$ and $\{\mathbf{F}_n^q, \mathbf{M}_\theta^q\}$, should be applied at points p and q, respectively, it is desirable, at least practically, if only the normal forces $\mathbf{F}_n^p$ and $\mathbf{M}_n^q$ need to be applied. As a matter of fact, this is the direct consequence of the current contact model, as will be demonstrated below.

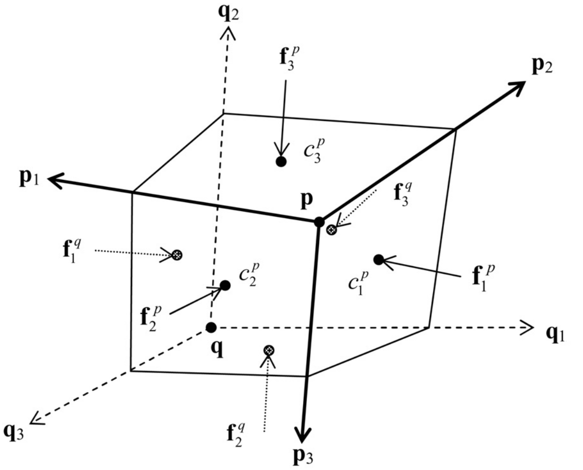

Fig. 3. An equilibrum distributed contact force system.

Let

$$\mathbf{f}_i^p = -W'(V) A_i^p \mathbf{n}_i^p, \quad \mathbf{f}_i^q = -W'(V) A_i^q \mathbf{n}_i^q \quad (i = 1, 2, 3)$$

be the forces acting at the six surface centres of the overlap volume, as shown in Fig. 3. Then

$$\mathbf{F}_n^p = \mathbf{f}_1^p + \mathbf{f}_2^p + \mathbf{f}_3^p, \quad \mathbf{M}_\theta^p = \mathbf{r}_1^p \times \mathbf{f}_1^p + \mathbf{r}_2^p \times \mathbf{f}_2^p + \mathbf{r}_3^p \times \mathbf{f}_3^p \tag{22}$$

$$\mathbf{F}_n^q = \mathbf{f}_1^q + \mathbf{f}_2^q + \mathbf{f}_3^q, \quad \mathbf{M}_\theta^q = \mathbf{r}_1^q \times \mathbf{f}_1^q + \mathbf{r}_2^q \times \mathbf{f}_2^q + \mathbf{r}_3^q \times \mathbf{f}_3^q \tag{23}$$

It can be proved that $\{\mathbf{F}_n^p, \mathbf{M}_\theta^p\}$ and $\{\mathbf{F}_n^q, \mathbf{M}_\theta^q\}$ together are an equilibrium force-moment system and therefore can be replaced by an equilibrium pair of forces $\mathbf{F}_n^p$, $\mathbf{F}_n^q$ acting at a different point c, termed the (reference) contact point, but on the two different bodies. Assuming its coordinates are $\mathbf{x}_c$, this contact point can be determined by the condition that the total moment produced by $\mathbf{F}_n^p$ and $\mathbf{F}_n^q$ about this point should vanish, i.e.

$$\mathbf{r}_{1c}^p \times \mathbf{f}_1^p + \mathbf{r}_{2c}^p \times \mathbf{f}_2^p + \mathbf{r}_{3c}^p \times \mathbf{f}_3^p + \mathbf{r}_{1c}^q \times \mathbf{f}_1^q + \mathbf{r}_{2c}^q \times \mathbf{f}_2^q + \mathbf{r}_{3c}^q \times \mathbf{f}_3^q = 0 \tag{24}$$

where $\mathbf{r}_{ic}^p$ and $\mathbf{r}_{ic}^q (\mathrm{i} = 1, 2, 3)$ are, respectively, the position vectors from points c_i^p and c_i^q to c. The contact point satisfying the above condition is, however, not unique. In fact, if $\mathbf{x}_0$ is a solution to Eq. (24), then any point on the line defined by

$$\mathbf{x} = \mathbf{x}_0 + \alpha \mathbf{n}$$

where α is an arbitrary parameter, will be the solution as well. The contact point is actually chosen to be the intersection point of this line with the contact plane, i.e.

Table 1
Several forms of $W(V)$

	$W(V)$	$W'(V)$
Linear	$k_n V$	k_n
Hertz-type	$\frac{2}{3}k_n V^{3/2}$	$k_n V^{1/2}$
Power	$k_n V^m/m$	$k_n V^{m-1}$

the coordinates $\mathbf{X}_c$ satisfy the following additional condition

$$(\mathbf{x}_c - \mathbf{x}_m) \cdot \mathbf{n} = 0$$

By the definition of both the tangential contact plane and the contact point, the tangential contact forces such as the frictional forces can be further determined based on proper tangential contact laws.

2.4. *Choice of contact energy function W (V)*

The magnitude of the normal force $\mathbf{F}_\mathrm{n}^\mathrm{p}$ is dependent on $W'(V)$. Several possible options for $W(V)$ or $W'(V)$ are listed in Table 1, in which the parameter k_n is the penalty coefficient.

3. Final remarks

Based on the assumption that contact of two polyhedra is associated with a contact energy function, then a complete normal contact law for a polyhedron/polyhedron contact has been derived fully; in particular, no distinction between node/node, node/edge, edge/edge, edge/surface and surface/surface contact scenarios is required and also no overlap distance/gap is present in the model.

The proposed contact model also suggests a procedure to numerically compute all the contact characteristics. The main computational efforts associated with the model are the determination of the surface areas of the overlap volume and the overlap volume, if required. As very effective algorithms are available for such operations (see, for instance, Preparata and Shamos [4]), the corresponding computational costs are relatively small.

4. Acknowledgement

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