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CONSTITUTIVE RELATION FOR A PARTICULATE MEDIUM WITH THE EFFECT OF PARTICLE ROTATION

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Abstract—The constitutive behavior of granular assemblies is investigated taking into account the effect of particle rotation. Continuum fields are assumed by tensorial polynomial expansion for the discrete variables, namely, particle displacements and rotations. The strain measures for the packing are obtained from the particle displacement and rotation. From the principle of virtual work, the stress measures for the packing are expressed in terms of the contact forces, the contact moments and the geometric measures for the packing structure. The derived stress-strain relationship is then evaluated by an example of a randomly packed assembly of circular disks loaded in two different conditions. Deformation of the packing calculated from the constitutive equations is compared with the results obtained from the discrete method of computer simulation to show the applicability of the method.

1. INTRODUCTION

Deformation behavior of closely packed granular assemblies in a quasistatic condition is of interest to many fields, such as soil mechanics, powder mechanics or ceramic mechanics. In an assembly of granular particles, the deformation occurs mostly at particle contacts. Thus the system is often treated conceptually as an assembly of rigid particles connected by springs at contacts such that the system deforms under an applied load through the deformation of springs.

Mechanical behavior of such system is often analyzed by two approaches which account for the packing geometry and the local interactions of particles, namely, the discrete approach and the microstructural continuum approach. The discrete approach solves for the deformation of an assembly based on the governing equations for the movement of each particle interacting with its surrounding particles. Along this line of approach, computer simulation methodology can be found in the work by Serrano and Rodrigus-Ortiz (1973) and Kishino (1987) for quasi-static condition and in the work by Cundall and Strack (1972) for dynamic condition. However, this approach is cumbersome for systems composed of large number of particles. This situation is inevitable in the case of practical problems. For example, the number of particles is in the order of 10^6 for a cubic inch of sand. Hence it is desirable to represent the discrete system with a more tractable continuum model.

In the microstructural continuum method, the deformation behavior of the assembly is described by the continuum concepts of stress and strain. The constitutive relationship for a granular assembly is obtained based on the local kinematics and the mechanical behavior of two particles in contact. A number of studies have been attempted along this line of approach. For example, work can be found in Duffy (1959), Duffy and Mindlin (1957), Deresiewicz (1958), and Makhlouf and Stewart (1967) for regular packings, and Digby (1981), Walton (1987), Jenkins (1987), Chang (1987), and Bathurst and Rothenburg (1988) for random packings. However, these analyses are limited to the assumption that there is no gain or loss of contacts during deformation. Furthermore, these analyses assume uniform strain field and do not explicitly consider the rotation mode of particle movement.

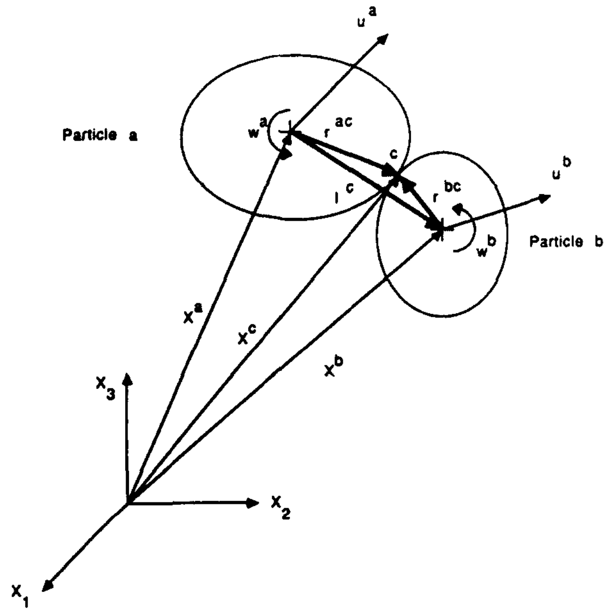

Fig. 1. Local kinematics for two particles.

In this study, we endeavor to obtain the constitutive relationship for granular systems considering a non-uniform strain field and taking into account the effect of particle rotation. This involves approximating the discrete variables, viz. displacement and rotation of particles, by continuum fields using tensor polynomial expansion. To make the analysis tractable, we assume that the local constitutive law is characterized by elastic springs connecting two particles, and we neglect the possible gain or loss of contacts during deformation. However, for analyses of particle assemblies under large deformation, these assumptions should be removed.

Since, in the microstructural continuum approach, the displacement and rotation are treated as two independent field variables, the granular material is thus a micro-polar medium (Toupin, 1964, Eringen, 1968, Kanatani, 1979). In contrast to Kanatani's work on the fluid-like behavior of granular material, this study is focused on the solid-like deformation behavior of granular material considering the particle interaction through contacts under relatively high stress levels in a quasi-static condition.

In this presentation, we first briefly derive the governing equations for the discrete method following the approach by Serrano and Rodrigus-Ortiz (1973). We then present the microstructural continuum approach, and deduce the constitutive relations of granular material, based on the approximation of the discrete variables (viz. displacement and rotation) by polynomial expansions. The packing structure, represented by position vectors and fabric tensors, are included in the description of kinematics. Principle of virtual work is used to express the stress in the media as a function of the packing structure, the contact forces, and the contact moments.

Using the derived constitutive relationship, an example is shown to analyze the deformation of a random packing. The computed deformation from the constitutive equations is compared with that obtained from discrete method to investigate the applicability of the microstructrual continuum method.

2. DISCRETE METHOD OF ANALYSIS

2.1. *Local kinematics*

In a granular assembly, let "*a*" and "*b*" denote two convex particles in contact at point *c* as shown in Fig. 1. Particles "*a*" and "*b*" are conceptually considered to be rigid and connected at the contact by springs. When the assembly is subjected to an increment of load, particles "a" and "b" undergo translations (i.e. u_i^a, u_i^b) and rotations (i.e. ω_i^a, ω_i^b). This results in the deformation of the springs connecting the two particles. Two types of springs are used to represent the contact resistance, namely, the rotation springs and the stretch springs. The rotation springs transmit the contact moment, and represent the rolling and torsional resistance at the contact of the two particles. The stretch springs transmit the contact forces, and represent the compression and sliding resistance at the contact of the two particles.

The angular rotation, θ_i^c, of the rotation springs at the contact of particles "a" and "b", is caused by the relative rotation of the two particles, that is

$$\theta_i^c = \omega_i^b - \omega_i^a. \tag{1}$$

The deformation, δ_i^c, of the stretch springs at the contact of particles "a" and "b", can be expressed in terms of the displacements (i.e. u_i^a and u_i^b), and the rotations (i.e. ω_i^a and ω_i^b) of the two particles, as follows:

$$\delta_i^c = (u_i^b - u_i^a) + e_{ijk}(\omega_j^b r_k^{bc} - \omega_j^a r_k^{ac}) \tag{2}$$

where r_k^{bc} and r_k^{ac} are the vectors joining the contact point c to the centers of particles "b" and "a" respectively, and quantity e_{ijk} is the permutation symbols used in tensor representation for cross product of vectors.

2.2. *Local constitutive law at contact*

The angular rotation of the rotation springs at the contact point c, θ_j^c, is related to the contact couple, m_i^c, by a general expression as follows:

$$m_i^c = G_{ij}^c \theta_j^c. \tag{3}$$

If the springs are characterized as linear elastic, the rotational stiffness tensor takes the form,

$$G_{ij}^c = G_n n_i n_j + G_s s_i s_j + G_t t_i t_j \tag{4}$$

where G_n, G_s and G_t are the rotational spring constants in the directions of the local coordinates n, s, and t respectively. The local coordinate system is constructed for each contact with three orthogonal base unit vectors: the vector **n** is normal to the contact area, and the vectors **s** and **t** can be chosen arbitrarily.

The stretch deformation of the springs at the contact point c, δ_j^c, is related to the contact force f_i^c by a general expression,

$$f_i^c = k_{ij}^c \delta_j^c. \tag{5}$$

For elastic stretch springs, the stiffness tensor is given by

$$K_{ij}^c = k_n n_i n_j + k_s s_i s_j + k_t t_i t_j \tag{6}$$

where k_n, k_s and k_t are the spring constants in the directions of local coordinate system n, s, t respectively.

2.3. *Local force and moment equilibrium*

Under a quasi-static condition, neglecting the gravitational force, the equilibrium equations for the particle "a" in the assembly can be expressed in terms of: (1) the force f_i^a and moment m_i^a externally applied at the centroid of the particle, and (2) the contact forces f_i^{ac} and contact couples m_i^{ac} transmitted from the neighbouring particles. The force and moment equilibrium equations are as follows:

$$f_j^a + \sum_c f_j^{ac} = 0 \tag{7}$$

$$m_j^a + \sum_c (m_j^{ac} + e_{jkl} r_k^{ac} f_l^{ac}) = 0 \tag{8}$$

where r_k^{ac} is the vector joining the centroid of particle "a" to the contact point c. Since the external forces are applied only to the boundary particles of the assembly, f_i^a and m_i^a are zero if the particle "a" is within the assembly.

2.4. *Governing equations for the system*

A set of governing equations for the discrete system can be set up based on the force equilibrium, local kinematics and local constitutive law. Substituting eqns (2) and (5) into eqn (7), it follows

$$f_i^a + \sum_c K_{ik}^c (u_k^b - u_k^a) + \sum_c K_{ik}^c e_{kjn} (\omega_j^b r_n^{bc} - \omega_j^a r_n^{ac}) = 0. \tag{9}$$

Equation (9) represents three equations that can be established for each particle in the assembly. Similarly, additional three equations can be established for each particle based on the moment equilibrium. Using eqns (1), (3) and (8), we obtain

$$m_i^a + \sum_c e_{ijk} r_j^{ac} K_{kn}^c \big((u_n^b - u_n^a) + e_{nqv} (\omega_q^b r_v^{bc} - \omega_q^a r_v^{ac})\big) = 0. \tag{10}$$

For a packing with N particles, the total number of equations is $6N$. The total number of variables is $12N$, consisting of $3N$ particle displacements, u_i, $3N$ particle rotations, ω_i, $3N$ particle forces, f_i, and $3N$ particle moments, m_i. Thus the set of simultaneous equations can be solved for a system with specified $6N$ known values of displacements, rotations, forces, or moments to obtain the other $6N$ unknown variables. The force and moment at each contact are in turn obtained from the local kinematics and local constitutive law.

3. MICROSTRUCTURAL CONTINUUM METHOD OF ANALYSIS

3.1. *Continuum field for displacement and rotation*

Let u_i be the displacement of the center of a particle in a granular assembly. For a small representative element consisting of sufficiently large number of particles, we express the continuum displacement field by a polynomial function

$$u_i = a_i + b_{ij} X_j + \frac{1}{2!} c_{ijk} X_j X_k + \cdots + \text{higher order terms} \tag{11}$$

where a_i, b_{ij} and c_{ijk} are coefficients, and X_j, X_k, etc. are the position vectors measured from the centroid of the volume V. The coefficient c_{ijk} has the following property: $c_{ijk} = c_{ikj}$. The position vector X_j can be measured with reference to a material frame either before or after deformation, depending on whether Lagrangian or Eulerian description is used. Since we deal with the small deformation problem, we shall not distinguish between Lagrangian and Eulerian representations.

Similarly, the rotation of a micro-element (i.e. particle), ω_i, termed as micro-rotation, is treated as an independent mode of deformation and represented by a continuum field given by

$$\omega_i = \alpha_i + \phi_{ij} X_j + \cdots + \text{higher order terms} \tag{12}$$

where α_i and ϕ_{ij} are coefficients.

Since the displacement and rotation fields are defined for a small volume of element, the higher order terms in eqns (11) and (12) may be neglected. In this work, in order to examine the effect of particle rotation, a quadratic form of u_i and a linear form of w_i are considered.

To investigate the deformation characteristics of a particle assembly, the coefficients of the polynomials in eqns (11) and (12) are evaluated by taking the mean values of the field variables, u_i and ω_i, and their derivatives for an element of particle assembly with volume V.

The mean displacement is defined by the volume average of u_i, i.e.

$$\bar{u}_i = \frac{1}{V}\int u_i \,\mathrm{d}v = \frac{1}{V}\int \left(a_i + b_{ij}X_j + \frac{1}{2!}c_{ijk}X_jX_k\right)\mathrm{d}v. \tag{13}$$

Since

$$\int X_k \,\mathrm{d}v = 0 \quad \text{and} \quad \frac{1}{V}\int X_jX_k \,\mathrm{d}v$$

is the moment of inertia I_{jk}, we obtain

$$\bar{u}_i = a_i + \frac{1}{2!}c_{ijk}I_{jk} \tag{14}$$

where a_i is approximately the mean displacement of the particles in the assembly if the higher order term is small compared to the first term.

The mean displacement gradient, defined by volume average, is given by

$$\bar{u}_{i,j} = \frac{1}{V}\int u_{i,j}\,\mathrm{d}v = \frac{1}{V}\int (b_{ij} + c_{ijk}X_k)\,\mathrm{d}v = b_{ij}. \tag{15}$$

Thus b_{ij} is the mean displacement gradient which is also equal to the $u_{i,j}$ at the centroid of the element.

The mean of the second derivative of displacement takes the form

$$\bar{u}_{i,jk} = c_{ijk}. \tag{16}$$

Similarly, the mean micro-rotation defined by volume average is given by

$$\bar{\omega}_i = \frac{1}{V}\int \omega_i\,\mathrm{d}v = \frac{1}{V}\int (\alpha_i + \phi_{ij}X_j)\,\mathrm{d}v = \alpha_i. \tag{17}$$

Thus the coefficient α_i is the mean of particle rotations.

The mean micro-rotation gradient is given by

$$\bar{\omega}_{i,j} = \frac{1}{V}\int \omega_{i,j}\,\mathrm{d}v = \phi_{ij}. \tag{18}$$

Thus the coefficient ϕ_{ij} is the mean micro-rotation gradient.

Assuming a quadratic function for u_i and a linear function for ω_i, and using eqns (15), (16), (17) and (18), eqns (11) and (12) are written as

$$u_i = a_i + \bar{u}_{i,j}X_j + \frac{1}{2!}\bar{u}_{i,jk}X_jX_k \tag{19}$$

$$\omega_i = \bar{\omega}_i + \bar{\omega}_{i,j}X_j. \tag{20}$$

With the continuum representation, the deformation characteristics for this packing can be described by the measures, $\bar{u}_{i,j}$, $\bar{u}_{i,jk}$, and $\bar{\omega}_{i,j}$.

3.2. *Kinematics in continuum field and strain in an assembly*

Using the particle displacement and rotation fields, the deformation of the stretch and rotation springs between particles can be described with the coefficients of the polynomials.

Substituting eqn (20) into eqn (1), the angular rotation of the rotation spring connection between two particles becomes,

$$\theta_i^c = l_j^c\bar{\omega}_{i,j} \tag{21}$$

where l_j^c represents the fabric vector $X_j^b - X_j^a$.

Furthermore, we define X^c as the position vector from the centroid of the assembly to the contact point between particles "a" and "b" such that

$$r_i^{ac} = X_i^c - X_i^a, \quad \text{and } r_i^{bc} = X_i^c - X_i^b. \tag{22}$$

Then, the stretch of the spring can be expressed as

$$\delta_i^c = (\varepsilon_i^b - \varepsilon_i^a) + e_{ijn}X_n^c(\omega_j^b - \omega_j^a) \tag{23}$$

where ε_i is a displacement vector, given by

$$\varepsilon_i = u_i + e_{ijm}\omega_m X_j. \tag{24}$$

Using eqns (19) and (20), eqn (24) is expressed into a polynomial form,

$$\varepsilon_i = a_i + \bar{\varepsilon}_{ij}X_j + \frac{1}{2!}\bar{\varepsilon}_{ijk}X_jX_k \tag{25}$$

where the coefficients $\bar{\varepsilon}_{ij}$ and $\bar{\varepsilon}_{ijk}$ take the following forms:

$$\bar{\varepsilon}_{ij} = \bar{u}_{i,j} + e_{ijm}\bar{\omega}_m \tag{26}$$

$$\bar{\varepsilon}_{ijk} = \bar{u}_{i,jk} + 2e_{ijm}\bar{\omega}_{m,k}. \tag{27}$$

Substituting eqns (25–27) and (21) into eqn (23), the stretch of the springs at the contact between two particles, due to translation and rotation of the particles, is thus expressed in terms of the coefficients of polynomials by

$$\delta_i^c = l_j^c\bar{\varepsilon}_{ij} + J_{jk}^c\bar{\varepsilon}_{ijk} + e_{ijn}X_n^c l_k^c\bar{\omega}_{j,k} \tag{28}$$

where the fabric tensor J_{jk}^c is introduced as $X_j^bX_k^b - X_j^aX_k^a$. Note that the fabric tensor is symmetric, that is, $J_{jk}^c = J_{kj}^c$. In the expression of the local kinematics of particles, the required geometric measures for the micro-structure are, X_i^c, l_i^c, and J_{ij}^c.

It is noted that although $\bar{\varepsilon}_{ij}$ in eqn (26) has a form similar to that of the micro-strain given by Eringen (1968) in the micropolar theory, it takes different meaning in the context of particle assembly. In an assembly of particles, the symmetrical part of $\bar{\varepsilon}_{ij}$ is equal to the symmetrical part of the displacement gradient, i.e.

$$\bar{\varepsilon}_{(ij)} = \bar{u}_{(i,j)} = 1/2(\bar{u}_{ij}+\bar{u}_{j,i}) \tag{29}$$

representing the mean stretch of the assembly.

The skew symmetric part of $\bar{\varepsilon}_{ij}$ in eqn (26) is given by

$$\bar{\varepsilon}_{[ij]} = \bar{u}_{[i,j]}+e_{ijm}\bar{\omega}_m \tag{30}$$

where the skew symmetrical tensor $\bar{u}_{[ij]} = 1/2(\bar{u}_{i,j}-\bar{u}_{j,i})$, representing the rigid body rotation tensor. The angular rotation $\bar{\psi}_m$ corresponding to the rigid body rotation is

$$\bar{\psi}_m = -1/2e_{ijm}\bar{u}_{i,j} \quad \text{or } e_{ijm}\bar{\psi}_m = -\bar{u}_{[i,j]}. \tag{31}$$

Using eqn (31), the skew symmetric part of $\bar{\varepsilon}_{ij}$ in eqn (30) becomes

$$\bar{\varepsilon}_{[ij]} = e_{ijm}(\bar{\omega}_m-\bar{\psi}_m) \tag{32}$$

which represents the mean value of the net particle spin (i.e. the difference of the mean particle rotation and the rigid body rotation of the assembly). Thus, we term the coefficient $\bar{\varepsilon}_{ij}$ as the "mean micro-strain" of the assembly and the coefficient $\bar{\varepsilon}_{ijk}$ as the "mean micro-strain of the second order". Neglecting the higher order terms, the variables of strain measures for this assembly can be selected to be $\bar{\varepsilon}_{ij}$, $\bar{\varepsilon}_{ijk}$ and $\bar{\omega}_{i,j}$.

3.3. *Stress in an assembly*

The principle of virtual work is used here to obtain the relationship between the external forces applied to the assembly and the internal forces between the particles of the assembly. Due to a virtual movement of each particle, δu_i^a and $\delta\omega_i^a$, the virtual work is given by

$$\begin{aligned}\delta(W_E+W_I) &= 0\\ &= \sum_a \delta u_i^a\left(f_i^a+\sum_c f_i^{ac}\right)+\sum_a \delta\omega_i^a\left(m_i^a+\sum_c (m_i^{ac}+e_{ikl}r_k^{ac}f_l^{ac})\right).\end{aligned} \tag{33}$$

Using the polynomial expansions in eqns (11) and (12) for δu_i^a and $\delta\omega_i^a$, and substituting r_k^{ac} from eqn (31), eqn (33) yields

$$\begin{aligned}0 = &\sum_a (\delta a_i+\delta b_{ij}X_j^a+\delta c_{ijk}X_jX_k+\cdots)\left(f_i^a+\sum_c f_i^{ac}\right)\\ &+\sum_a (\delta\alpha_i+\delta\phi_{ij}X_j^a+\cdots)\left(m_i^a+e_{ikl}X_k^a f_l^a+\sum_c (m_i^{ac}+e_{ikl}X_k^c f_l^{ac})\right).\end{aligned} \tag{34}$$

This equation must hold for any variation of the polynomial coefficients, δa_i, δb_{ij}, δc_{ijk}, $\delta\alpha_i$, $\delta\phi_{ij}$, etc. For example, corresponding to the coefficients, δa_i, we obtain the force equilibrium equation for the assembly

$$\sum_a f_i^a = -\sum_a\sum_c f_i^{ac} \tag{35}$$

and corresponding to the coefficients, $\delta\alpha_i$, we obtain the moment equilibrium equation for the assembly

$$\sum_a (m_i^a + e_{ikl} X_k^a f_l^a) = -\sum_a \sum_c (m_i^{ac} + e_{ikl} X_k^{ac} f_l^{ac}). \quad (36)$$

Similarly, corresponding to the polynomial coefficients, δb_{ij}, δc_{ijk} and $\delta \phi_{ij}$, we obtain the following set of equations:

$$\sum_a X_i^a f_j^a = -\sum_a X_i^a \sum_c f_j^{ac} \quad (37)$$

$$\sum_a X_i^a X_j^a f_k^a = -\sum_a X_i^a X_j^a \sum_c f_k^{ac} \quad (38)$$

$$\sum_a X_i^a (m_j^a + e_{jkl} X_k^a f_l^a) = -\sum_a X_i^a \sum_c (m_j^{ac} + e_{jkl} X_k^{ac} f_l^{ac}). \quad (39)$$

Each of the above equations shows the relationship between the external forces of the assembly and the internal contact forces within the assembly. If more terms of the polynomial coefficients are selected, more equations of such relationships can be established.

In terms of continuum concept of stress, we relate the forces in eqns (37), (38), and (39) to the quantities termed as (1) stretch stress, (2) first moment of stretch stress, and (3) polar stress.

(1) *Stretch stress*. To differentiate from couple stress, we term the Cauchy stress σ_{ij} as the stretch stess in the granular assembly. In a representative element of granular assembly with volume V, using the equilibrium condition

$$\sigma_{ij,i} = 0 \quad (40)$$

we define the mean field of stress by

$$\bar{\sigma}_{ij} = \frac{1}{V}\int_V \sigma_{ij}\,\mathrm{d}v = \frac{1}{V}\int_V (\sigma_{kj} X_i)_{,k}\,\mathrm{d}v. \quad (41)$$

Introducing divergence theorem, the volume integral in eqn (41) can be converted into a surface integral as follows:

$$\bar{\sigma}_{ij} = \frac{1}{V}\int_S X_i \sigma_{kj} n_k\,\mathrm{d}S \quad (42)$$

where S represents the boundary surface of the volume V, and n_k is the normal vector outward to the surface. For discrete forces f_j^a on the boundary surface S, the surface integral in eqn (42) can be expressed by a summation of the boundary forces, given by

$$\bar{\sigma}_{ij} = \frac{1}{V}\sum_a X_i^a f_j^a. \quad (43)$$

Equation (43) can also be written in terms of the internal contact forces with the aid of eqn (37). On the right hand side of eqn (37), in the summation over all particles, each contact is counted twice because each contact is associated with a pair of particles. For example, the contact point c is associated with particles "a" and "b". Thus eqn (43) can be written as a summation over all contacts

$$\bar{\sigma}_{ij} = -\frac{1}{V}\sum_c (X_i^a f_j^{ac} + X_i^b f_j^{bc}). \tag{44}$$

Note that $f_j^{ac} = -f_j^{bc} = f_j^c$ and the fabric vector $l_i^c = X_i^b - X_i^a$. Hence the mean stress of the assembly is

$$\bar{\sigma}_{ij} = \frac{1}{V}\sum_c l_i^c f_j^c. \tag{45}$$

This leads to the familiar results by Christoffersen *et al.* (1981) and Rosenberg and Selvaudurai (1981) for the volume average of stress.

(2) *First moment of stretch stress.* Due to the non-vanishing second derivative of displacement $u_{i,jk}$, the stress is no longer uniform in the assembly. To account for the stress non-uniformity, we define a quantity $\bar{T}_{ijk}$ as the mean of the first moment of stretch stress in the granular assembly, similar to that used in the theory of stress mean (Truesdell and Toupin, 1960). It is given by

$$\bar{T}_{ijk} = \frac{1}{V}\int_V [\sigma_{ik}X_j + \sigma_{jk}X_i]\,\mathrm{d}v \tag{46}$$

where V is the volume of the assembly.

Applying divergence theorem and equilibrium equation (eqn (40)) to eqn (46), the volume integral can be expressed into a surface integral as follows

$$\bar{T}_{ijk} = \frac{1}{V}\int_V (\sigma_{mk}X_iX_j)_{,m}\,\mathrm{d}v = \frac{1}{V}\int_S X_iX_j\sigma_{mk}n_m\,\mathrm{d}S \tag{47}$$

where n_m is the normal vector outward to the surface. For discrete forces f_k^a on the boundary surface S, the surface integral can be expressed by a summation of the external forces applied to the boundary surface of the assembly. It is given by

$$\bar{T}_{ijk} = \frac{1}{V}\sum_a X_i^a X_j^a f_k^a. \tag{48}$$

The mean of the first moment of stretch stress in eqn (48) can also be described by the internal contact forces with the aid of eqn (38). Because each contact point is associated with a pair of particles, the summation of eqn (38) can be written as a summation over all contacts. Thus eqn (48) becomes

$$\bar{T}_{ijk} = -\frac{1}{V}\sum_c (X_i^a X_j^a f_k^{ac} + X_i^b X_j^b f_k^{bc}). \tag{49}$$

Note that $f_k^{ac} = -f_k^{bc} = f_k^c$ and the fabric tensor $J_{ij}^c = X_i^b X_j^b - X_i^a X_j^a$. Hence the mean of the first moment of the stretch stress for the assembly is given by

$$\bar{T}_{ijk} = \frac{1}{V}\sum_c J_{ij}^c f_k^c \tag{50}$$

where V is the volume of the assembly. Note that the fabric tensor is symmetric, i.e. $J_{jk}^c = J_{kj}^c$. Thus the first moment of the stretch stress tensor $\bar{T}_{ijk} = \bar{T}_{jik}$.

(3) *Polar stress.* Since stress couples are expected to exist at particle contacts throughout the assembly, the stress representation for such media should be chosen to include the couple stress defined as that in the micropolar theory (Eringen, 1968).

From the balance law of angular momentum, the equilibrium conditions of couple stress can be expressed as follows:

$$m_{ij,i} + e_{jmn}\sigma_{mn} = 0 \tag{51}$$

where the couple stress tensor m_{ij}, defined in the micropolar theory for an infinitesimal element of a continuum media, is the moment about the centroid of the infinitesimal element, per unit area of the ith face in the jth direction (right hand rule is applied).

Since we are dealing with an assembly of finite volume, it is convenient, in our derivation, to refer the moment about the centroid of the assembly. Let X_n be the position vector measured from the centroid of the assembly to the centroid of the infinitesimal element, we introduce a polar stress M_{ij} as the moment stress per unit area about the centroid of an assembly. The polar stress is thus a function of both couple and stretch stresses

$$M_{ij} = m_{ij} + e_{jnm}\sigma_{im}X_n. \tag{52}$$

Using this definition of polar stress tensor M_{ij}, the moment equilibrium equation can be reduced to a simple form given by

$$M_{ij,i} = 0. \tag{53}$$

In a granular assembly, we define the mean polar stress by

$$\bar{M}_{ij} = \frac{1}{V}\int M_{ij}\,\mathrm{d}v \tag{54}$$

where V is the volume of the assembly.

Applying divergence theorem to eqn (54) and using the moment equilibrium equation (eqn (53)), eqn (54) is expressed as a surface integral, given by

$$\bar{M}_{ij} = \frac{1}{V}\int_V (M_{kj}X_i)_{,k}\,\mathrm{d}v = \frac{1}{V}\int_S X_i M_{kj} n_k\,\mathrm{d}S$$

$$= \frac{1}{V}\int_S X_i(m_{kj} + e_{jmn}X_m\sigma_{kn})n_k\,\mathrm{d}S. \tag{55}$$

For discrete moments m_j^a on the boundary surface S, the mean polar stress can be expressed as a summation of external forces and moments, given by

$$\bar{M}_{ij} = \frac{1}{V}\sum_a X_i^a(m_j^a + e_{jkl}X_k^a f_l^a). \tag{56}$$

The mean polar stress in eqn (56) can also be described by the internal contact forces and moments with the aid of eqn (39). The expression of the summation over all particles in eqn (39) can be written as a summation over all contacts. Equation (56) becomes

$$\bar{M}_{ij} = -\frac{1}{V}\sum_c ((X_i^a m_j^{ac} + X_i^b m_j^{bc}) + e_{jkl}(X_i^a X_k^{ac} f_l^{ac} + X_i^b X_k^{bc} f_l^{bc})). \tag{57}$$

Note that $f_j^{ac} = -f_j^{bc} = f_j^c$, $m_j^{ac} = -m_j^{bc} = m_j^c$, $X_j^{ac} = X_j^{bc} = X_j^c$, and the fabric vector $l_i^c = X_i^b - X_i^a$. Equation 57 becomes

$$\bar{M}_{ij} = \frac{1}{V}\sum_c (l_i^c m_j^c + e_{jkl} l_i^c X_k^c f_l^c). \tag{58}$$

3.4. *Constitutive relationship*

A set of constitutive equations are proposed to relate the strain measures: $\bar{\varepsilon}_{ij}$, $\bar{\varepsilon}_{ijk}$, and $\bar{\omega}_{i,j}$ to the stress measures: $\bar{\sigma}_{ij}$, $\bar{T}_{ijk}$, and $\bar{M}_{ij}$. The relationship between stress and strain can be obtained based on the following relationships: (a) stresses versus contact forces and moments (eqns (45), (50), (58)), (b) contact forces and moments versus contact displacement and rotation (eqns (3), (5)), and (c) strains versus contact displacement and rotation (eqns (21), (28)). Applying eqns (5), (28) into eqn (45), eqns (5), (28) into eqn (50), and eqns (3), (5), (21), (28) into eqn (58), the set of constitutive equations can be obtained:

$$\bar{\sigma}_{ij} = A_{ijkl}\bar{\varepsilon}_{kl} + B_{ijklm}\bar{\varepsilon}_{klm} + C_{ijkl}\bar{\omega}_{k,l} \tag{59}$$

$$\bar{T}_{ijp} = B_{lpkij}\bar{\varepsilon}_{kl} + E_{ijpklm}\bar{\varepsilon}_{klm} + F_{ijpkl}\bar{\omega}_{k,l} \tag{60}$$

$$\bar{M}_{ij} = C_{ikjl}\bar{\varepsilon}_{kl} + F_{mlkji}\bar{\varepsilon}_{klm} + H_{ijkl}\bar{\omega}_{k,l} \tag{61}$$

where the constitutive coefficients are expressed in terms of packing structure measures: l_i^c, J_{ij}^c and X_i^c, and the local constitutive constants: K_{ij}^c and G_{ij}^c, given by

$$A_{ijkl} = \frac{1}{V}\sum_c l_i^c K_{jk}^c l_l^c \tag{62}$$

$$B_{ijklm} = \frac{1}{V}\sum_c l_i^c K_{jk}^c J_{ml}^c \tag{63}$$

$$C_{ijkl} = \frac{1}{V}\sum_c l_i^c K_{jm}^c e_{mkn} X_n^c l_l^c \tag{64}$$

$$E_{ijpklm} = \frac{1}{V}\sum_c J_{ij}^c K_{pk}^c J_{ml}^c \tag{65}$$

$$F_{ijpkl} = \frac{1}{V}\sum_c J_{ij}^c K_{pm}^c e_{mkn} X_n^c l_l^c \tag{66}$$

$$H_{ijkl} = \frac{1}{V}\sum_c l_i^c G_{jk}^c l_l^c + \frac{1}{V}\sum_c l_i^c e_{jmn} X_m^c K_{nv}^c e_{vku} X_u^c l_l^c. \tag{67}$$

The condition of non-negative energy is essential for the requirement of stability of the material. This set of constitutive equations satisfy the requirement of non-negative internal energy since the local constitutive law is selected such that the internal energy is always positive for each contact. The non-negative energy of the system can also be observed from the symmetrical properties of the following constitutive coefficient tensors:

$$A_{ijkl} = A_{lkji};\quad E_{ijpklm} = E_{mlkpji};\quad \text{and } H_{ijkl} = H_{lkji}.$$

These symmetrical properties can be shown clearly from the matrix form of the constitutive equations. By defining a stress vector that consists of the following components,

$$\{\bar{\sigma}\} = \langle \bar{\sigma}_{11}, \bar{\sigma}_{12}, \ldots, \bar{\sigma}_{32}, \bar{\sigma}_{33}, \bar{T}_{111}, \bar{T}_{112}, \ldots, \bar{T}_{332}, \bar{T}_{333}, \bar{M}_{11}, \bar{M}_{12}, \ldots, \bar{M}_{32}, \bar{M}_{33} \rangle$$

and a strain vector that consists of the following components,

$$\{\bar{\varepsilon}\} = \langle \bar{\varepsilon}_{11}, \bar{\varepsilon}_{21}, \ldots, \bar{\varepsilon}_{23}, \bar{\varepsilon}_{33}, \bar{\varepsilon}_{111}, \bar{\varepsilon}_{2111}, \ldots, \bar{\varepsilon}_{233}, \bar{\varepsilon}_{333}, \bar{\omega}_{1,1}, \bar{\omega}_{2,1}, \ldots, \bar{\omega}_{2,3}, \bar{\omega}_{3,3} \rangle$$

the constitutive equations (i.e. eqns (59)–(61)) can be written in a matrix form

$$\{\bar{\sigma}\} = [C]\{\bar{\varepsilon}\}. \tag{68}$$

The constitutive matrix $[C]$ is symmetric.

4. EXAMPLE OF TWO DIMENSIONAL CIRCULAR PARTICLES

A random packing of equal sized circular disks is used here for the evaluation of the proposed method. The structure of this packing is shown in Fig. 2 which is obtained by digitizing a photograph of an assembly of aluminum rods randomly placed in a box of 7 in × 8.1 in. Radius of each rod is 0.25 in. Total number of particles is 276, total number of contacts 695, and the average coordination number 5.03. The contact normal distribution for this packing is shown in Fig. 3.

4.1. *Discrete method*

Constants for the springs between the disks in contact are assumed to be as follows: $k_n = 1000$ lb/in, $k_s = 100$ lb/in, and $G_z = 100$ lb/rad. Two loading conditions, as schematically shown in Fig. 4, are applied to simulate: (a) a symmetric shear stress $\sigma_{xy} = \sigma_{yx}$ and a normal stress σ_{yy}, (b) a polar stress M_{xz}. The packing is deformed through external forces applied to the boundary particles of the assembly. Using eqns (45), (50) and (58), the stresses corresponding to the two sets of applied forces are given in Table 1. Since the packing is not symmetrical about x and y axis, the applied forces on boundary particles

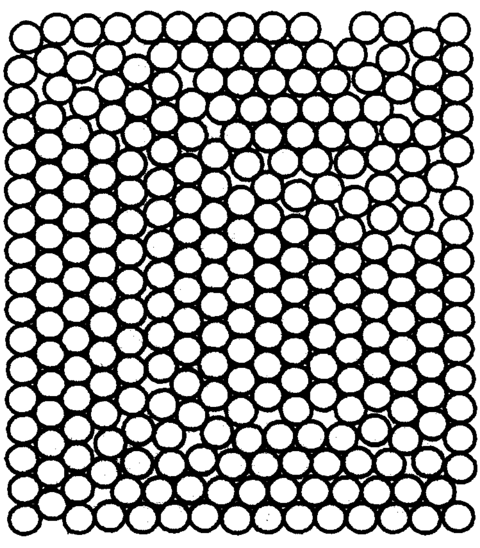

Fig. 2. A randomly packed assembly of circular disks in the example.

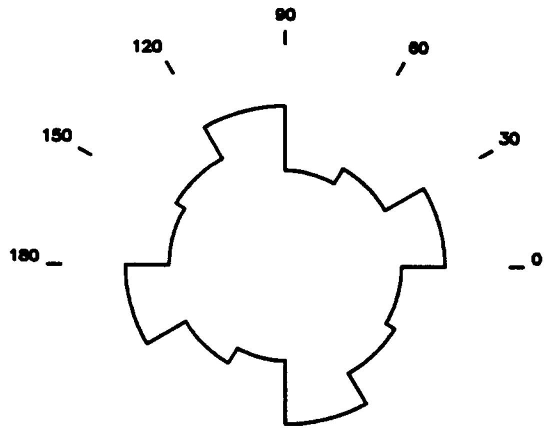

Fig. 3. Contact normal distribution for the random packing.

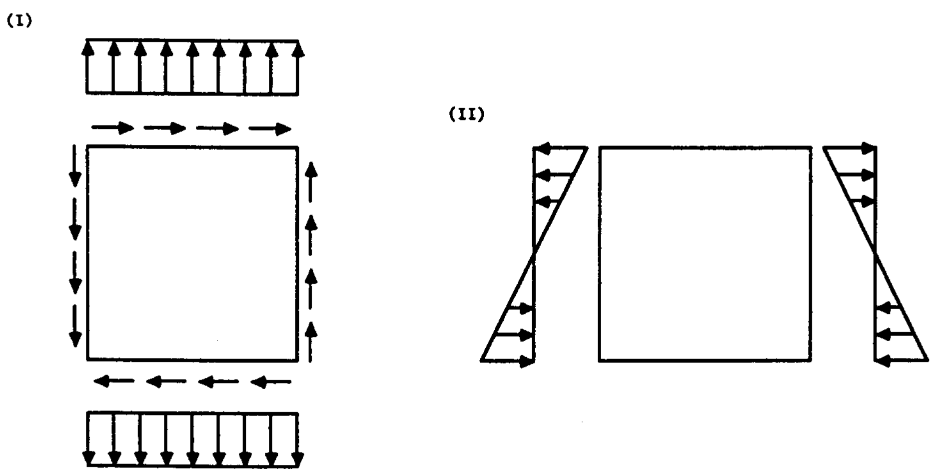

Fig. 4. Schematic plot for two loading conditions: (I) normal and shear stress, and (II) moment stress.

Table 1. Applied stress for the two loading conditions

Applied stress	Loading condition	
	I	II
σ_{xx}(lb/in^2)	−0.064	−0.0055
σ_{yx}(lb/in^2)	1.087	0.2136
σ_{xy}(lb/in^2)	1.081	0.0000
σ_{yy}(lb/in^2)	1.638	0.0000
M_{xz}(lb–in/in^2)	0.1637	−11.3320
M_{yz}(lb–in/in^2)	0.1639	−1.9114
T_{xxx}(lb–in/in^2)	−0.0003	0.6976
T_{xyx}(lb–in/in^2)	−0.0468	11.3320
T_{yyx}(lb–in/in^2)	0.0452	1.9114
T_{xxy}(lb–in/in^2)	0.1169	0.0000
T_{yxy}(lb–in/in^2)	0.2091	0.0000
T_{yyy}(lb–in/in^2)	0.0330	0.0000

cause a small polar stress in the first loading case and small shear and normal stresses in the second loading case.

Based on eqns (9) and (10), three equations can be set up for each particle, thus a set of 828 simultaneous equations is formulated for the 276 particles. The computed displacement and rotation for particles, relative to those of the particle located nearest to

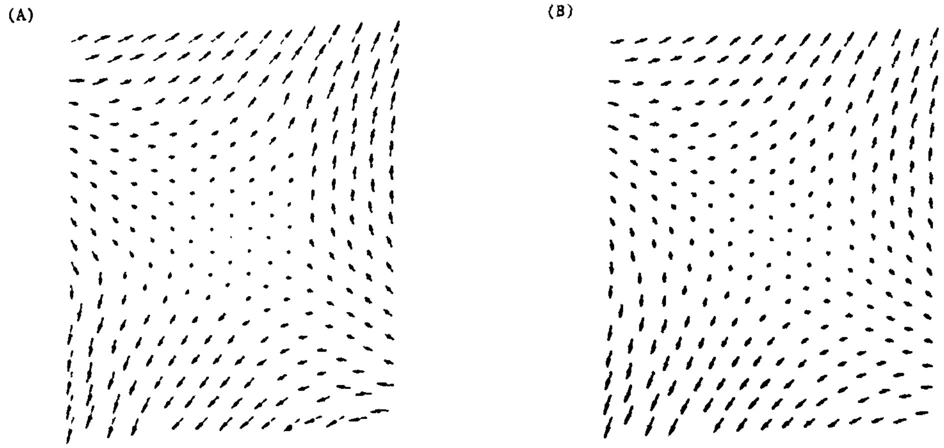

Fig. 5. Comparison of the particle displacement fields obtained from the discrete method and the continuum method for loading case I. (A) Discrete method. (B) Continuum method.

the centroid of the assembly, are plotted with amplified scales in Figs 5, 6 and 7 and compared with the results calculated from microstructural continuum method. The particle displacement field for the first and second loading cases is shown in Figs 5 and 6, respectively. The particle rotation field for the second loading case is shown in Fig. 7. The particle rotations for the first loading case are negligibly small compared to that of the second case, therefore are not shown in plot.

To represent the discrete variables by continuum fields, the computed u_x, u_y and ω_z for the 276 particles are then used to fit polynomial functions by the least square method. For this example, the polynomial forms are assumed as follows:

$$u_x = a_x + \bar{u}_{x,x}x + \bar{u}_{x,y}y + \bar{u}_{x,xx}x^2 + \bar{u}_{x,yx}xy + \bar{u}_{x,yy}y^2 \tag{69}$$

$$u_y = a_y + \bar{u}_{y,x}x + \bar{u}_{y,y}y + \bar{u}_{y,xx}x^2 + \bar{u}_{y,yx}xy + \bar{u}_{y,yy}y^2 \tag{70}$$

$$\omega_z = \bar{\omega}_z + \bar{\omega}_{z,x}x + \bar{\omega}_{z,y}y. \tag{71}$$

The coefficients computed from the least square method are listed in Table 2 and compared with the results obtained from the microstructural continuum method. The degree of agreement between the discrete values and polynomial approximation is shown by the

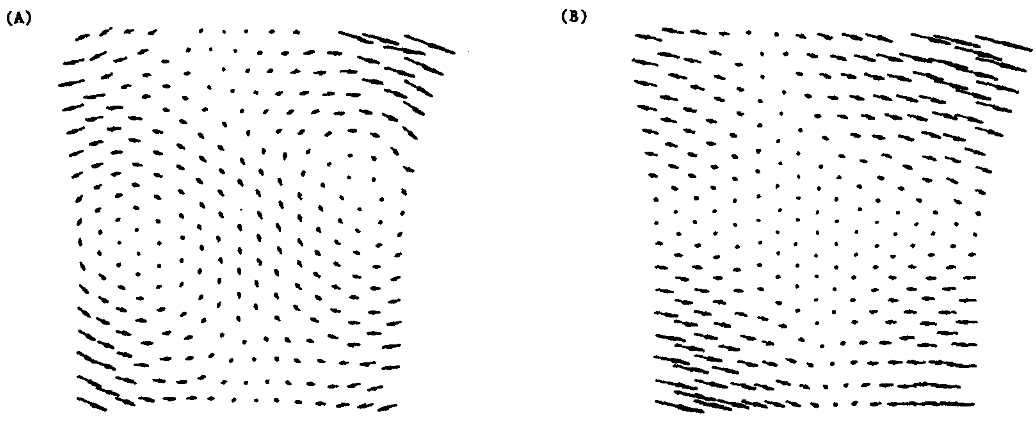

Fig. 6. Comparison of the particle displacement fields obtained from the discrete method and the continuum method for loading case II. (A) Discrete method. (B) Continuum method.

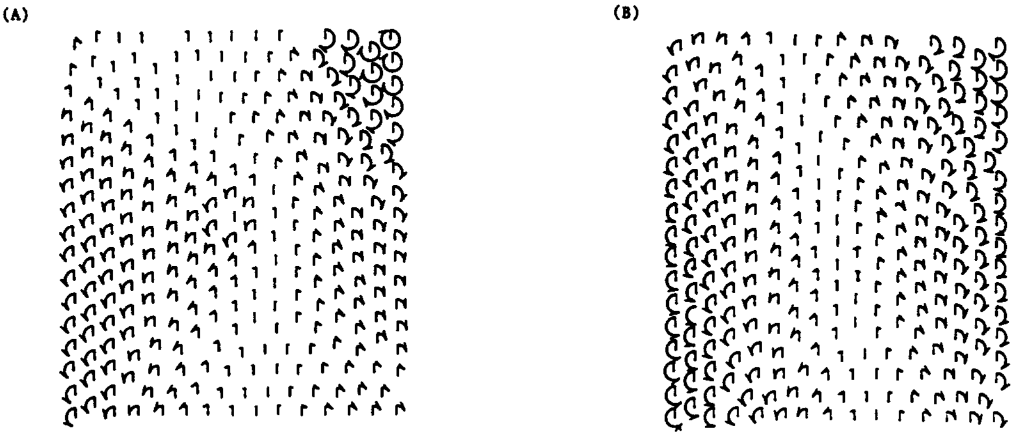

Fig. 7. Comparison of the particle rotation fields obtained from the discrete method and the continuum method for loading case II. (A) Discrete method. (B) Continuum method.

Table 2. Comparison of strains obtained from continuum and discrete methods for the two loading cases

Strain measures	Loading case I		Loading case II	
	Microstructural continuum	Discrete	Microstructural continuum	Discrete
$\bar{u}_{x,x}$	−4.25	−3.74	1.23	5.84
$\bar{u}_{x,y}+\bar{\omega}_z$	13.43	15.64	8.78	4.20
$\bar{u}_{y,x}-\bar{\omega}_z$	12.46	14.90	−5.44	−0.99
$\bar{u}_{y,y}$	13.96	15.84	−0.36	−2.59
$\bar{u}_{x,xx}$(1/in)	−0.05	−0.05	0.78	1.58
$\bar{u}_{x,xy}$(1/in)	−0.08	−0.15	8.38	20.27
$\bar{u}_{x,yy}$(1/in)	−0.02	−0.16	3.16	6.00
$\bar{u}_{y,xx}$(1/in)	0.26	0.16	−8.27	−9.71
$\bar{u}_{y,xy}$(1/in)	0.23	1.1	−4.10	−2.22
$\bar{u}_{y,yy}$(1/in)	0.13	0.16	−2.32	−3.60
$\bar{\omega}_{z,x}$(rad./in)	0.34	0.93	−14.98	−18.52
$\bar{\omega}_{z,y}$(rad./in)	0.15	0.59	−3.69	−6.85

*All numbers $\times 10^{-4}$.

goodness of fit, R, ($R = 1$ represents a perfect fit). The goodness of fit, listed in Table 3 for this example, shows that the displacements and rotations can be reasonably approximated by the assumed polynomial functions. The strain energy for stretch springs and for rotation springs are also listed in Table 3. In the first loading case, the strain energy for stretch springs is 99.55% of the total applied external work. Strain energy for rotation springs is only 0.45%. In the second loading case, the strain energy for stretch springs is about 96% of the total applied external work. Strain energy for rotation springs is 4%.

Table 3. Goodness of fit for the computed particle displacement and rotation and the work done in this system

Goodness of fit	Loading condition	
	I	II
u_x	0.9950	0.9984
u_y	0.9855	0.9995
ω_z	0.6188	0.8887
Work done (lb–in)	I	II
By stretch springs	0.3525	1.204
By rotation springs	0.0018	0.046
Total	0.3543	1.250

4.2. *Microstructural continuum method*

The microstructural continuum method is applied to solve the same problem by assuming that the variables u_x, u_y and ω_z have the same polynomial forms as that in eqns (69), (70) and (71). Following eqns (62)–(67), using constants k_n = 1000 lb/in, k_s = 100 lb/in, and G_z = 100 lb/rad, the constitutive matrix in eqn (68) is obtained. Thus deformation behavior of the packing can be described by the small system of eqn (68), instead of a large system of 828 simultaneous equations as in the discrete method.

The applied stress $\{\bar{\sigma}\}$ in eqn (68) is already given in Table 1, which is computed from the applied forces using eqns (43), (48) and (56). The $\{\bar{\varepsilon}\}$ in eqn (68) is thus computed. Then, using eqns (26) and (27), values of $\bar{u}_{i,j}$ and $\bar{u}_{i,jk}$ are obtained. The values of $\bar{\varepsilon}_{xx}$, $\bar{\varepsilon}_{yy}$, $\bar{\varepsilon}_{xy}$, $\bar{\varepsilon}_{yx}$, $\bar{\omega}_{z,x}$, $\bar{\omega}_{z,y}$, $\bar{u}_{x,xx}$, $\bar{u}_{x,xy}$, $\bar{u}_{x,yy}$, $\bar{u}_{y,xx}$, $\bar{u}_{y,xy}$, $\bar{u}_{y,yy}$ are listed and compared with that obtained from discrete method in Table 2. From the comparison, the results obtained from the microstructural continuum method show reasonable agreement with that from the discrete method.

Using the values in Table 2, the particle rotations, ω_i, and the particle displacements, u_i, are computed from eqns (19) and (20) for comparison with that obtained from the discrete method. For the first loading case, comparisons of the displacement fields in Fig. 5 show good agreement between the discrete and microstructural continuum methods. For the second loading case, Fig. 6 shows local vortices in the displacement field obtained from the discrete method. This pattern is not exhibited in the results obtained from the microstructural continuum method. Similarly, the local variations, observed in the particle rotation field from discrete method, are not shown in the results from the microstructural continuum method. However, the general trends of the rotation field and displacement field are reasonably in good agreement between the two methods. Higher order terms of stress and strain should be considered if the local variations are of interest in the analysis.

5. SUMMARY AND CONCLUSION

A set of constitutive relationships is presented for granular medium. The discrete variables (i.e. displacements and rotations of particles) are assumed to be continuum polynomial functions so that the discrete system can be treated as a continuum system to derive the stress-strain relationship for the medium. The strain measures for the packing account for both the particle displacement and the particle rotation. Based on the principle of virtual work, the stress measures for the packing are expressed in terms of contact forces and contact moments.

The derived stress–strain relationship is illustrated by an example of a randomly packed particles loaded in two different conditions. The results for this example are obtained from the microstructural continuum method assuming a quadratic polynomial for the particle displacements and a linear polynomial for the particle rotations. The calculated particle displacements and particle rotations show reasonable agreement with that obtained from the discrete method.

The microstructural continuum method is a practical way to solve problems involving enormously large number of particles. The total number of equations describing the constitutive relationship of a granular assembly is determined by the number of terms selected in the polynomials. For simplicity, it is desired to use smaller system of constitutive equations. The smallest system of a set of constitutive equations, obtained by selecting a linear polynomial for particle displacements and a constant for particle rotations, has the same form as that given by Chang (1987). When the mode of rotation is completely neglected in the smallest system, the constitutive relations can be further reduced to a form similar to that given by Walton (1987), Jenkins (1987) and Bathurst and Rothenburg (1988).

However, the smaller set of equations results in an approximate set of solutions for particle displacements and rotations. Consequently, each individual particle is not necessarily in force and moment equilibrium. Accuracy of the solutions depends on the approximation involved in the polynomial representation for particle displacements and particle rotations. The present approach provides a flexible method so that one can select the number of terms of polynomial functions to obtain a desired balance between the amount of computing effort and the accuracy of solution.

The proposed constitutive model is useful, when corporated in a finite element method, for the analysis of boundary value problems involving complicated boundary conditions for a granular media which are often encountered in practical situations.

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