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Statics and kinematics of discrete Cosserat-type granular materials

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Abstract

A theoretical framework is presented for the statics and kinematics of discrete Cosserat-type granular materials. In analogy to the force and moment equilibrium equations for particles, compatibility equations for closed loops are formulated in the two-dimensional case for relative displacements and relative rotations at contacts. By taking moments of the equilibrium equations, micromechanical expressions are obtained for the static quantities average Cauchy stress tensor and average couple stress tensor. In analogy, by taking moments of the compatibility equations, micromechanical expressions are obtained for the (infinitesimal) kinematic quantities average rotation gradient tensor and average Cosserat strain tensor in the two-dimensional case. Alternatively, these expressions for the average Cauchy stress tensor and the average couple stress tensor are obtained from considerations of the equivalence of the continuum force and couple traction vectors acting on a plane and the resultant of the discrete forces and couples acting on this plane. In analogy, the expressions for the average rotation gradient tensor and the average Cosserat strain tensor are obtained from considerations of the change of length and change of rotation of a line element in the two-dimensional case. It is shown that the average particle stress tensor is always symmetrical, contrary to the average stress tensor of an equivalent homogenized continuum. Finally, discrete analogues of the virtual work and complementary virtual work principles from continuum mechanics are derived.

Keywords: Granular materials; Micromechanics; Statics; Kinematics; Cosserat continuum

1. Introduction

Micromechanics of granular materials deals with the study of relations between microscopic quantities and macroscopic quantities. A major objective of micromechanics is to formulate micromechanical constitutive relations. For assemblies of semi-rigid particles the microscopic level is that of contacts. The relevant microscopic static quantities are contact force and contact couple and the associated kinematic quantities are relative displacement and relative rotation at contacts.

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Granular materials are special in the sense that they can transmit couples and that besides translational degrees of freedom, they also possess rotational degrees of freedom. The description of granular materials as Cosserat continua, or micropolar continua (Cosserat and Cosserat, 1909; see also Eringen, 1999), takes this into account. For the quasi-static deformations considered here the couple stress and rotation gradient tensors are also important, besides the classical Cauchy stress and strain tensors.

In micromechanical studies expressions for these macroscopic tensors in terms of contact quantities are required. The micromechanical expression for the average Cauchy stress tensor has been reported many times (for example, Drescher and de Josselin de Jong, 1972; Rothenburg and Selvadurai, 1981; Mehrabadi et al., 1982; Kruyt and Rothenburg, 1996), although some controversy still remains about its symmetry (Bardet and Vardoulakis, 2001). Conflicting expressions have been given for the couple stress tensor (Chang and Ma, 1990, 1992; Oda and Iwashita, 2000). Although it is clear that kinematics is equally important as statics, the corresponding kinematic tensors have unfortunately not received as much attention. Expressions for the (infinitesimal) strain tensor, or more accurately the (infinitesimal) displacement gradient tensor, have been given by Rothenburg (1980), Kruyt and Rothenburg (1996), Bagi (1996) and Kuhn (1997). These expressions do not include the effect of particle rotation. For the rotation gradient tensor an expression has only been (effectively) postulated by Satake (2001). The objective of this study is therefore to give a reappraisal of various micromechanical expressions for the macroscopic tensors, and in particular to clarify the role of particle rotation in the expression for the strain tensor.

These micromechanical expressions will be formulated using two different approaches. In the first approach, moments are taken of the discrete force and moment equilibrium equations for contact forces and contact couples and of the discrete compatibility equations for relative displacements and relative rotations at contacts. These discrete compatibility equations have not been reported before. In the second approach micromechanical expressions are obtained using the continuum-mechanical meaning of these tensors. In addition, an alternative view on the issue of the symmetry of the average stress tensor is presented. To complete the theoretical framework for the statics and kinematics of inherently discrete granular materials, discrete analogues of the virtual work and complementary virtual work principles of continuum mechanics are derived.

In this paper the summation convention is used, by which a summation is implied over repeated subscripts. Furthermore, the usual sign convention from continuum mechanics is employed, so tensile stresses and strains are considered positive.

The outline of this study is as follows. In Section 2 the concept of homogenization is discussed. In Section 3 the relevant micromechanical quantities are defined. Section 4 deals with the micromechanical expressions for the average Cauchy stress tensor and average couple stress tensor. For the two-dimensional case, micromechanical expressions for the average Cosserat strain tensor and the average rotation gradient tensor are formulated in Section 5. Discrete virtual work and virtual complementary work principles are given in Section 6. Finally, findings from this study are discussed.

2. Homogenization

In general the geometry of an assembly of particles will exhibit significant inhomogeneity, i.e. it will deviate essentially from that of a crystal. This geometrical inhomogeneity will result in mechanical inhomogeneity. Furthermore, the particles are semi-rigid with stress concentrations occurring near the contact points. Thus, the stress and strain fields inside of the particles will also vary greatly.

As an illustration, the stress field τ_{ij} inside a particle of radius R that is loaded by two diametrically placed normal forces P is given in Fig. 1 (see for example, Timoshenko and Goodier (1970)). It is clear that the length scale associated with the variation of the stress inside the particle is much smaller than the particle radius R.

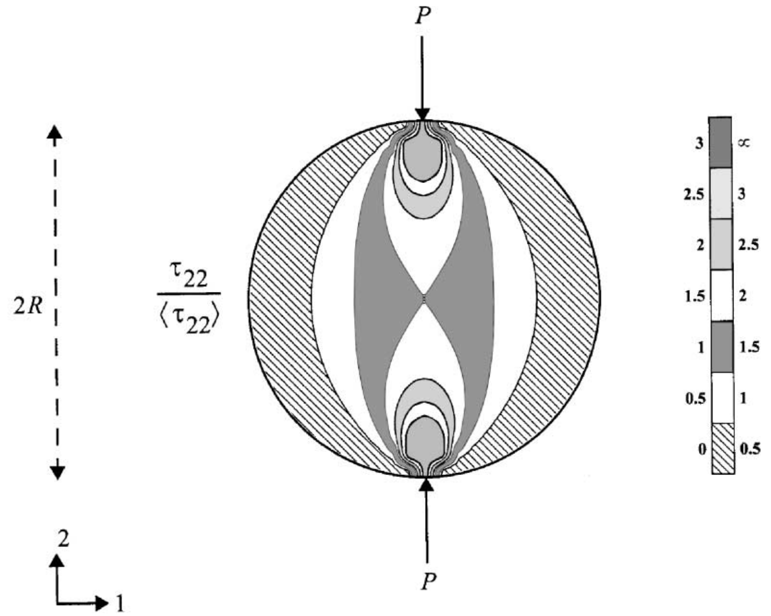


Fig. 1. Nondimensional vertical stress field inside a disk; $\langle\tau_{22}\rangle$ is the average vertical stress inside the disk.

Experiments on photoelastic materials (for example, Drescher and de Josselin de Jong, 1972; Oda and Konishi, 1974) show that the average stresses of particles are also very inhomogeneous. An important manifestation of this inhomogeneity is the occurrence of force chains that carry a large part of the applied load.

Since the detailed of knowledge of the precise stress field is generally not required in studies of the macroscopic behaviour of granular materials, it is natural to replace the assembly of particles by an equivalent homogenized continuum, as illustrated in Fig. 2. For this homogenization process to be meaningful, the length scale λ of the variation of the homogenized stress σ_{ij} must be significantly larger than the particle radius R. So we require $R \ll \lambda < \Lambda$, where Λ is a macroscopic length scale.

Homogenized granular materials may best be described as Cosserat continua (see for example, Eringen, 1999), since the particles can transmit couples at contacts and they also possess rotational degrees of freedom, besides the classical translational degrees of freedom. The basic kinematic quantities of the equivalent homogenized Cosserat continuum are therefore the displacement field $U_i(\boldsymbol{x})$ and rotation field $\omega_i(\boldsymbol{x})$. The basic static quantities are the homogenized Cauchy stress tensor σ_{ij} and the couple stress tensor μ_{ij}.

There is no a priori need for averages of the particle stress τ_{ij} and the average of the homogenized stress σ_{ij} to be equal. This issue will be discussed in Section 4.4.

The mechanical behaviour of the discrete assembly of particles and the homogenized continuum has to be equivalent. Thus the force traction vector over a boundary B of the homogenized stress tensor σ_{ij} must be equal to the resultant of the discrete forces that act on the boundary of the assembly

$$\int_B n_j \sigma_{ji} \, \mathrm{d}B = \sum_{\beta \in B} f_i^\beta \tag{1}$$

where n_i is the outward unit normal vector, the sum is over the contacts β at the boundary B and f_i^β is the force acting at contact β.

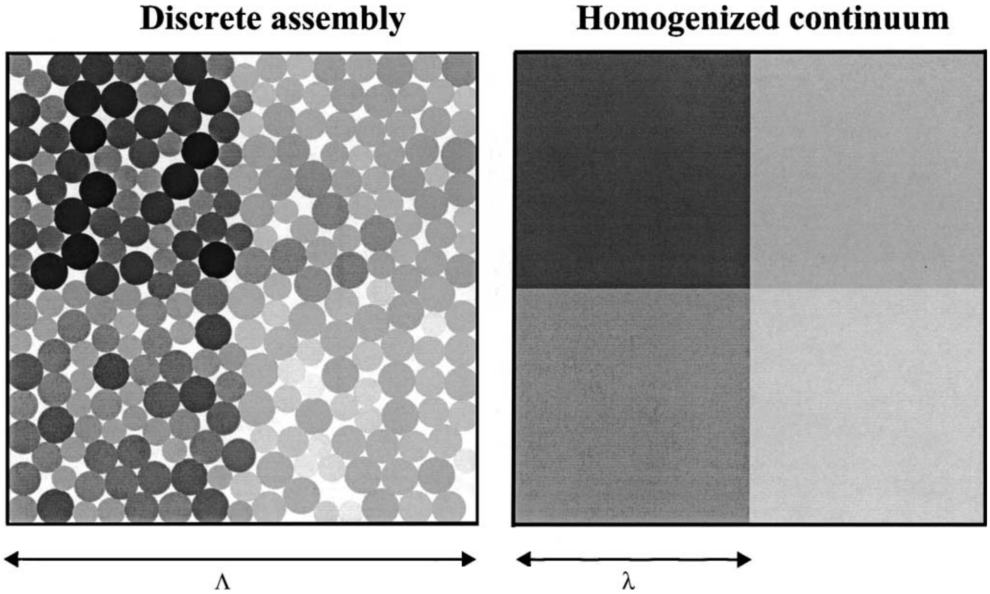


Fig. 2. Discrete assembly and homogenized continuum; greyscale indicates level of stress.

Similar to (1), the couple traction vector over a boundary B of the homogenized couple stress tensor μ_{ij} must be equal to the resultant of the discrete couples acting on the boundary of the assembly

$$\int_B n_j \mu_{ji} \, \mathrm{d}B = \sum_{\beta \in B} \kappa_i^\beta \tag{2}$$

where κ_i^β is the couple acting at contact β. Note that this relation does not involve contact forces.

Since the length scales of the homogenized continuum are assumed to be large in comparison to the particle radius R, it is possible to define a position-dependent contact density $m_V(\boldsymbol{x})$, i.e. the number of contacts per volume. Similarly, it is feasible to define a position-dependent average (over contacts) $\overline{\Psi}(\boldsymbol{x})$ of a general contact quantity Ψ^c (like normal and tangential components of the contact force). The contact density $m_V(\boldsymbol{x})$ and the average $\overline{\Psi}(\boldsymbol{x})$ satisfy

$$\sum_{c \in C} 1 = \int_V m_V(\boldsymbol{x}) \, \mathrm{d}V \qquad \sum_{c \in C} \Psi^c = \int_V m_V(\boldsymbol{x}) \overline{\Psi}(\boldsymbol{x}) \, \mathrm{d}V \tag{3}$$

where the sum is over the set of contacts $c \in C$ in volume V.

In the derivations in this study often a sum over contacts occurs of the product of a contact property Ψ^c and a function of *position* $\phi(\boldsymbol{x})$ that varies slowly over length scales of the order of magnitude of the particle radius R. So the indicated sums are of the type $(1/V) \sum_{c \in C} \phi(\boldsymbol{C}^c) \Psi^c$, where $\boldsymbol{C}^c$ is the position vector of the point of contact c, i.e. the sums are volume-additive. Since $\phi(\boldsymbol{x})$ is assumed to be slowly varying we may write $\overline{\phi \Psi}(\boldsymbol{x}) = \phi(\boldsymbol{x}) \overline{\Psi}(\boldsymbol{x})$. Thus, under the assumptions just described, a sum over contacts may be replaced by an equivalent homogenized integral over the volume

$$\sum_{c \in C} \phi(\boldsymbol{C}^c) \Psi^c = \int_V m_V(\boldsymbol{x}) \phi(\boldsymbol{x}) \overline{\Psi}(\boldsymbol{x}) \, \mathrm{d}V \tag{4}$$

3. Micromechanics

In this section the important micromechanical quantities are introduced. Firstly, the relevant contact quantities are defined. Then the discrete force and moment equilibrium equations are given. To obtain kinematic analogues of these static equilibrium equations, the concept of loops, or *polygons*, is introduced. These polygons are then used to formulate compatibility equations for relative displacement and relative rotations at contacts. In effect, a derivation of the infinitesimal-strain compatibility equations in continuum mechanics is also based on loop considerations (see for example, Boresi and Chong, 2000).

3.1. Contact quantities

The important static quantities at the contact between particles p and q are the contact force f_i^{pq} and the contact couple κ_i^{pq} (exerted by particle q on particle p). The associated kinematic variables at the contact are the relative displacement Δ_i^{pq} and the relative rotation Ω_i^{pq} that are defined by

$$\begin{aligned} \Delta_i^{pq} &= \left[U_i^q + e_{ijk}\omega_j^q r_k^{qp}\right] - \left[U_i^p + e_{ijk}\omega_j^p r_k^{pq}\right] \\ \Omega_i^{pq} &= \omega_i^q - \omega_i^p \end{aligned} \tag{5}$$

where U_i^p and ω_i^p are the (increments of) displacement and rotation of particle p and e_{ijk} is the three-dimensional permutation symbol. The vector from the centre of particle p, X_i^p, to the contact point C_i^{pq} is denoted by $r_i^{pq} = C_i^{pq} - X_i^p$, with an analogous definition for r_i^{qp}. These vectors are depicted in Fig. 3 for the two-dimensional case.

For a contact between particle p and the boundary at point β, the relative displacement and the relative rotation are defined by

$$\begin{aligned} \Delta_i^{p\beta} &= \left[U_i^\beta\right] - \left[U_i^p + e_{ijk}\omega_j^p r_k^{p\beta}\right] \\ \Omega_i^{p\beta} &= \omega_i^\beta - \omega_i^p \end{aligned} \tag{6}$$

where U_i^β and ω_i^β are the displacement and rotation at the boundary. This means that there may be a difference between the displacement and rotation of the particle and those of the boundary, i.e. slip is allowed in the formulation.

The relative displacement Δ_i^{pq} is the sum of two parts, δ_i^{pq} due to displacements of particle centres and ρ_i^{pq} due to particle rotations

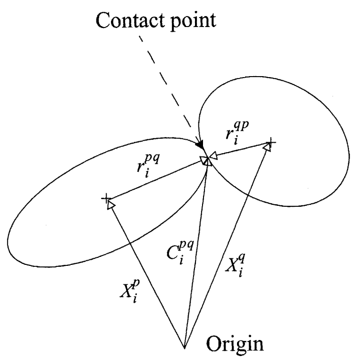


Fig. 3. Geometrical vectors.

$$\begin{aligned} \delta_i^{pq} &= U_i^q - U_i^p \\ \rho_i^{pq} &= e_{ijk}\omega_j^q r_k^{qp} - e_{ijk}\omega_j^p r_k^{pq} \end{aligned} \tag{7}$$

Note that the kinematic contact quantities Δ_i^{pq} and Ω_i^{pq} equal zero for rigid body motions of the whole assembly, contrary to δ_i^{pq}. Therefore the pair $\{\Delta_i^{pq}, \Omega_i^{pq}\}$ constitutes a better measure of deformation at contacts than the pair $\{\delta_i^{pq}, \Omega_i^{pq}\}$. Hence it is desirable to formulate the micromechanical expressions for the strain and rotation gradient tensors in terms involving Δ_i^{pq} and Ω_i^{pq}.

Note that the forces and couples at contacts satisfy Newton's third law

$$f_i^{qp} = -f_i^{pq} \qquad \kappa_i^{qp} = -\kappa_i^{pq} \tag{8}$$

and the relative displacements and relative rotations at contacts satisfy a similar relation

$$\Delta_i^{qp} = -\Delta_i^{pq} \qquad \Omega_i^{qp} = -\Omega_i^{pq} \tag{9}$$

The exact relation between static quantities f_i^{pq} and κ_i^{pq}, and kinematic quantities Δ_i^{pq} and Ω^{pq} is described by the contact constitutive relation.

3.2. Equilibrium equations

In the absence of body forces, the quasi-static force and moment *equilibrium equations* are

$$\sum_q f_j^{pq} + f_j^{p\beta} = 0 \tag{10}$$

$$\sum_q \left(\kappa_j^{pq} + e_{jkl}C_k^{pq} f_l^{pq}\right) + \left(\kappa_j^{p\beta} + e_{jkl}C_k^{p\beta} f_l^{p\beta}\right) = 0 \tag{11}$$

where the sums are over the particles q that are in contact with particle p, $f_i^{p\beta}$ is the force and $\kappa_i^{p\beta}$ is the couple exerted by the boundary on particle p (if present), C_k^{pq} is the position vector of the point of contact between particles p and q and $C_i^{p\beta}$ is the position vector of the point of contact between particle p and the boundary. Note that multiple contacts between two particles are not allowed in the current formulation.

An alternative form of the moment equilibrium equation (11) is obtained by considering the moments with respect to the particle centres

$$\sum_q \kappa_j^{pq} + \kappa_j^{p\beta} + e_{jkl}\sum_q r_k^{pq} f_l^{pq} + e_{jkl} r_k^{p\beta} f_l^{p\beta} = 0 \tag{12}$$

In the sequel, (11) will mostly be used instead of (12), since (11) contains absolute positions C_i^{pq} instead of relative positions r_i^{pq}. The absolute positions do have a continuum equivalent, contrary to the relative positions.

3.3. Polygons

In order to formulate compatibility equations for the relative displacements and relative rotations at contacts in the *two-dimensional* case, it is advantageous to consider the graph representation of a granular assembly (Satake, 1992) (see also Fig. 4). In this graph representation the internal nodes (or vertices) of the graph are formed by the centres of the particles and the boundary nodes of the graph are formed by the contact points at the boundary. Branches (or edges) of the graph are formed by the contacts, corresponding either to two particles in contact, or to a contact between a particle and the boundary. In addition, boundary branches between adjacent contact points at the boundary are included in the graph. The number of particles is N_p and the number of contact points at the boundary is N_c^{B}. Hence the number of nodes N_v in

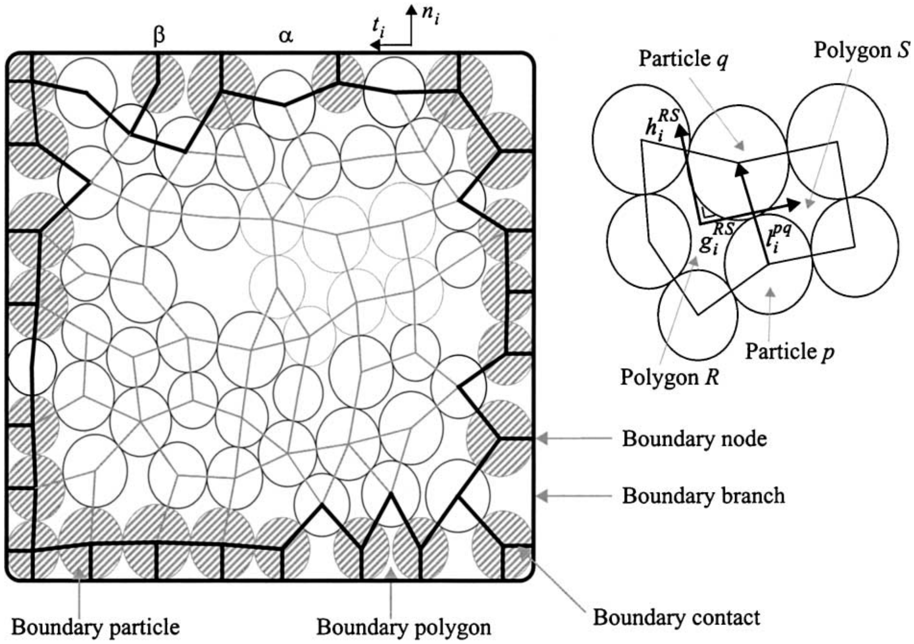


Fig. 4. Polygons, branch vector, polygon vector and rotated polygon vector.

the graph is $N_v = N_p + N_c^B$. The set of all contacts C consists of the set C^I of all internal contacts (between two particles) and the set C^B of all boundary contacts (between a particle and the boundary). The number of internal contacts in C^I is N_c^I, the number of boundary contacts is N_c^B and the total number of contacts is N_c, with $N_c = N_c^I + N_c^B$. The number of branches N_e in the graph is $N_e = N_c + N_c^B$, since the number of boundary branches equals N_c^B.

Branch vectors l_i^{pq} are defined as the vectors that connect the centres of particles p and q that are in contact. These branch vectors form closed loops, or polygons, as depicted in Fig. 4. For future reference the *polygon vector* h_j^{RS} (Rothenburg, 1980; Kruyt and Rothenburg, 1996) is also defined in Fig. 4: it is the vector that is obtained by counter-clockwise rotation over 90° of the *rotated polygon vector* g_i^{RS} that connects the centres of adjacent polygons R and S.

Contacts can be identified in two ways: by the particles involved, or by the polygons involved. The first way will be indicated by using lowercase superscripts, while the second way will be indicated by uppercase superscripts. The adopted convention for the equivalence of contact RS with contact pq is that the vectors g_i^{RS} and l_i^{pq} form a right-handed system. For example, in Fig. 4 contact RS (and not SR) is equivalent to contact pq.

The polygons shown in Fig. 4 include "boundary" polygons, i.e. those polygons that share an edge with the boundary. The boundary polygons are indicated by thick lines in Fig. 4. It is easily verified that the number of these boundary polygons equals the number of boundary contacts N_c^B. The number of internal polygons is N_l^I and the total number of polygons is $N_l = N_l^I + N_c^B$.

The branch vector for a boundary contact of particle p with the boundary is denoted by $l_i^{p\beta}$. It is the vector from the centre of particle p to the contact point $C_i^{p\beta}$, i.e. $l_i^{p\beta} = C_i^{p\beta} - X_i^p$. This definition of the branch vector for boundary contacts was also given by Bagi (1999). The polygon vector h_j^{RS} for a boundary contact between two polygons R and S is defined from the midpoint of the boundary branch of polygon R to the midpoint of the boundary branch of polygon S.

Euler's relation for a connected graph is (see for example, Liu, 1968)

$$N_v - N_e + N_l = 1 \tag{13}$$

where N_v is the number of nodes (vertices), N_l is the number of polygons (loops) and N_e is the number of edges of the graph. Using the relations $N_v = N_p + N_c^B$ and $N_e = N_c + N_c^B$, it follows that

$$N_p - N_c + N_l = 1 \tag{14}$$

A geometrical relation between branch vectors l_i^c and polygon vectors h_j^c is (Kruyt and Rothenburg, 1996)

$$I_{ij} = \frac{1}{A} \sum_{c \in C} l_i^c h_j^c \tag{15}$$

where I_{ij} is the two-dimensional identity tensor and A is the area of the region of interest. This relation is based on the fact that the polygons tessellate the area. Statistics of branch vectors l_i^c and polygon vectors h_j^c for isotropic assemblies were studied by Kruyt and Rothenburg (2001). Note that (15) is valid for any particle shape, not only for disks as shown in Fig. 4.

3.4. Compatibility equations

Using the polygons introduced in the previous section, compatibility equations for the relative displacements and relative rotations at contacts will be derived in the two-dimensional case. In this case, rotation ω^p of particle p and the relative rotation Ω^{pq} between particles p and q are scalar quantities. The part of relative displacement due to rotation, ρ_i^{pq}, is now given by

$$\rho_i^{pq} = e_{ji} r_j^{qp} \omega^q - e_{ji} r_j^{pq} \omega^p \tag{16}$$

where e_{ij} is the two-dimensional permutation tensor.

Consider a closed loop (or polygon) R as shown in Fig. 5. A quantity ψ^{RS} associated with a branch RS is considered that is defined as the *difference* between values associated with the nodes that form the branch, i.e.

$$\psi^{RS} = \Phi^{H(RS)} - \Phi^{T(RS)} \tag{17}$$

where $H(RS)$ and $T(RS)$ denote the "head" node and the "tail" node of the directed branch RS, respectively. For instance, in Fig. 5 $H(AB) = b$ and $T(AB) = a$. Then it follows that

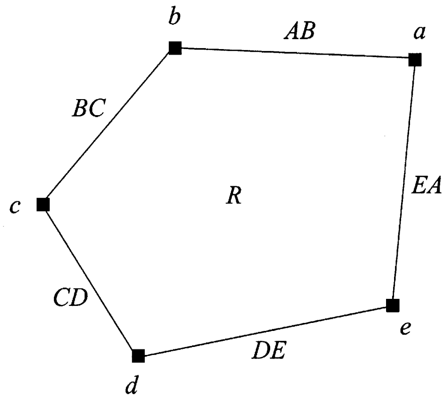
$$\sum_S \psi^{RS} = 0 \tag{18}$$

where the sum is over the branches (sides) of polygon R. This *loop identity* is the discrete analogue of the continuum relation $\oint_C \psi \, ds = \oint_C (d\Phi/ds) \, ds = 0$ for a closed contour C.

Using this loop identity with $\Phi \equiv U_i$ gives the compatibility equations of Rothenburg (1980) and Kruyt and Rothenburg (1996) for relative displacements δ_i^{RS} corresponding to the displacement of the particle centres, as defined in (7)

$$\sum_S \delta_i^{RS} + \delta_i^{R\alpha} = 0 \tag{19}$$

where $\delta_i^{R\alpha}$ is the relative displacement corresponding to the boundary branch of polygon R (if present), defined in terms of displacements at the boundary nodes by $\delta_i^{R\alpha} = u_i^{H(R\alpha)} - u_i^{T(R\alpha)}$.



$$\sum_S \psi^{RS} = \psi^{AB} + \psi^{BC} + \psi^{CD} + \psi^{DE} + \psi^{EA}$$
$$= (\Phi^b - \Phi^a) + (\Phi^c - \Phi^b) + (\Phi^d - \Phi^c) + (\Phi^e - \Phi^d) + (\Phi^a - \Phi^e)$$
$$= 0$$

Fig. 5. Nodes and branches of a polygon *R* and the loop identity.

Similarly, using this loop identity with $\Phi \equiv \omega$ gives the compatibility equations for relative rotations Ω^{RS}

$$\sum_S \Omega^{RS} + \Omega^{R\alpha} = 0 \tag{20}$$

where $\Omega^{R\alpha}$ is the relative rotation corresponding to the boundary branch of polygon *R* (if present), defined in terms of rotations at the boundary nodes by $\Omega^{R\alpha} = \omega^{H(R\alpha)} - \omega^{T(R\alpha)}$.

It is desirable to express the Eq. (19) in terms of the kinematic contact quantities Δ_i^{RS} and Ω^{RS}, since these form a better measure of deformation than δ_i^{RS} and Ω^{RS} as discussed in Section 3.1. This is possible by using the loop identity with $\Phi \equiv -e_{ji}X_j\omega$. It follows that

$$\sum_S \xi_i^{RS} + \xi_i^{R\alpha} = 0 \tag{21}$$

where

$$\xi_i^{RS} = -e_{ji}\left(X_j^S\omega^S - X_j^R\omega^R\right) \tag{22}$$

By adding (19) and (21) it follows

$$\sum_S \left(\delta_i^{RS} + \xi_i^{RS}\right) + \delta_i^{R\alpha} + \xi_i^{R\alpha} = 0 \tag{23}$$

The term ξ_i^{pq} that corresponds to two particles *p* and *q* can be rewritten as

$$\xi_i^{pq} = -e_{ji}C_j^{pq}(\omega^q - \omega^p) + e_{ji}\left(r_j^{qp}\omega^q - r_j^{pq}\omega^p\right) \tag{24}$$

since $X_j^q = C_j^{pq} - r_j^{qp}$ and $X_j^p = C_j^{pq} - r_j^{pq}$ (see also Fig. 3).

Hence we obtain the compatibility equations involving the relative displacements Δ_i^{RS}

$$\sum_S \Delta_i^{RS} + \delta_i^{R\alpha} + \xi_i^{R\alpha} = e_{ji} \sum_S C_j^{RS} \Omega^{RS} \tag{25}$$

Note that the boundary terms $\delta_i^{R\alpha}$ and $\xi_i^{R\alpha}$ that correspond to boundary branches are well-defined in terms of macroscopic kinematics at the boundary $\{U_i^\beta, \omega^\beta\}$.

Since the polygons constitute a "fundamental system of circuits", as defined in graph theory (Liu, 1968), the compatibility equations are independent. Hence, given the set of all relative displacements $\{\Delta_i^c\}$ and relative rotations $\{\Omega^c\}$ at contacts, the displacement field $\{U_i^p\}$ and the rotation field $\{\omega^p\}$ can be reconstructed up to a rigid body motion of the whole assembly, as follows from Euler's relation (14).

4. Stress and couple stress tensors

In this section moments are taken of the discrete equilibrium equations. By multiplying these equations by 1 and summing over all particles, the continuum equilibrium equations are retrieved. By multiplying the equilibrium equations by position vector and summing over all particles, micromechanical expression for the average Cauchy stress tensor and the average couple stress tensor are obtained. An alternative approach to obtaining these expressions is presented that is based on the continuum-mechanical meaning of these tensors.

4.1. Continuum equilibrium equations

Continuum equivalents of the discrete equilibrium equations (10) and (11) are obtained by multiplying these equations with 1 and summing over all particles.

From the force equilibrium equation (10) we find

$$\sum_p \sum_q f_j^{pq} + \sum_p f_j^{p\beta} = 0 \tag{26}$$

The first, double sum consists of terms $f_j^{pq} + f_j^{qp}$, which equal zero since $f_j^{qp} = -f_j^{pq}$. The second sum has a continuum equivalent of $\int_B n_k \sigma_{kj} \, \mathrm{d}B$ (see (1)), which can be expressed as $\int_V \partial\sigma_{kj}/\partial x_k \, \mathrm{d}V$ using the divergence theorem. It follows that the continuum equivalent of the discrete force equilibrium equations is

$$\frac{\partial \sigma_{kj}}{\partial x_k} = 0 \tag{27}$$

since the result holds for any subvolume. This is identical to the classical continuum force equilibrium equations for quasi-static deformations without body forces.

Similarly, we find from the discrete moment equilibrium equation (11)

$$\sum_p \sum_q \left(\kappa_j^{pq} + e_{jkl} C_k^{pq} f_l^{pq}\right) + \sum_p \left(\kappa_j^{p\beta} + e_{jkl} C_k^{p\beta} f_l^{p\beta}\right) = 0 \tag{28}$$

The first, double sum consists of terms $(\kappa_j^{pq} + e_{jkl} C_k^{pq} f_l^{pq}) + (\kappa_j^{qp} + e_{jkl} C_k^{qp} f_l^{qp})$, which equal zero since $\kappa_j^{qp} = -\kappa_j^{pq}$, $C_k^{qp} = C_k^{pq}$ and $f_l^{qp} = -f_l^{pq}$. Thus we find

$$\sum_p \left(\kappa_j^{p\beta} + e_{jkl} C_k^{p\beta} f_l^{p\beta}\right) = 0 \tag{29}$$

The sum in this relation has a continuum equivalent of $\int_B n_m \{\mu_{mj} + e_{jkl} x_k \sigma_{ml}\} \, \mathrm{d}B$ (see (1) and (2)). Using the divergence theorem, this can be expressed as $\int_V \partial(\mu_{mj} + e_{jkl} x_k \sigma_{ml})/\partial x_m \, \mathrm{d}V$. Hence the continuum equivalent of the discrete moment equilibrium equations is

$$\frac{\partial}{\partial x_m}(\mu_{mj} + e_{jkl}x_k\sigma_{ml}) = 0 \tag{30}$$

since the result holds for any subvolume. Using the continuum force equilibrium equation (27), this can simplified to

$$\frac{\partial \mu_{mj}}{\partial x_m} + e_{jkl}\sigma_{kl} = 0 \tag{31}$$

which is identical to the continuum moment equilibrium equations for quasi-static deformations (see for example, Eringen, 1999). It should be noted that it is not possible to obtain this result without using (2), i.e. in the form where the couple traction vector does not involve contact forces. In effect, the second term of (31) corresponds to the moment due to contact forces.

4.2. Stress and couple stress tensors: moments of equilibrium equations

An expression for the average homogenized stress tensor is obtained by multiplying the force equilibrium equation (10) by X_i^p and summing over all particles

$$\sum_p \sum_q X_i^p f_j^{pq} + \sum_p X_i^p f_j^{p\beta} = 0 \tag{32}$$

In the first double sum, each contact between two particles p and q contributes $X_i^p f_j^{pq} + X_i^q f_j^{qp}$. Since $f_j^{qp} = -f_j^{pq}$, this term can be written as $-(X_i^q - X_i^p) f_j^{pq}$, or $-l_i^{pq} f_j^{pq}$. It is easily verified that this product is a proper contact quantity, i.e. $l_i^{pq} f_j^{pq} = l_i^{qp} f_j^{qp}$. Hence the first term can be written as $-\sum_{c\in C^{\mathrm{I}}} l_i^c f_j^c$. Using the definition of the branch vector for a boundary contact, $l_i^{p\beta} = C_i^{p\beta} - X_i^p$, we obtain

$$-\sum_{c\in C^{\mathrm{I}}\cup C^{\mathrm{B}}} l_i^c f_j^c + \sum_{\beta\in B} C_i^\beta f_j^\beta = 0 \tag{33}$$

The second term in this equation has a continuum equivalent of $\int_B x_i n_k \sigma_{kj}\,\mathrm{d}B$. Applying the divergence theorem, this can be expressed as $\int_V \partial(x_i\sigma_{kj})/\partial x_k\,\mathrm{d}V$. Using the continuum force equilibrium equation (27), it follows that the micromechanical expression for the average homogenized stress tensor $\langle\sigma_{ij}\rangle$ becomes

$$\langle\sigma_{ij}\rangle = \frac{1}{V}\int_V \sigma_{ij}\,\mathrm{d}V = \frac{1}{V}\sum_{c\in C} l_i^c f_j^c \tag{34}$$

An expression for the average homogenized couple stress tensor is obtained by multiplying the moment equilibrium equation (11) by X_i^p and summing over all particles

$$\sum_p \sum_q X_i^p \left(\kappa_j^{pq} + e_{jkl} C_k^{pq} f_l^{pq}\right) + \sum_p X_i^p \left(\kappa_j^{p\beta} + e_{jkl} C_k^{p\beta} f_l^{p\beta}\right) = 0 \tag{35}$$

In the first term of the double sum, the contribution of each contact between two particles p and q is $X_i^p \kappa_j^{pq} + X_i^q \kappa_j^{qp}$. Since $\kappa_j^{qp} = -\kappa_j^{pq}$, this contribution can be expressed as $-(X_i^q - X_i^p)\kappa_j^{pq}$, or $-l_i^{pq}\kappa_j^{pq}$. It is easily verified that this product is a proper contact quantity, i.e. $l_i^{pq}\kappa_j^{pq} = l_i^{qp}\kappa_j^{qp}$. Hence the first term in the double sum can be written as $-\sum_{c\in C^{\mathrm{I}}} l_i^c \kappa_j^c$. By a similar argument it follows that the second term of the double sum can be written as $-e_{jkl}\sum_{c\in C^{\mathrm{I}}} l_i^c C_k^c f_l^c$. Using the definition of the branch vector for a boundary contact, $l_i^{p\beta} = C_i^{p\beta} - X_i^p$, we obtain

$$-\sum_{c\in C^{\mathrm{I}}\cup C^{\mathrm{B}}} l_i^c \kappa_j^c - e_{jkl}\sum_{c\in C^{\mathrm{I}}\cup C^{\mathrm{B}}} l_i^c C_k^c f_l^c + \sum_{\beta\in B} C_i^\beta\left(\kappa_j^\beta + e_{jkl} C_k^\beta f_l^\beta\right) = 0 \tag{36}$$

The continuum equivalent of the third term is $\int_B x_i n_m\{\mu_{mj} + e_{jkl}x_k\sigma_{ml}\}\,\mathrm{d}B$, which can be written as $\int_V \partial(x_i[\mu_{mj} + e_{jkl}x_k\sigma_{ml}])/\partial x_m\,\mathrm{d}V$, using the divergence theorem. Employing the continuum force and moment equilibrium equations (27) and (31), it follows that the average couple stress tensor $\langle\mu_{ij}\rangle$ is given by

$$\langle\mu_{ij}\rangle = \frac{1}{V}\int_V \mu_{ij}\,\mathrm{d}V = \frac{1}{V}\left\{\sum_{c\in C} l_i^c\kappa_j^c + e_{jkl}\left[\sum_{c\in C} C_k^c l_i^c f_l^c - \int_V x_k\sigma_{il}\,\mathrm{d}V\right]\right\} \tag{37}$$

Using (4) for the equivalence of a sum over contacts with a volume integral, expression (34) for the homogenized stress tensor can be written as

$$\int_V \sigma_{ij}\,\mathrm{d}V = \int_V m_V(\boldsymbol{x})\overline{l_i f_j}(\boldsymbol{x})\,\mathrm{d}V \tag{38}$$

Since this relation holds for any volume V it follows that

$$\sigma_{ij}(\boldsymbol{x}) = m_V(\boldsymbol{x})\overline{l_i f_j}(\boldsymbol{x}) \tag{39}$$

Similarly, the term $\sum_{c\in V} C_k^c l_i^c f_l^c$ in (37) can be written as $\int_V m_V(\boldsymbol{x})x_k\overline{l_i f_l}(\boldsymbol{x})\,\mathrm{d}V$, or using the previous equation, as $\int_V x_k\sigma_{ij}(\boldsymbol{x})\,\mathrm{d}V$. Hence the last two terms in (37) cancel, and the micromechanical expression for the average couple stress tensor becomes

$$\langle\mu_{ij}\rangle = \frac{1}{V}\int_V \mu_{ij}\,\mathrm{d}V = \frac{1}{V}\sum_{c\in C} l_i^c\kappa_j^c \tag{40}$$

The right-hand side of this equation has a homogenized equivalent $(1/V)\int_V m_V(\boldsymbol{x})\overline{l_i\kappa_j}(\boldsymbol{x})\,\mathrm{d}V$. Since this relation holds for any volume V it follows that

$$\mu_{ij}(\boldsymbol{x}) = m_V(\boldsymbol{x})\overline{l_i\kappa_j}(\boldsymbol{x}) \tag{41}$$

For future reference it is convenient to derive a relation that is based on the moment equilibrium equation (12) that involves relative coordinates. By multiplying these moment equilibrium equations by 1 and summing over all particles we obtain

$$\sum_p\sum_q\left(\kappa_j^{pq} + e_{jkl}r_k^{pq}f_l^{pq}\right) + \sum_p\left(\kappa_j^{p\beta} + e_{jkl}r_k^{p\beta}f_l^{p\beta}\right) = 0 \tag{42}$$

In the first term of the double sum each contact between particles p and q contributes $\kappa_j^{pq} + \kappa_j^{qp}$, which equals zero, since $\kappa_j^{qp} = -\kappa_j^{pq}$. The contribution of each contact in the second term in the double sum is $e_{jkl}(r_k^{pq}f_l^{pq} + r_k^{qp}f_l^{qp})$. Since $l_i^{pq} = r_i^{pq} - r_i^{qp}$ and $f_j^{qp} = -f_j^{pq}$, this can be expressed as $e_{jkl}\sum_{c\in C^{\mathrm{I}}} l_k^c f_l^c$. Using the definition of the boundary branch vector l_i^{β}, the contribution of the contact forces in the single sum is $e_{jkl}\sum_{c\in C^{\mathrm{B}}} l_k^c f_l^c$. Hence we find

$$\sum_{\beta\in B}\kappa_j^{\beta} + e_{jkl}\sum_{c\in C^{\mathrm{I}}\cup C^{\mathrm{B}}} l_k^c f_l^c = 0 \tag{43}$$

4.3. Stress and couple stress tensors: continuum-mechanical meaning

An alternative approach to formulating the micromechanical expression for the Cauchy stress tensor is based on a consideration of the equivalence of the resulting force F_i^{B} acting on a boundary B and the integral of the force traction vector, i.e. $\int_B n_j\sigma_{ji}\,\mathrm{d}B = F_i^{\mathrm{B}}$ (see also (1)). This approach has also been used by Rothenburg and Selvadurai (1981), Mehrabadi et al. (1982), Jagota et al. (1988) and Oda and Iwashita (2000).

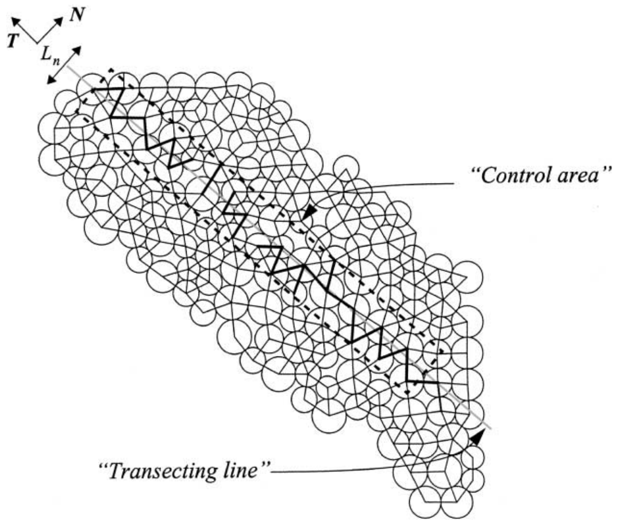


Fig. 6. Contacts corresponding to transecting line.

Consider a plane with area A and unit normal vector N_i at spatial position x_i. A sketch of the two-dimensional case is given in Fig. 6, where the equivalent of the plane in two dimensions is a transecting line with length L. The contacts whose corresponding particles are on opposite sides of the plane are considered to contribute to the resultant of the forces acting on the plane. Such contacts are denoted by a thick line in Fig. 6. The number of contacts in the "control volume" ("control area" in the two-dimensional case depicted in Fig. 6) determined by the area of the plane and the perpendicular distance L_n is $m_V(\boldsymbol{x})AL_n$, where $m_V(\boldsymbol{x})$ is the position-dependent contact density. For such a local contact density to be meaningful, the dimensions of the plane must be such that $L \ll \lambda$, where λ is the length scale associated with variations of the homogenized stress (see also Fig. 2).

The fraction of these contacts whose branch vector l_i intersects the plane, and hence contributes to the resultant force acting on the plane, is $(l_jN_j)/L_n$, compare Buffon's problem (see Santalo, 1976).

By a suitable averaging procedure, we find that the resulting force $F_i^{\mathrm{B}}(\boldsymbol{N};\boldsymbol{x})$ acting on the plane with normal N_i then is given by

$$(m_V(\boldsymbol{x})AL)\overline{\left(\frac{l_jN_j}{L_n}\right)f_i} = m_V(\boldsymbol{x})AN_j\overline{l_jf_i}(\boldsymbol{x}) = F_i^{\mathrm{B}}(\boldsymbol{N};\boldsymbol{x}) \equiv AN_j\sigma_{ji}(\boldsymbol{x}) \tag{44}$$

Since this relation must be satisfied by any N_i, we retrieve (39) for the local homogenized stress tensor.

A similar argument for the equivalence of the resulting couple κ_i^{B} acting on the plane and the integral of the couple traction vector, i.e. $\int_B n_j\mu_{ji}\,\mathrm{d}B = \kappa_i^{\mathrm{B}}$ (see also (2)), retrieves the analogous expression for the couple stress tensor (41). This approach was also used by Oda (1999) and Oda and Iwashita (2000).

4.4. Symmetry of the average particle stress tensor

To analyse the issue of the symmetry of average particle stress $\langle\tau_{ij}\rangle$, it is necessary to consider the origin of the discrete couples κ_i^{β}. The force traction vector of the particle stress acting on the *small* contact area C of two particles in contact (see Fig. 7) will in general not be uniform. Its action can be replaced by a force f_i^c and a couple κ_i^c acting at the contact point such that

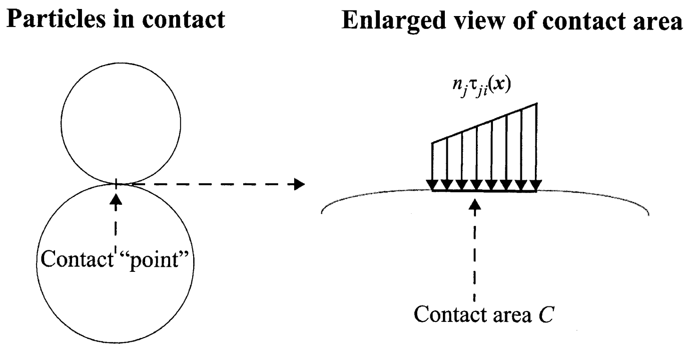


Fig. 7. Particle stress distribution on contact area C.

$$\int_C n_j\tau_{ji}(\boldsymbol{x})\,\mathrm{d}B = f_i^c \qquad \int_C e_{ijk}x_j\{n_l\tau_{lk}(\boldsymbol{x})\}\,\mathrm{d}B = e_{ijk}C_j^c f_k^c + \kappa_i^c \tag{45}$$

where C_i^c is the position vector of the centroid of the contact area.

The particle stress τ_{ij} also satisfies the continuum force equilibrium equation (27). Using this equation and the divergence theorem, it follows that the average particle stress $\langle\tau_{ij}\rangle$ is given by

$$\langle\tau_{ij}\rangle = \frac{1}{V}\int_V \tau_{ij}\,\mathrm{d}V = \frac{1}{V}\int_V \frac{\partial}{\partial x_l}(x_i\tau_{lj})\,\mathrm{d}V = \frac{1}{V}\int_B x_i n_l \tau_{lj}\,\mathrm{d}B \tag{46}$$

From this equation and (45) it follows that the anti-symmetric part of the average particle stress tensor is

$$e_{ijk}\langle\tau_{jk}\rangle = \frac{1}{V}\sum_{\beta\in B}\{e_{ijk}x_j^\beta f_k^\beta + \kappa_i^\beta\} \tag{47}$$

From this equation and (29), it follows that the average particle stress $\langle\tau_{ij}\rangle$ is always symmetrical, i.e. $e_{ijk}\langle\tau_{jk}\rangle = 0$, contrary to the average stress $\langle\sigma_{ij}\rangle$ of the equivalent homogenized continuum! When contact couples are absent, the average stress $\langle\sigma_{ij}\rangle$ of the equivalent homogenized continuum is also symmetrical, as follows from (34) and (43).

Therefore the averages of particle stress and homogenized stress are not necessarily always equal. Since the average particle stress is always symmetrical, the behaviour of the stresses inside the particles is completely "classical".

5. Strain and rotation gradient tensors

In this section micromechanical expressions will be given for the Cosserat strain and rotation gradient tensors in the two-dimensional case. The two methods used are analogous to those employed in Section 4 to obtain the micromechanical expressions for the stress and couple stress tensors. The first method employs taking moments of the compatibility equations, while the second method uses the continuum-mechanical meanings of these tensors. Contrary to the expressions for stress and couple stress tensors, the expressions for the strain and rotation gradient tensors are only valid in the two-dimensional case.

5.1. Strain and rotation gradient tensors: moments of compatibility equations

Firstly the micromechanical expression for the rotation gradient tensor will be considered, since it turns out that the expression for the rotation gradient tensor is required in obtaining the expression for the Cosserat strain tensor.

The micromechanical expression for the average rotation gradient is obtained by taking a moment of the compatibility equations for relative rotations (20), i.e. by multiplying by a vector Y_j^R associated with polygon R and adding all equations we find

$$\sum_R \sum_S \Omega^{RS} Y_j^R + \sum_R \Omega^{R\alpha} Y_j^R = 0 \tag{48}$$

The vector Y_j^R is chosen equal to the centre of polygon R if the polygon is an internal polygon and equal to the midpoint of the boundary branch if the polygon is a boundary polygon.

In the double sum in the previous equation each contact that corresponds to polygons R and S contributes $\Omega^{SR} Y_j^S + \Omega^{RS} Y_j^R$. Since $\Omega^{SR} = -\Omega^{RS}$, this can be written as $-\Omega^{RS} g_j^{RS}$, where g_j^{RS} is the rotated polygon vector $g_j^{RS} = Y_j^S - Y_j^R$ defined in Section 3.3. Note that the product $\Omega^{RS} g_j^{RS}$ is a well-defined contact quantity, i.e. $\Omega^{RS} g_j^{RS} = \Omega^{SR} g_j^{SR}$. Hence the double sum can be written as $-\sum_{c\in C} \Omega^c g_j^c$. The second sum of (48) has a continuum equivalent of $\int_B (\mathrm{d}\omega/\mathrm{d}s) x_j \,\mathrm{d}s$ where $\mathrm{d}s$ is the length of an infinitesimal line element along the boundary. After using the relation $t_j = \mathrm{d}x_j/\mathrm{d}s$ for the unit tangential vector along the boundary (see also Fig. 4), $e_{jk} t_k = n_j$ and performing a partial integration along the closed boundary B, it follows that $\int_B (\mathrm{d}\omega/\mathrm{d}s) x_j \,\mathrm{d}s = e_{jk} \int_B \omega n_k \,\mathrm{d}s$. Finally, it follows from the divergence theorem that the micromechanical expression for the average rotation gradient tensor is given by

$$\left\langle \frac{\partial \omega}{\partial x_j} \right\rangle = \frac{1}{A} \int_A \frac{\partial \omega}{\partial x_j} \mathrm{d}A = \frac{1}{A} \sum_{c\in C} \Omega^c h_j^c \tag{49}$$

where $h_i^c = e_{ji} g_j^c$ is the polygon vector defined in Section 3.3.

Using the two-dimensional version of (4) for the equivalence of a sum over contacts with a surface integral, the right-hand side of (49) has a homogenized equivalent $(1/A) \int_A m_A(\boldsymbol{x}) \overline{\Omega h_j}(\boldsymbol{x}) \,\mathrm{d}A$, where $m_A(\boldsymbol{x})$ is the two-dimensional contact density, i.e. the number of contacts per area. Since (49) holds for any A, it follows that

$$\frac{\partial \omega}{\partial x_j}(\boldsymbol{x}) = m_A(\boldsymbol{x}) \overline{\Omega h_j}(\boldsymbol{x}) \tag{50}$$

The Cosserat strain tensor ε_{ij} is defined by (see for example, Eringen, 1999)

$$\varepsilon_{ij} = \frac{\partial u_j}{\partial x_i} - e_{ij}\omega \tag{51}$$

The micromechanical expression for the Cosserat strain tensor is obtained by taking a moment of the compatibility equations for relative displacements (25), i.e. by multiplying by the vector Y_j^R associated with polygon R and adding all equations we find

$$\sum_R \sum_S \Delta_i^{RS} Y_j^R + \sum_R \delta_i^{R\alpha} Y_j^R + \sum_R \xi_i^{R\alpha} Y_j^R = e_{ki} \sum_R \sum_S C_k^{RS} \Omega^{RS} Y_j^R \tag{52}$$

In the first double sum the contribution of each contact that corresponds to polygons R and S is $\Delta_i^{SR} Y_j^S + \Delta_i^{RS} Y_j^R$. Since $\Delta_i^{SR} = -\Delta_i^{RS}$, this can be written as $-\Delta_i^{RS} g_j^{RS}$. Note that the product $\Delta_i^{RS} g_j^{RS}$ is a well-defined contact quantity, i.e. $\Delta_i^{RS} g_j^{RS} = \Delta_i^{SR} g_j^{SR}$. Hence this double sum can be written as $-\sum_{c\in C} \Delta_i^c g_j^c$. By a similar argument it follows that the double sum on the right-hand side can be expressed as $-e_{ki} \sum_{c\in C} C_k^c \Omega^c g_j^c$. The continuum equivalent of the first boundary term in (48) is $\int_B (\mathrm{d}u_i/\mathrm{d}s) x_j \,\mathrm{d}s$, while that of the second boundary term is $-e_{ki}\int_B [\mathrm{d}(x_k\omega)/\mathrm{d}s]x_j\,\mathrm{d}s$. By performing a partial integration of the first boundary term along the closed boundary B and using $g_i^c = e_{ij}h_j^c$, we find

$$-e_{jk}\sum_{c\in C}\Delta_i^c h_k^c - \int_B u_i t_j\,\mathrm{d}s - e_{ki}\int_B x_j\frac{\mathrm{d}}{\mathrm{d}s}(x_k\omega)\,\mathrm{d}s = -e_{ki}e_{jl}\sum_{c\in C}C_k^c\Omega^c h_l^c \tag{53}$$

Using the two-dimensional version of (4) for the equivalence of a sum over contacts with a surface integral, the term $\sum_{c\in C}C_k^c\Omega^c h_l^c$ can be written as $\int_A x_k m_A(\boldsymbol{x})\overline{\Omega h_l}(\boldsymbol{x})\,\mathrm{d}A$. Employing the micromechanical expression for the rotation gradient (50), this term can be expressed as $\int_A x_k(\partial\omega/\partial x_l)\,\mathrm{d}A$. This last term equals $\int_A \partial(x_k\omega)/\partial x_l\,\mathrm{d}A - \int_A I_{lk}\omega\,\mathrm{d}A$, where I_{lk} is the two-dimensional identity tensor. Hence we obtain

$$-e_{jk}\sum_{c\in C}\Delta_i^c h_k^c + e_{jk}\int_B u_i n_k\,\mathrm{d}s = e_{ki}\int_B x_j\frac{\mathrm{d}}{\mathrm{d}s}(x_k\omega)\,\mathrm{d}s - e_{ki}e_{jl}\left[\int_A\frac{\partial}{\partial x_l}(x_k\omega)\,\mathrm{d}A - \int_A I_{lk}\omega\,\mathrm{d}A\right] \tag{54}$$

Using the divergence theorem and $-e_{jl}n_l = t_j = \mathrm{d}x_j/\mathrm{d}s$, it follows after some algebra that

$$\int_A\left(\frac{\partial u_i}{\partial x_k} - e_{ki}\omega\right)\mathrm{d}A = \sum_{c\in C}\Delta_i^c h_k^c \tag{55}$$

Hence we obtain the micromechanical expression for the average Cosserat strain tensor

$$\langle\varepsilon_{ij}\rangle = \frac{1}{A}\int_A\varepsilon_{ij}\,\mathrm{d}A = \frac{1}{A}\sum_{c\in C}h_i^c\Delta_j^c \tag{56}$$

Using the two-dimensional version of (4) for the equivalence of a sum over contacts with a surface integral, the right-hand side of (56) has a homogenized equivalent $\int_A m_A(\boldsymbol{x})\overline{h_i\Delta_j}(\boldsymbol{x})\,\mathrm{d}A$. Since this equation holds for any A, it follows that

$$\varepsilon_{ij}(\boldsymbol{x}) = m_A(\boldsymbol{x})\overline{h_i\Delta_j}(\boldsymbol{x}) \tag{57}$$

5.2. Strain and rotation gradient tensors: continuum-mechanical meaning

In this section an alternative view is presented for the micromechanical expressions for the average strain and rotation gradient tensors, using the continuum-mechanical meaning of these tensors. It is analogous to the presentation in Section 4.3 for the micromechanical expression for the stress and couple stress tensors. An analogous, yet more complex, formulation for the displacement gradient tensor was given by Rothenburg (1980).

The continuum-mechanical meaning of the displacement gradient $\partial u_j/\partial x_i$ is that the relative displacement $\mathrm{d}u_i$ of points separated by a vector $\mathrm{d}x_i$ is given by $\mathrm{d}u_i = (\partial u_i/\partial x_j)\,\mathrm{d}x_j$. Similarly, the relative rotation $\mathrm{d}\omega$ is given in terms of the rotation gradient $\partial\omega/\partial x_j$ by $\mathrm{d}\omega = (\partial\omega/\partial x_j)\,\mathrm{d}x_j$.

Consider a line with unit directional vector T_i and unit normal vector N_i at spatial position x_i that transects an assembly (see Fig. 8). The length of this transecting line is L. Consider the contacts whose centres of the corresponding polygons are on opposite sides of this transecting line. These contacts are indicated by a thick line in Fig. 8. It is observed that these contacts form a *chain* that, on average, is oriented along the transecting line.

It is easily verified that the difference in displacement $\mathrm{d}u_i$ between the ending and the starting point of the chain is given by $\sum_{c\in\mathrm{Chain}}\delta_i^c$ (see also Fig. 9(a)), where the sum is over the contacts c in the chain. The difference in position between the ending and starting point of the chain is $\mathrm{d}x_i = LT_i$.

The number of contacts in the "control area" determined by the length of the transecting line and the perpendicular distance L_n is $m_A(\boldsymbol{x})LL_n$, where $m_A(\boldsymbol{x})$ is the position-dependent contact density. For such a

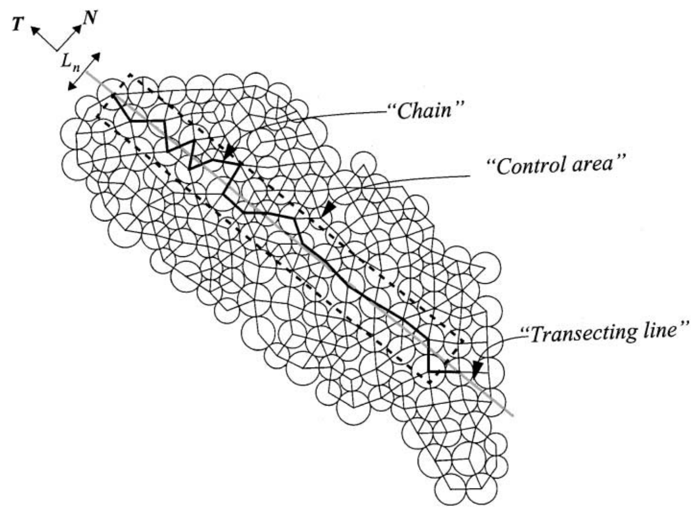


Fig. 8. Contacts corresponding to the "chain".

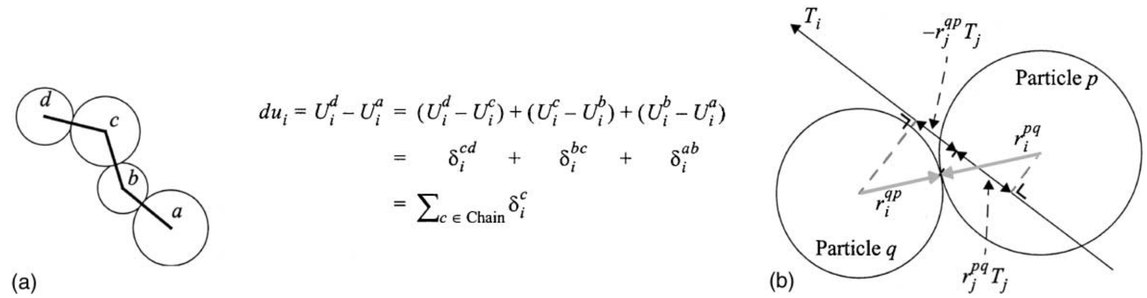


Fig. 9. (a) Relative displacement of a line element and (b) average rotation of a line element.

local contact density to be meaningful, the dimensions of the transecting line must be such that $L \ll \lambda$, where λ is the length scale associated with variations of the homogenized stress (see also Fig. 2).

The fraction of these contacts whose rotated polygon vector g_i intersects the line, and hence contributes to the difference in displacement of the chain, is $(g_j N_j)/L_n$, compare Buffon's problem (see Santalo, 1976). By a suitable averaging procedure and using $g_j N_j = h_j T_j$, we find that the relative displacement $\mathrm{d}u_i$ between the ending and starting point of the chain is given by

$$\frac{\partial u_i}{\partial x_j}\,\mathrm{d}x_j = \mathrm{d}u_i = (m_A L L_n)\overline{\left(\frac{g_j N_j}{L_n}\right)\delta_i} = m_A(\boldsymbol{x})\overline{\delta_i h_j}(L T_j) = m_A(\boldsymbol{x})\overline{\delta_i h_j}\,\mathrm{d}x_j \tag{58}$$

Since this relation holds for any orientation T_i of the transecting line, it follows that the displacement gradient is given by

$$\frac{\partial u_j}{\partial x_i}(\boldsymbol{x}) = m_A(\boldsymbol{x})\overline{h_i \delta_j}(\boldsymbol{x}) \tag{59}$$

Consider a contact between two particles p and q. For such a contact its average rotation (weighted by length along the line segment) is $-[r_j^{qp}\omega^q - r_j^{pq}\omega^p]T_j = e_{kj}\rho_k^{pq}T_j$ (see also Fig. 9(b)). The term ρ_k^{pq} has been defined in (7). Hence the average rotation $\bar{\omega}$ for the line segment is given by $L\bar{\omega} = \sum_{c\in\text{Chain}} e_{kj}\rho_k^c T_j$. In terms of averages this becomes, using $g_j N_j = h_j T_j$

$$L\bar{\omega} = (m_A L L_n)\overline{\left(\frac{g_j N_j}{L_n}\right) e_{kj}\rho_k^{pq} T_j} \Rightarrow \bar{\omega}(\boldsymbol{x}) = m_A(\boldsymbol{x}) T_k \overline{h_k \rho_j}(\boldsymbol{x}) e_{ji} T_i \tag{60}$$

For $\bar{\omega}$ to be a meaningful homogenized quantity, it must be independent of T_j. Hence it follows that $\overline{h_k\rho_j}(\boldsymbol{x})e_{ji}$ must be isotropic and $e_{ji}\bar{\omega} = e_{kj}\overline{h_i\rho_j}(\boldsymbol{x})$. By adding this relation to the relation for the displacement gradient tensor (59), we retrieve expression (57) for the Cosserat strain tensor.

An argument based on the difference in rotation $d\omega$ between the ending and the starting point of the chain, similar to that leading to expression (59) for the displacement gradient tensor, retrieves the analogous expression for the rotation gradient tensor (50).

6. Virtual work and complementary virtual work

To complete the theoretical framework for the discrete kinematics and statics, discrete virtual work and complementary work principles are derived, in analogy to the continuous virtual work and complementary work principles in continuum mechanics (see for example, Washizu, 1968). These discrete principles are valid in the two-dimensional and the three-dimensional case.

6.1. Virtual work

Consider an arbitrary displacement and rotation field $\{U_i^{*p}, \omega_i^{*p}\}$. By multiplying the force equilibrium equation (10) by a virtual displacement U_i^{*p} and the moment equilibrium equation (12) by a virtual rotation ω_i^{*p} and summing these over all particles we find

$$\sum_p \sum_q f_i^{pq}\left(U_i^{*p} + e_{ijk}\omega_j^{*p} r_k^{pq}\right) + \sum_p \sum_q \kappa_i^{pq}\omega_i^{*p} + \sum_p f_i^{p\beta}\left(U_i^{*p} + e_{ijk}\omega_j^{*p} r_k^{p\beta}\right) + \sum_p \kappa_i^{p\beta}\omega_i^{*p} = 0 \tag{61}$$

In the first double sum each internal contact between particles p and q contributes a term $f_i^{pq}\{U_i^{*p} + e_{ijk}\omega_j^{*p} r_k^{pq}\} + f_i^{qp}\{U_i^{*q} + e_{ijk}\omega_j^{*q} r_k^{qp}\}$. Since $f_i^{pq} = -f_i^{qp}$, this combination can be expressed as $-f_i^{pq}\Delta_i^{*pq}$. It is easily verified that this product is a well-defined contact quantity, since $f_i^{pq}\Delta_i^{*pq} = f_i^{qp}\Delta_i^{*pq}$. In a similar manner, it follows that each contact in the second double sum contributes $-\kappa_i^{pq}\Omega_i^{*pq}$. In the boundary terms, we employ the definitions of the relative displacement and relative rotation at the boundary, i.e. $U_i^{*p} + e_{ijk}\omega_j^{*p} r_k^{p\beta} = U_i^{*\beta} - \Delta_i^{*p\beta}$ and $\omega_i^{*p} = \omega_i^{*\beta} - \Omega_i^{*p\beta}$, respectively (compare (6)). Here $U_i^{*\beta}$ and $\omega_i^{*\beta}$ are the virtual displacement and rotation at the boundary, respectively. Finally, the *virtual work principle* is obtained

$$\sum_{c\in C} f_i^c \Delta_i^{*c} + \sum_{c\in C} \kappa_i^c \Omega_i^{*c} = \sum_{\beta\in B} f_i^\beta U_i^{*\beta} + \sum_{\beta\in B} \kappa_i^\beta \omega_i^{*\beta} \tag{62}$$

6.2. Complementary virtual work

In analogy to the method employed by Washizu (1968), the complementary virtual work principle is derived by multiplying the definitions of relative displacements and relative rotations by an arbitrary virtual contact force f_i^{*c} and virtual contact couple κ_i^{*c}, respectively, and summing over all contacts. The virtual forces and virtual couples must satisfy the equilibrium equation (10) and (12). In addition, the virtual forces and couples will satisfy (8).

Using these relations in the definitions (5) and (6) of relative displacements and relative rotations at internal and boundary contacts results in

$$\begin{aligned}
\Delta_i^{pq} f_i^{*pq} &= -\left[U_i^q + e_{ijk}\omega_j^q r_k^{qp}\right] f_i^{*qp} - \left[U_i^p + e_{ijk}\omega_j^p r_k^{pq}\right] f_i^{*pq} \\
\Delta_i^{p\beta} f_i^{*p\beta} &= U_i^\beta f_i^{*p\beta} - \left[U_i^p + e_{ijk}\omega_j^p r_k^{p\beta}\right] f_i^{*p\beta} \\
\Omega_i^{pq} \kappa_i^{*pq} &= -\omega_i^q \kappa_i^{*qp} - \omega_i^p \kappa_i^{*pq} \\
\Omega_i^{p\beta} \kappa_i^{*p\beta} &= \omega_i^\beta \kappa_i^{*q\beta} - \omega_i^p \kappa_i^{*p\beta}
\end{aligned} \tag{63}$$

By summing these expressions over all internal contacts we find

$$\begin{aligned}
\sum_{c\in C^{\mathrm{I}}} \Delta_i^c f_i^{*c} &= \frac{1}{2}\sum_p \sum_q \Delta_i^{pq} f_i^{*pq} = -\sum_p \sum_q \left[U_i^p + e_{ijk}\omega_j^p r_k^{pq}\right] f_i^{*pq} \\
\sum_{c\in C^{\mathrm{I}}} \Omega_i^c \kappa_i^{*c} &= \frac{1}{2}\sum_p \sum_q \Omega_i^{pq} \kappa_i^{*pq} = -\sum_p \sum_q \omega_i^p \kappa_i^{*pq}
\end{aligned} \tag{64}$$

and by summing these expressions over all boundary contacts we find

$$\begin{aligned}
\sum_{c\in C^{\mathrm{B}}} \Delta_i^c f_i^{*c} &= \sum_p \Delta_i^{p\beta} f_i^{*p\beta} = \sum_{\beta\in B} U_i^\beta f_i^{*\beta} - \sum_p \left[U_i^p + e_{ijk}\omega_j^p r_k^{p\beta}\right] f_i^{*p\beta} \\
\sum_{c\in C^{\mathrm{B}}} \Omega_i^c \kappa_i^{*c} &= \sum_p \Omega_i^{p\beta} \kappa_i^{*p\beta} = \sum_{\beta\in B} \omega_i^\beta \kappa_i^{*\beta} - \sum_p \omega_i^p \kappa_i^{*p\beta}
\end{aligned} \tag{65}$$

By adding the previous two equations and taking into account that the virtual forces and couples satisfy the equilibrium equations (10) and (12), we obtain after some algebra the *complementary virtual work principle*

$$\sum_{c\in C} \Delta_i^c f_i^{*c} + \sum_{c\in C} \Omega_i^c \kappa_i^{*c} = \sum_{\beta\in B} U_i^\beta f_i^{*\beta} + \sum_{\beta\in B} \omega_i^\beta \kappa_i^{*\beta} \tag{66}$$

7. Discussion and concluding remarks

A theoretical framework is presented for the static and kinematics of discrete Cosserat-type granular materials. In analogy to the equilibrium equations for forces and moments at contacts, compatibility equations have been formulated for the relative displacements and relative rotations at contacts in the two-dimensional case. These kinematic equations are based on polygons (closed loops).

By taking moments of the equilibrium and compatibility equations, micromechanical expressions for the average Cauchy stress, couple stress, Cosserat strain and rotation gradient tensors have been obtained. Alternatively, these expressions are also found from considerations of the continuum-mechanical meaning of these tensors, i.e. of the resulting force and couple acting on a plane and of the change of displacement and change of rotation of a line element.

To complete the theoretical framework for the discrete kinematics and statics, discrete virtual work and complementary work principles have been derived.

It is possible to define uniform field expressions for the kinematic and static quantities at contacts in the two-dimensional case. The relative displacements and relative rotations at contacts that correspond to uniform strain and uniform rotation gradient are given by

$$\Delta_i^c = l_k^c \varepsilon_{ki} \qquad \Omega^c = l_k^c \frac{\partial \omega}{\partial x_k} \tag{67}$$

Similarly, the forces and couples at contacts that correspond to uniform stress and uniform couple stress are given by

$$f_i^c = h_k^c \sigma_{ki} \qquad \kappa^c = h_k^c \mu_k \tag{68}$$

These uniform field expressions (67) and (68) are consistent with (the two-dimensional versions of) the micromechanical expressions (34) for the average stress tensor, (40) for the average couple stress tensor, (56) for the average Cosserat strain tensor and (49) for the average rotation gradient, as follows from the geometrical identity (15). Uniform field expressions for relative displacements and forces at contacts have been employed by Kruyt and Rothenburg (2002a,b) to derive rigorous bounds for the effective elastic moduli of two-dimensional assemblies with bonded contacts.

The theoretical framework is summarised in Table 1. Note that the two-dimensional case is considered in order to emphasize the dualities present and that the boundary terms have been omitted for clarity in the equilibrium and compatibility equations.

It may be expedient to point out that in the formulation of the micromechanical expressions for Cosserat strain and rotation gradient tensors and of the compatibility equations for relative displacement and relative rotations, it is not necessary that contacts are fixed (i.e. that particles corresponding to a contact remain in contact during deformation). The resulting equations are equally valid when a contact is broken due to deformation. However, the direct relation between (increments of) force and relative displacement at contacts through the contact constitutive relation is lost when the contact is broken.

The micromechanical expression (34) for the average stress tensor is identical to that obtained by many others (for example, Drescher and de Josselin de Jong, 1972; Rothenburg, 1980; Rothenburg and Selvadurai, 1981; Mehrabadi et al., 1982; Chang and Ma, 1990, 1992; Kruyt and Rothenburg, 1996). Sometimes the transpose of (34) is given, i.e. $\langle \sigma_{ij} \rangle = (1/V) \sum_{c \in C} f_i^c l_j^c$. This difference arises when the continuum force equilibrium equations $\partial \sigma_{jk} / \partial x_k = 0$ are used instead of (27). Although expression (34) was formulated for the case where body forces are absent, it can be shown that it also is valid when these are present (Kruyt, 1993; Bagi, 1999).

A slightly different expression for the average stress tensor was given by Bardet and Vardoulakis (2001). The difference with (34) is only significant for small assemblies. However, as shown in Appendix A, their expression does not correspond to the continuum-mechanical meaning of the stress tensor for small as-

Table 1
Micromechanical framework for kinematics and statics

Statics		Kinematics	
Force	f_i^c	Δ_i^c	Relative displacement
Couple	κ^c	Ω^c	Relative rotation
Equilibrium equations for particles	$\sum_q f_j^{pq} = 0$ $\sum_q \kappa^{pq} + \sum_q e_{ij} C_i^{pq} f_j^{pq} = 0$	$\sum_S \Delta_i^{RS} + \sum_S e_{ij} C_j^{RS} \Omega^{RS} = 0$ $\sum_S \Omega^{RS} = 0$	Compatibility equations for polygons
Stress	$\langle \sigma_{ij} \rangle = \frac{1}{A} \sum_{c \in C} l_i^c f_j^c$	$\langle \varepsilon_{ij} \rangle = \frac{1}{A} \sum_{c \in C} h_i^c \Delta_j^c$	Strain
Couple stress	$\langle \mu_i \rangle = \frac{1}{A} \sum_{c \in C} l_i^c \kappa^c$	$\left\langle \frac{\partial \omega}{\partial x_j} \right\rangle = \frac{1}{A} \sum_{c \in C} h_j^c \Omega^c$	Rotation gradient
Virtual work	$\sum_{c \in C} f_i^c \Delta_i^{*c} + \sum_{c \in C} \kappa_i^c \Omega_i^{*c}$ $= \sum_{\beta \in B} f_i^\beta U_i^{*\beta} + \sum_{\beta \in B} \kappa^\beta \omega^{*\beta}$	$\sum_{c \in C} \Delta_i^c f_i^{*c} + \sum_{c \in C} \Omega_i^c \kappa_i^{*c}$ $= \sum_{\beta \in B} U_i^\beta f_i^{*\beta} + \sum_{\beta \in B} \omega^\beta \kappa^{*\beta}$	Complementary virtual work
Uniform kinematics	$\Delta_i^c = l_k^c \varepsilon_{ki}$ $\Omega^c = l_k^c \frac{\partial \omega}{\partial x_k}$	$f_i^c = h_k^c \sigma_{ki}$ $\kappa^c = h_k^c \mu_k$	Uniform statics
Branch vector	l_i^c	h_i^c	Polygon vector
Geometry	$I_{ij} = \frac{1}{A} \sum_{c \in C} l_i^c h_j^c$		Geometry

semblies. Therefore, we disagree with one of their conclusions that, even in the absence of contact couples, the average homogenized stress tensor need not be symmetric.

The current micromechanical expression (40) for the average couple stress tensor is also given by Oda (1999) and Oda and Iwashita (2000), although their arguments for neglecting some terms involving contact forces that arise in their formulation are rather arbitrary. As discussed in Section 2, contributions of contact forces should not be present.

Chang and Ma (1990, 1992) give

$$\langle \mu_{ij} \rangle = \frac{1}{V} \sum_{c \in C} l_i^c \left[\kappa_j^c + e_{jkl} \zeta_k^c f_l^c \right] \tag{69}$$

where $\zeta_i^{pq} = (1/2)(r_i^{qp} + r_i^{pq})$. Once more, this expression involves contact forces, which should not be present. The difference with (40) may be small, since for equal-sized disks $\zeta_i^{pq} \equiv 0$.

Chang and Liao (1990) proposed an expression for what they called the average "polar stress" Π_{ij}

$$\langle \Pi_{ij} \rangle = \frac{1}{V} \int_V \Pi_{ij} \, \mathrm{d}V \equiv \frac{1}{V} \int_V \left[\mu_{ij} + e_{jkl} x_k \sigma_{il} \right] \mathrm{d}V = \frac{1}{V} \sum_{c \in C} l_i^c \left[\kappa_j^c + e_{jkl} C_k^c f_l^c \right] \tag{70}$$

Note that "polar stress" satisfies the continuum equation $\partial \Pi_{ji} / \partial x_j = 0$ (see (30)). The expression (70), which is also given by Bardet and Vardoulakis (2001), does not separate the contribution due to the couple stress from that due to what is called the "first moment of stress". It is therefore of limited use in micromechanical studies.

The current expressions for the Cosserat strain tensor (56) and for the rotation gradient tensor (49) involve the kinematic contact quantities Δ_i^c and Ω_i^c that equal zero for rigid body motions of the whole assembly, unlike δ_i^c. Expressions for the average displacement gradient tensor obtained previously by Kruyt and Rothenburg (1996), Bagi (1996) and Kuhn (1997) were formulated in terms of δ_i^c, and therefore did not account for the effect of particle rotation. Hence expression (56) for the average Cosserat strain tensor gives a true measure deformation.

It has been shown by Cambou et al. (2000) and Bagi (2001) that micromechanical expressions for the displacement gradient tensor that are based on partitioning area into polygons, as employed here, are always consistent with the macroscopic displacement gradient tensor that is determined from the boundary displacements, contrary to formulations that are based on least-square fits of the displacements (see for example, Liao et al., 1997; Oda and Iwashita, 2000). These least-square fit methods are therefore of limited use in micromechanical studies.

The current compatibility equations for the relative displacements and relative rotations at contacts are only valid in the two-dimensional case. It is recommended to try to formulate compatibility equations in the three-dimensional case, using the three-dimensional graph representation of Satake (1997). Such equations could be employed to formulate micromechanical expressions for the Cosserat strain and rotation gradient tensors for the three-dimensional case.

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Appendix A

In this appendix the current micromechanical expression (34) for the average homogenized stress tensor is compared with that given by Bardet and Vardoulakis (2001). To this end a simple example without contact couples is analysed that closely resembles the first example given by Bardet and Vardoulakis (2001).

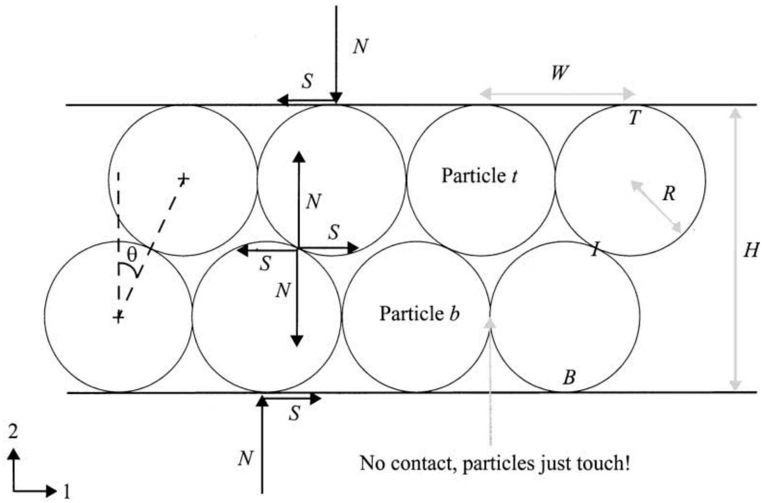

Fig. 10. Example assembly.

Consider an assembly as depicted in Fig. 10 consisting of layers of two equal-sized disks with radius R that constitute a "chain". The geometry is such that for the particles in adjacent chains just touch, so there is effectively zero contact force. Therefore, in each chain consisting of particles t and b there are effectively three contacts: contact I corresponding to the contact between particles t and b, and contacts T and B that correspond to the contacts with the top and bottom walls, respectively. At the boundary there are normal and tangential forces N and S, respectively. The angle of the chain with the vertical direction is θ. The width occupied by a single chain is $W = 2R$, while its width is $H = 2R\cos\theta + 2R$ and its area $A = WH$.

In the current notation the expression of Bardet and Vardoulakis (2001) for the average stress tensor is

$$A\langle\sigma_{ij}\rangle = \sum_{c\in\{I\}} l_i^c f_j^c = \sum_{c\in\{B,T\}} Z_i^{p\beta} f_j^{p\beta} \tag{A.1}$$

where $Z_i^{p\beta}$ is the coordinate of the centre of the particle that corresponds to contact β with the boundary.

The current expression (34) for the average stress tensor is

$$A\langle\sigma_{ij}\rangle = \sum_{c\in\{B,T,I\}} l_i^c f_j^c = \sum_{c\in\{B,T\}} C_i^{p\beta} f_j^{p\beta} \tag{A.2}$$

where $C_i^{p\beta}$ is the coordinate of the contact point β of the contact between particle p and the boundary.

The contact forces are

$$f_i^{bB} = \begin{bmatrix} S \\ N \end{bmatrix} \qquad f_i^{bt} = \begin{bmatrix} -S \\ -N \end{bmatrix} \qquad f_i^{tT} = \begin{bmatrix} -S \\ -N \end{bmatrix} \tag{A.3}$$

With respect to a coordinate system that is centred at the contact point I, we have for the various geometrical vectors

$$l_i^{bB} = \begin{bmatrix} 0 \\ -R \end{bmatrix} \qquad l_i^{bt} = \begin{bmatrix} 2R\sin\theta \\ 2R\cos\theta \end{bmatrix} \qquad l_i^{tT} = \begin{bmatrix} 0 \\ R \end{bmatrix} \tag{A.4}$$

$$C_i^{bB} = \begin{bmatrix} -R\sin\theta \\ -R\cos\theta - R \end{bmatrix} \qquad C_i^{tT} = \begin{bmatrix} R\sin\theta \\ R\cos\theta + R \end{bmatrix} \tag{A.5}$$

$$Z_i^{bB} = \begin{bmatrix} -R\sin\theta \\ -R\cos\theta \end{bmatrix} \qquad Z_i^{tT} = \begin{bmatrix} R\sin\theta \\ R\cos\theta \end{bmatrix} \tag{A.6}$$

The expressions for the average stress tensors become

Current

$$\langle\sigma_{ij}\rangle = \begin{bmatrix} -\dfrac{S}{2R}\dfrac{\sin\theta}{1+\cos\theta} & -\dfrac{N}{2R}\dfrac{\sin\theta}{1+\cos\theta} \\ -\dfrac{S}{2R} & -\dfrac{N}{2R} \end{bmatrix} \tag{A.7}$$

Bardet and Vardoulakis (2001)

$$\langle\sigma_{ij}\rangle = \begin{bmatrix} -\dfrac{S}{2R}\dfrac{\sin\theta}{1+\cos\theta} & -\dfrac{N}{2R}\dfrac{\sin\theta}{1+\cos\theta} \\ -\dfrac{S}{2R}\dfrac{\cos\theta}{1+\sin\theta} & -\dfrac{N}{2R}\dfrac{\cos\theta}{1+\sin\theta} \end{bmatrix} \tag{A.8}$$

The continuum meaning of the stress tensor is that the resulting force F_i^{B} acting on a boundary is given by $F_i^{\mathrm{B}} = \int_B n_j\sigma_{ji}\,\mathrm{d}B$. Therefore it is expected here that the stresses $\langle\sigma_{21}\rangle$ and $\langle\sigma_{22}\rangle$ are given by $\langle\sigma_{21}\rangle = -S/W = -S/(2R)$ and $\langle\sigma_{22}\rangle = -N/W = -N/(2R)$. The current expression conforms to these expectations, but the expression of Bardet and Vardoulakis (2001) does not. However, the difference between the two expressions becomes negligible for large assemblies, $N_p \to \infty$.

When moment equilibrium is satisfied for the particles we have

$$S = N\frac{\sin\theta}{1+\cos\theta} \tag{A.9}$$

Under this condition the stress tensor according to the current expression is symmetric, unlike that given by Bardet and Vardoulakis (2001).

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