

A thermomechanical approach to the development of micropolar constitutive models of granular media

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Summary. In this paper, we lay the groundwork for the development of micropolar (Cosserat) constitutive relations for granular media within the framework of the theory of thermomechanics. Expressions for the free energy and the dissipation function have been derived using a micromechanical analysis of a cluster consisting of a particle and its immediate neighbors (i.e., “the first ring”). Fluctuations in particle displacements and rotations within this mesoscale assembly as well as fluctuations in strain and curvature are represented by internal variables. Using thermomechanical techniques previously employed for classical materials, a non-local micropolar model is constructed and then subsequently applied to a granular material undergoing simple shear. The effects of the boundaries through particle rotations are discussed.

1 Introduction

Non-invasive experimental studies in conjunction with advanced discrete element simulations have given remarkable insight into the evolution of microstructural properties of a deforming granular material. In particular, studies on quasi-static deformations which have provided benchmarks critical to the future development of micromechanical constitutive models include those by Oda and co-workers [1]–[3], Bardet and Proubet [4], Rothenburg and Bathurst [5], Howell et al. [6], and Calvetti et al. [7]. In recent years, our group has been engaged in the development of micropolar models in which key experimental and numerical results on contact and force anisotropy, void evolution and interparticle rolling resistance are addressed in an effort to capture shear bands (Tordesillas and Walsh [8], Tordesillas et al. [9]). Our model relies on a homogenization procedure which is based on the consideration of a mesodomain consisting of a particle and its first ring of neighbors. The underlying assumption is that gradients in the properties of two adjacent particles (e.g., gradients as expressed through differences in rotations and in displacements) can be represented by their mean gradients. This assumption has been adopted in previous micromechanical models (see, for example, Chang and Ma [10]). However, there is mounting evidence which suggests that local fluctuations in both particle displacements and particle rotations have a significant influence on the bulk behaviour of granular media – *even at low to moderate strains* (Calvetti et al. [7], Kuhn [11], Kuhn and Bagi [12], Radjai and Roux [13], Didwania et al. [14]). Another challenge confronting the development of effective homogenization methods relates to the question of how friction-controlled interparticle slip, as well as particle rearrangements (non-affine motions), are to be accounted

for (Valanis [15], Peters [16]). These factors govern energy dissipation, and their proper characterisation is critical to the development of robust constitutive models.

The objective of this study is to explore the efficacy of thermomechanics theory as a framework for developing micropolar models of granular media. To achieve this, we apply thermomechanical techniques which are based upon the use of internal variables: in this case, we use internal variables to represent the aforementioned kinematic fluctuations. While the underlying ideas date back to the pioneering work of Ziegler [17], and Collins and Houlsby [18], the procedure we adopt here follows that of Valanis [19]. Other important contributions are due to Houlsby and Puzrin [20], and Collins and co-workers [21], [22] for the use of thermomechanics principles to establish a hierarchy of classical plasticity models for geomaterials. We refer the reader to the recent review by Collins and Hilder [22] and the references cited therein for a comprehensive background on the developments in this field.

In this paper, the theory of thermomechanics is applied to a micropolar continuum to capture the effects of particle rotations within a granular assembly. The dominant influence of particle rotations on the bulk behavior of granular media is now well established. Our earlier paper Tordesillas and Walsh [8] presents a summary of the effects of rotations as established from experiments and discrete element simulations.

So how does the so-called “thermomechanics approach” differ from conventional constitutive developments? The standard practice in mechanics is to develop material models by initially proposing constitutive relations, and then imposing the laws of thermodynamics to these relations. The thermomechanics approach, however, guarantees the fulfillment of these laws at the outset by proceeding in the reverse manner: that is, by constructing constitutive models directly from the Laws of Thermodynamics. To characterize the material, internal variables are used in addition to the normal state variables. For example, the internal variables may take the form of plastic strain or generalized stress variables (Houlsby and Puzrin [20]). In Valanis [19], the internal variables are linked to the non-affine motions of the particle assembly, expressed through local fluctuations in the particle displacements.

In this paper, the internal variables represent fluctuations in particle displacements and rotations, as well as fluctuations in strain and curvature. The rearrangements of the constituent particles during the material’s deformation are reflected in the changes in the internal variables. The evolution of the internal variables, in turn, reflects the dissipation of energy in the material. In a similar fashion to the method proposed by Valanis [19], the constitutive relations in the current formulation depend on both the internal variables and their gradients. This is because gradient theories can predict the appearance of localized deformation under uniform boundary conditions – a well-known characteristic of geomaterials. Finally, we note that although our current formulation focuses on the aforementioned kinematic fluctuations, there is scope to build on the proposed approach to account for other important state variables in future model refinements.

The following section discusses the physical interpretation of the proposed internal variables. In Sect. 3, generalized constitutive relations are developed for a micropolar continuum using thermomechanical principles. It is shown that the constitutive relations obey the laws of conservation of linear and angular momentum for micropolar continua. A range of micropolar constitutive models may be derived from the general constitutive laws by specifying relations for the free energy and the dissipation function. In Sect. 4, we derive specific expressions for the free energy and the dissipation function from a micromechanical analysis of a mesodomain comprising of a particle and its immediate neighbors. To keep the analysis simple, we neglect the evolution of contact anisotropy. Results for a granular assembly undergoing a simple shear deformation are presented in Sect. 5, with the effects of the boundaries explored by examining the particle rotations.

2 Internal variables from local variations

Continuum mechanics is based on the premise that the physical nature of real objects can be represented mathematically by constitutive laws acting on material bodies. A set of constitutive laws defines a particular material’s response to a given input process, typically the stress or strain history of the material. The material’s response is described through constitutive variables that are assigned to each point in the body.

Ideally, the values of the constitutive variables given to each point should describe the exact state of the object to be modelled. In reality, however, these constitutive variables may fluctuate on small scales in a way that is either difficult to deal with mathematically or impossible to observe experimentally. It is only possible, therefore, to determine the values of these constitutive variables on a macroscopic scale and, using that information, assign a statistical average to each point in the body. In this case, the constitutive variables should not be thought of as referring to a particular point in the body. Instead, they should be considered indicative of the state of a small region of the object, i.e., a “mesodomain” associated with that point.

In the event that the constitutive variables undergo large variations within the mesodomain, the average constitutive response of the domain may not be indicative of the actual behavior of the object. In this case additional variables, which are so-called internal variables, may be required to properly describe the state of the body. To define these internal variables, first consider a field A' which represents the actual values of a constitutive variable within a cubic mesodomain $\mathcal{D}(X_i)$ centred around a point X_i . A' is a function of two variables: the location of the mesodomain X_i and the position x_i relative to the centre of the mesodomain \mathcal{D} . These coordinate systems are illustrated in Fig. 1. The field A' can be expressed as

$$A'(X_i, x_i) = A(X_i, x_i) + B(X_i, x_i), \tag{1}$$

where $A(X_i, x_i)$ is a linearly varying field made up of the average/macroscopic value of A' and its material gradient,

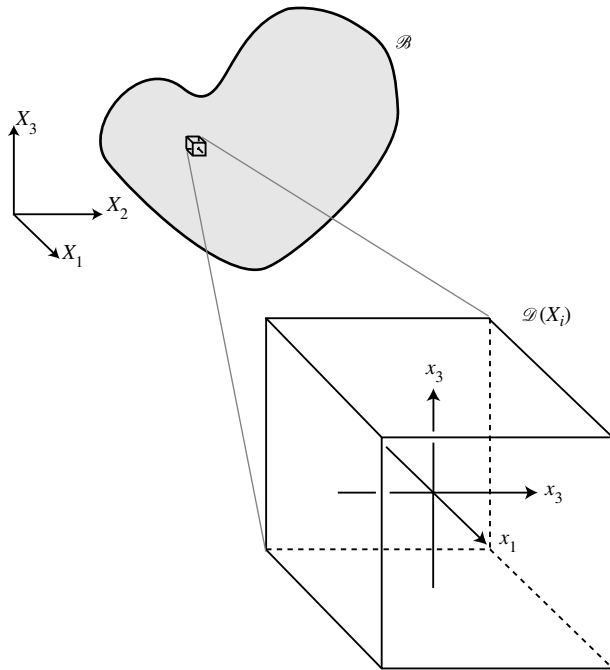


Fig. 1. The X_i -coordinates are used to indicate a location within the body \mathcal{B} . The x_i -coordinates for a mesodomain $\mathcal{D}(X_i)$ indicate a location relative to the centre of the mesodomain

$$A(X_i, x_i) = \bar{A}(X_i) + \bar{A}_{,i}(X_i)x_i, \quad (2)$$

and $B(X_i, x_i)$ represents the remaining microscale variation in the field $A'(X_i, x_i)$. A two-dimensional example is given in Fig. 2. Since

$$\begin{aligned} \bar{A} &= \frac{1}{V_{\mathcal{D}}} \int_{V_{\mathcal{D}}} A' dV, \\ &= \frac{1}{V_{\mathcal{D}}} \int_{V_{\mathcal{D}}} [\bar{A}(X_i) + \bar{A}_{,i}(X_i)x_i + B(X_i, x_i)] dV, \\ &= \frac{1}{V_{\mathcal{D}}} \int_{V_{\mathcal{D}}} \bar{A}(X_i) dV + \frac{1}{V_{\mathcal{D}}} \int_{V_{\mathcal{D}}} B(X_i, x_i) dV, \end{aligned} \quad (3)$$

it follows that

$$\int_{V_{\mathcal{D}}} B(X_i, x_i) dV = 0, \quad (4)$$

where $V_{\mathcal{D}}$ is the volume of mesodomain $\mathcal{D}(X_i)$, and the integrals $\int_{V_{\mathcal{D}}} dV$ are made relative to the local coordinate system x_i such that $dV = dx_1 dx_2 dx_3$.

The internal variation B is a function of both the location of the mesodomain X_i and the position within that domain x_i . To obtain an expression for the internal variation in terms of X_i alone, a weighting function $\phi(x_i)$ is introduced, such that

$$\int_{V_{\mathcal{D}}} \phi(x_i) dV = \frac{1}{V_{\mathcal{D}}}. \quad (5)$$

Using the weighting function, a variable \hat{B} is defined as

$$\hat{B}(X_i) = \int_{V_{\mathcal{D}}} B(X_i, x_i) \phi(x_i) dV. \quad (6)$$

In this way, A' is represented at each point X_i by the macroscopic component of the field \bar{A} , and a variable representing the internal variation of that field within the associated mesodomain, \hat{B} .

In this paper, two sets of internal variables are introduced to describe the local particle motions. One describes the internal fluctuations in the displacement field, while the other describes the internal fluctuations in the rotation field. Concentrating on the displacement for

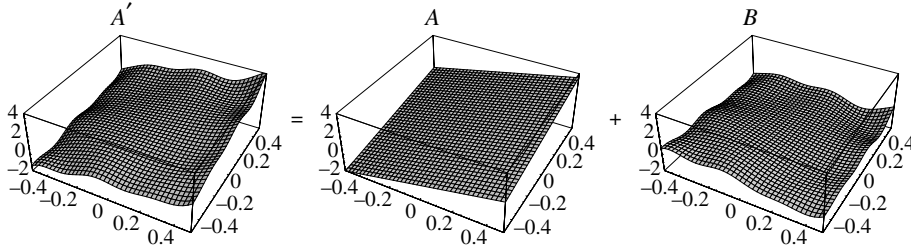


Fig. 2. The field A' can be divided into two components: $A(X_i, x_i)$ the linearly varying field made up of the average/macroscopic value of A' and its material gradient, and $B(X_i, x_i)$ representing the remaining microscale variation

the time being, an internal variable field q_i is defined as the difference between the actual displacement field u'_i and the field u_i :

$$q_i = u'_i - u_i, \quad (7)$$

where u_i is composed of the average displacement for the domain $\bar{u}_i = (1/V_{\mathcal{D}}) \int_{V_{\mathcal{D}}} u'_i dv$, and its material gradient, namely

$$u_i = \bar{u}_i + \bar{u}_{i,j} x_j. \quad (8)$$

As mentioned earlier, particles in a micropolar material can rotate independently of their neighborhood. Consequently, a rotation field ω'_i is needed, in addition to the displacement field u'_i , to describe the particle motion. The field ω'_i gives the rotation of the particle about its own centre of mass. It can be related to the displacement field via

$$\omega'_i = -\frac{1}{2} e_{ijk} u'_{j,k} + \psi'_i, \quad (9)$$

where ψ'_i is the particle spin.

In order to develop a thermomechanical approach for micropolar materials, a field m_i is introduced that describes the internal variation of the rotation field in the mesodomain. Similar to the internal displacement field, the internal rotation field can be defined in terms of the actual rotation ω'_i and the field ω_i :

$$m_i = \omega'_i - \omega_i. \quad (10)$$

Like the field u_i defined in Eq. (8), the field ω_i is composed of the average rotation for the microdomain $\bar{\omega}_i$ and its gradient $\bar{\omega}_{i,j}$,

$$\omega_i = \bar{\omega}_i + \bar{\omega}_{i,j} x_j, \quad (11)$$

where $\bar{\omega}_i = (1/V_{\mathcal{D}}) \int_{V_{\mathcal{D}}} \omega'_i dv$. The constitutive relations derived in the next section depend on the macroscopic and local rotation fields, as well as their gradients. Gradient theories, like this one, can describe the appearance of localized deformation under uniform boundary conditions. Such localized deformation is common in geotechnical materials: examples include the formation of shear bands in granular materials (Oda and Kazama [2]) and the appearance of bands of localized cracking in rocks and concrete (Read and Hegemeier [23]).

For a micropolar material, the state of deformation is expressed in terms of a microstrain tensor ϵ'_{ij} and a curvature tensor κ'_{ij} as follows:

$$\epsilon'_{ij} = u'_{i,j} + e_{ijk} \omega'_k, \quad (11)$$

$$\kappa'_{ij} = \omega'_{i,j}. \quad (12)$$

The average microstrain and curvature tensors are given by

$$\bar{\epsilon}_{ij} = \frac{1}{V_{\mathcal{D}}} \int_{V_{\mathcal{D}}} \epsilon'_{ij} dV, \quad (13)$$

$$\bar{\kappa}_{ij} = \frac{1}{V_{\mathcal{D}}} \int_{V_{\mathcal{D}}} \kappa'_{ij} dV. \quad (14)$$

Two additional tensors η_{ij} and ζ_{ij} are defined as

$$\eta_{ij} = \epsilon'_{ij} - \bar{\epsilon}_{ij}, \quad (15)$$

$$\zeta_{ij} = \kappa'_{ij} - \bar{\kappa}_{ij}. \quad (16)$$

Interparticle motions, which are governed by friction and rolling resistance, are accompanied by energy dissipation in a granular material. These motions consist of interparticle slip and interparticle rolling which can be expressed in terms of the microstrain and curvature (Tordesillas and Walsh [8]). Discrete element simulations reveal a strong correlation between energy dissipation and regions of nonuniform deformation (e.g., Kuhn [11]), which suggest that fluctuations in microstrain and/or curvature may have a stronger influence on energy dissipation than the average values, $\bar{\epsilon}_{ij}$ and $\bar{\kappa}_{ij}$. Accordingly, in this analysis, the energy dissipation is linked to η_{ij} and ζ_{ij} . Additional dissipative effects that occur in response to changes in $\bar{\epsilon}_{ij}$ and/or $\bar{\kappa}_{ij}$ can also be readily incorporated in the present analysis but this is beyond the scope of this paper.

3 Constitutive relations from thermodynamics

Constitutive relations incorporating the previously defined internal variables can be found from the laws of thermodynamics. First consider the internal energy inside the mesodomain. The total internal energy of a mesodomain $U_{\mathcal{D}}(X_i)$ can be expressed as

$$U_{\mathcal{D}}(X_i) = \int_{V_{\mathcal{D}}} U(X_i, x_i) dV, \quad (17)$$

where $U(X_i, x_i)$ is the local internal energy density.

From the First Law of Thermodynamics, a variation in the internal energy for a mesodomain is equal to the variation in the work done on the mesodomain $\delta W_{\mathcal{D}}$ and the heat flow into that domain $\delta Q_{\mathcal{D}}$. Thus

$$\delta U_{\mathcal{D}} = \delta W_{\mathcal{D}} + \delta Q_{\mathcal{D}}. \quad (18)$$

The heat flow into the domain can be written as

$$\delta Q_{\mathcal{D}} = - \int_{S_{\mathcal{D}}} h_i n_i dS, \quad (19)$$

where h_i is the heat flux and n_i represents the components of a unit vector normal to the surface of the mesodomain $S_{\mathcal{D}}$. The work done on the domain may be expressed as follows:

$$\delta W_{\mathcal{D}} = \int_{S_{\mathcal{D}}} \{T'_i \delta u'_i + \Omega'_i \delta \omega'_i\} dS + \int_{V_{\mathcal{D}}} \{f_i \delta \bar{u}_i + g_i \delta \bar{\omega}_i\} dV, \quad (20)$$

where $\delta u'_i$ is a variation in the actual displacement field on the surface of the mesodomain, $\delta \omega'_i$ is a variation in the actual rotation field on the surface of the mesodomain, T'_i represents the applied traction, Ω'_i represents the applied couples, $\delta \bar{u}_i$ is a variation in the average displacement field, $\delta \bar{\omega}_i$ is a variation in the average rotation field, f_i is the body force field and g_i is the body moment field. The fields f_i and g_i are assumed to be constant within the mesodomain.

As noted earlier, energy dissipation is linked to the changes in the fields η_{ij} and ζ_{ij} . This relationship may be introduced through the Second Law of Thermodynamics, expressed by the Clausius-Duhem inequality. The Clausius-Duhem inequality ensures that the external entropy supply for any domain is less than or equal to the entropy production inside the domain. Ignoring the effects of body heating, the inequality may be written as

$$\int_v \delta s dV \geq - \int_s \frac{h_i}{\theta} n_i dS, \quad (21)$$

where s is the entropy and θ is the temperature (Lubliner [25]). Rearranging the inequality and using Gauss' theorem, it can be shown that

$$\int_v \left\{ \delta s + \left(\frac{h_i}{\theta} \right)_{,i'} \right\} dV \geq 0, \quad (22)$$

where the subscripted primed indices represent derivatives with respect to the local coordinate system, i.e., $\partial(\cdot)/\partial x_i = (\cdot)_{,i'}$. As the inequality can be applied to any domain, regardless of its size, it can be said that

$$\theta \delta s + h_{i,i'} - \frac{h_i \theta_{,i'}}{\theta} \geq 0. \quad (23)$$

Houlsby and Puzrin [20] note that, in slow processes, the dissipation function $D = \theta \delta s + h_{i,i'}$ is much larger than the term $-h_i \theta_{,i'}/\theta$. For this reason it is argued that the expression derived from the Clausius-Duhem inequality in Eq. (23) can be replaced by

$$D = \theta \delta s + h_{i,i'} \geq 0. \quad (24)$$

Here it is assumed that the dissipation function D can be split into two components, i.e., $D = D^n + D^\zeta$; D^n describes the dissipation due to the field η_{ij} ,

$$D^n = P_{ij} \delta \eta_{ij}, \quad (25)$$

while D^ζ describes the dissipation due to the field ζ_{ij} ,

$$D^\zeta = N_{ij} \delta \zeta_{ij}, \quad (26)$$

where P_{ij} and N_{ij} are the dissipative stress and couple stress fields, respectively. Moreover, it is stipulated that

$$D > 0 \quad (27)$$

if any of the following are true:

$$\|P_{ij}\| > 0, \quad (28)$$

$$\|\delta \eta_{ij}\| > 0, \quad (29)$$

$$\|N_{ij}\| > 0, \quad (30)$$

or

$$\|\delta \zeta_{ij}\| > 0, \quad (31)$$

where for a tensor A_{ij} , $\|A_{ij}\| = \sqrt{A_{ij} A_{ij}}$.

Applying Gauss' divergence theorem to Eq. (19) and then combining this with Eqs. (18), (20) and (24) gives the following expression:

$$\delta U_{\mathcal{Q}} = \int_{s_{\mathcal{Q}}} \{T'_i \delta u'_i + \Omega'_i \delta \omega'_i\} dS + \int_{V_{\mathcal{Q}}} \{f_i \delta \bar{u}_i + g_i \delta \bar{\omega}_i + \theta \delta s - D\} dV, \quad (32)$$

Next a stress field σ'_{ij} and a couple stress field μ'_{ij} are introduced such that

$$T'_i = \sigma'_{ji} n_j; \Omega'_i = \mu'_{ji} n_j. \quad (33)$$

The average stress $\bar{\sigma}_{ij}$ and couple stress $\bar{\mu}_{ij}$ are defined as

$$\bar{\sigma}_{ij} = \frac{1}{V_{\mathcal{Q}}} \int_{V_{\mathcal{Q}}} \sigma'_{ij} dV; \bar{\mu}_{ij} = \frac{1}{V_{\mathcal{Q}}} \int_{V_{\mathcal{Q}}} \mu'_{ij} dV. \quad (34)$$

Using these fields the internal variation in the stress and couple stress can be written as

$$Q_{ij} = \sigma'_{ij} + \sigma_{ij}; \quad M_{ij} = \mu'_{ij} - \mu_{ij}, \quad (35)$$

where the stress field σ_{ij} and the couple stress field μ_{ij} are defined locally as

$$\sigma_{ij} = \bar{\sigma}_{ij} + \bar{\sigma}_{ij,k}x_k; \quad \mu_{ij} = \bar{\mu}_{ij} + \bar{\mu}_{ij,k}x_k. \quad (36)$$

Equation (32) now yields:

$$\begin{aligned} \delta U_{\mathcal{D}} &= \int_{S_{\mathcal{D}}} \left\{ \sigma'_{ji} n_j \delta u'_i + \mu'_{ji} n_j \delta \omega'_i \right\} dS + \int_{V_{\mathcal{D}}} \{ f_i \delta \bar{u}_i + g_i \delta \bar{\omega}_i + \theta \delta s - D \} dV \\ &= \int_{V_{\mathcal{D}}} \left\{ \left[\sigma'_{ji} \delta u'_i + \mu'_{ji} \delta \omega'_i \right]_{,j'} + f_i \delta \bar{u}_i + g_i \delta \bar{\omega}_i + \theta \delta s - D \right\} dV. \end{aligned} \quad (37)$$

Examining the terms inside the square brackets leads to:

$$\begin{aligned} \int_{V_{\mathcal{D}}} \left[\sigma'_{ji} \delta u'_i + \mu'_{ji} \delta \omega'_i \right]_{,j'} dV &= \int_{V_{\mathcal{D}}} \{ (\bar{\sigma}_{ji,j} + Q_{ji,j'}) (\delta \bar{u}_i + \delta \bar{u}_{i,k} x_k + \delta q_i) \\ &\quad + (\bar{\sigma}_{ji} + \bar{\sigma}_{ji,k} x_k + Q_{ji}) (\delta \bar{u}_{i,j} + \delta q_{i,j'}) \\ &\quad + (\bar{\mu}_{ji,j} + M_{ji,j'}) (\delta \bar{\omega}_i + \delta \bar{\omega}_{i,k} x_k + \delta m_i) \\ &\quad + (\bar{\mu}_{ji} + \bar{\mu}_{ji,k} x_k + M_{ji}) (\delta \bar{\omega}_{i,j} + \delta m_{i,j'}) \} dV \\ &= \int_{V_{\mathcal{D}}} \{ (\bar{\sigma}_{ji,j} + Q_{ji,j'}) \delta \bar{u}_i + Q_{ji,j'} (\delta \bar{u}_{i,k} x_k + \delta q_i) \\ &\quad + \sigma_{ji} \delta \bar{u}_{i,j} + (\bar{\sigma}_{ji} + \bar{\sigma}_{ji,k} x_k + Q_{ji}) \delta q_{i,j'} \\ &\quad + (\bar{\mu}_{ji,j} + M_{ji,j'}) \delta \bar{\omega}_i + M_{ji,j'} (\delta \bar{\omega}_{i,k} x_k + \delta m_i) \\ &\quad + \bar{\mu}_{ji} \delta \bar{\omega}_{i,j} + (\bar{\mu}_{ji} + \bar{\mu}_{ji,k} x_k + M_{ji}) \delta m_{i,j'} \} dV, \end{aligned} \quad (38)$$

where use has been made of the following:

$$\int_{V_{\mathcal{D}}} q_i dV = \int_{V_{\mathcal{D}}} m_i dV = 0 \quad (39)$$

and

$$\int_{V_{\mathcal{D}}} Q_{ij} dV = \int_{V_{\mathcal{D}}} M_{ij} dV = 0. \quad (40)$$

The ‘‘local’’ derivative of the internal displacement field, $q_{i,j'}$, can be related to derivatives of the global coordinate system X_i by considering the actual displacement field u'_i . Note that for the actual displacement the following is true:

$$\frac{\partial u'_i}{\partial X_j} = \frac{\partial u'_i}{\partial x_j} \quad (41)$$

or

$$\frac{\partial \bar{u}_i}{\partial X_j} + \frac{\partial q_i}{\partial X_j} + \frac{\partial \bar{u}_{i,k}}{\partial X_j} x_k = \frac{\partial q_i}{\partial x_j} + \bar{u}_{i,k} \frac{\partial x_k}{\partial x_j}, \quad (42)$$

where the \bar{u}_i term has vanished on the right-hand side of Eq. (41) as \bar{u}_i is constant in x_i . Therefore

$$\bar{u}_{i,j} + q_{i,j} + \bar{u}_{i,jk}x_k = q_{i,j'} + \bar{u}_{i,j}, \quad (42)$$

or

$$q_{i,j'} = q_{i,j} + \bar{u}_{i,jk}x_k. \quad (43)$$

In a similar fashion, it can also be shown that

$$m_{i,j'} = m_{i,j} + \bar{\omega}_{i,jk}x_k, \quad (44)$$

$$Q_{ij,k'} = Q_{ij,k} + \bar{\sigma}_{ij,kl}x_l, \quad (45)$$

and

$$M_{ij,k'} = M_{ij,k} + \bar{\mu}_{ij,kl}x_l. \quad (46)$$

Currently the equation for the internal energy is a function of the internal fields q_i , m_i , Q_{ij} and M_{ij} . The equations that follow can be greatly simplified however by introducing the variables q_i^* , m_i^* , Q_{ij}^* and M_{ij}^* where

$$q_i^* = q_i + \bar{u}_{i,k}x_k, \quad (47)$$

$$m_i^* = m_i + \bar{\omega}_{i,k}x_k, \quad (48)$$

$$Q_{ij}^* = Q_{ij} + \bar{\sigma}_{ij,k}x_k, \quad (49)$$

and

$$M_{ij}^* = M_{ij} + \bar{\mu}_{ij,k}x_k, \quad (50)$$

Note that $q_{i,j}^* = q_{i,j'}$, $m_{i,j}^* = m_{i,j'}$, $Q_{ij,k}^* = Q_{ij,k'}$ and $M_{ij,k}^* = M_{ij,k'}$. Also, the two variables η_{ij} and ζ_{ij} may be written as

$$\eta_{i,j} = q_{i,j}^* + e_{ijk}m_k^*, \quad (51)$$

$$\zeta_{i,j} = m_{i,j}^*. \quad (52)$$

With the identities in Eqs. (47)–(50), the variation in the internal energy can be expressed as

$$\begin{aligned} \delta U = & (\bar{\sigma}_{ji,j} + f_i)\delta\bar{u}_i + Q_{ji}^*\delta q_i^* + \bar{\sigma}_{ji}\delta\bar{u}_{i,j} + Q_{ij}^*\delta q_{i,j}^* + (\bar{\mu}_{ji,j} + g_i)\delta\bar{\omega}_i + M_{ji}^*\delta m_i^* \\ & + \bar{\mu}_{ji}\delta\bar{\omega}_{i,j} + M_{ij}^*\delta m_{i,j}^* + \theta\delta s - D. \end{aligned} \quad (53)$$

The local internal energy density is a function of the displacement and displacement gradient, the rotation and the rotation gradient, the newly defined q_i^* and m_i^* and their gradients, and of the entropy, i.e.,

$$U = U(\bar{u}_i; \bar{u}_{i,j}; q_i^*; q_{i,j}^*; \bar{\omega}_i; \bar{\omega}_{i,j}; m_i^*; m_{i,j}^*; s). \quad (54)$$

As it stands, the expression for the internal energy in Eq. (54) violates the principle of objectivity. Due to the dependence on the displacement, the model predicts that the internal energy will vary with a change in the reference frame. One way to correct this is to remove the dependence on the displacement. However, the same result can be obtained, along with other insights into the material behavior, by stipulating that for all infinitesimal rigid body motions the internal energy remains constant, i.e.,

$$\delta U = 0. \quad (55)$$

From Eq. (54), the variation of the local internal energy density can also be expressed as

$$\begin{aligned} \delta U = & \frac{\partial U}{\partial \bar{u}_i} \delta \bar{u}_i + \frac{\partial U}{\partial \bar{u}_{i,j}} \delta \bar{u}_{i,j} + \frac{\partial U}{\partial q_i^*} \delta q_i^* + \frac{\partial U}{\partial q_{i,j}^*} \delta q_{i,j}^* + \frac{\partial U}{\partial \bar{\omega}_i} \delta \bar{\omega}_i + \frac{\partial U}{\partial \bar{\omega}_{i,j}} \delta \bar{\omega}_{i,j} \\ & + \frac{\partial U}{\partial m_i^*} \delta m_i^* + \frac{\partial U}{\partial m_{i,j}^*} \delta m_{i,j}^* + \frac{\partial U}{\partial s} \delta s. \end{aligned} \quad (56)$$

Under pure heating conditions, the internal variables, the displacements and the rotations remain constant. Comparing Eq. (53) and Eq. (56) leads to

$$\frac{\partial U}{\partial s} = \theta. \quad (57)$$

Granular materials typically undergo isothermal deformation. Under these conditions, the free energy is a more useful energy function to use in place of the internal energy, as the free energy is expressed in terms of the temperature of the system rather than the entropy.

Like the internal energy, the total free energy of a mesodomain $\psi_{\mathcal{D}}$ can be expressed as

$$\psi_{\mathcal{D}}(X_i) = \int_{\mathcal{V}_{\mathcal{D}}} \psi(X_i, x_i) dV, \quad (58)$$

where $\psi(X_i, x_i)$ is the free energy density.

As noted in Collins and Houslyby [17], the free energy can be expressed in terms of the internal energy using a Legendre transform. The two functions are related by

$$\psi = U - \theta s. \quad (59)$$

Under isothermal conditions

$$\delta \psi = \delta U - \theta \delta s, \quad (60)$$

and consequently

$$\begin{aligned} \delta \psi = & (\bar{\sigma}_{ji,j} + f_i) \delta \bar{u}_i + Q_{ji,j}^* \delta q_i^* + \bar{\sigma}_{ji} \delta \bar{u}_{i,j} + Q_{ji}^* \delta q_{i,j}^* + (\bar{\mu}_{ji,j} + g_i) \delta \bar{\omega}_i + M_{ji,j}^* \delta m_i^* \\ & + \bar{\mu}_{ji} \delta \bar{\omega}_{i,j} + M_{ji}^* \delta m_{i,j}^* - D. \end{aligned} \quad (61)$$

The local free energy is a function of the state and internal variables, which now include θ :

$$\psi = \psi(\bar{u}_i; \bar{u}_{i,j}; q_i^*; q_{i,j}^*; \bar{\omega}_i; \bar{\omega}_{i,j}; m_i^*; m_{i,j}^*; \theta). \quad (62)$$

At constant temperatures, the variation of the free energy can be written as

$$\begin{aligned} \delta \psi = & \frac{\partial \psi}{\partial \bar{u}_i} \delta \bar{u}_i + \frac{\partial \psi}{\partial \bar{u}_{i,j}} \delta \bar{u}_{i,j} + \frac{\partial \psi}{\partial q_i^*} \delta q_i^* + \frac{\partial \psi}{\partial q_{i,j}^*} \delta q_{i,j}^* \\ & + \frac{\partial \psi}{\partial \bar{\omega}_i} \delta \bar{\omega}_i + \frac{\partial \psi}{\partial \bar{\omega}_{i,j}} \delta \bar{\omega}_{i,j} + \frac{\partial \psi}{\partial m_i^*} \delta m_i^* + \frac{\partial \psi}{\partial m_{i,j}^*} \delta m_{i,j}^*. \end{aligned} \quad (63)$$

By combining the two expressions for the variation of the free energy density, Eq. (61) and Eq. (63), and enforcing the condition that the dissipation be greater than zero if $\|\delta \eta_{ij}\| > 0$ or $\|\delta \zeta_{ij}\| > 0$, then

$$\begin{aligned} & \left[\bar{\sigma}_{ji,j} + f_i - \frac{\partial \psi}{\partial \bar{u}_i} \right] \delta \bar{u}_i + \left[\bar{\sigma}_{ji} - \frac{\partial \psi}{\partial \bar{u}_{i,j}} \right] \delta \bar{u}_{i,j} + \left[Q_{ji,j}^* - \frac{\partial \psi}{\partial q_i^*} \right] \delta q_i^* + \left[Q_{ji}^* - \frac{\partial \psi}{\partial q_{i,j}^*} \right] \delta q_{i,j}^* \\ & + \left[\bar{\mu}_{ji,j} + g_i - \frac{\partial \psi}{\partial \bar{\omega}_i} \right] \delta \bar{\omega}_i + \left[\bar{\mu}_{ji} - \frac{\partial \psi}{\partial \bar{\omega}_{i,j}} \right] \delta \bar{\omega}_{i,j} + \left[M_{ji,j}^* - \frac{\partial \psi}{\partial m_i^*} \right] \delta m_i^* + \left[M_{ji}^* - \frac{\partial \psi}{\partial m_{i,j}^*} \right] \delta m_{i,j}^* > 0. \end{aligned} \quad (64)$$

Increments in the state and internal variables can be chosen that will violate this inequality unless the following equations hold:

$$\bar{\sigma}_{ji} - \frac{\partial \psi}{\partial \bar{u}_{i,j}} = 0, \quad (65)$$

$$\bar{\sigma}_{ji,j} + f_i - \frac{\partial \psi}{\partial \bar{u}_i} = 0, \quad (66)$$

$$Q_{ji}^* - \frac{\partial \psi}{\partial Q_i^*} = 0, \quad (67)$$

$$\bar{\mu}_{ji} - \frac{\partial \psi}{\partial \bar{\omega}_{i,j}} = 0, \quad (68)$$

and

$$\bar{\mu}_{ji,j} + g_i - \frac{\partial \psi}{\partial \bar{\omega}_i} = 0. \quad (69)$$

It may also be shown that

$$\left(Q_{ji}^* - \frac{\partial \psi}{\partial Q_{i,j}^*} \right) \delta q_{i,j}^* + \left(M_{ji,j}^* - \frac{\partial \psi}{\partial m_i^*} \right) \delta m_i^* + \left(M_{ji}^* - \frac{\partial \psi}{\partial m_{i,j}^*} \right) \delta m_{i,j}^* > 0, \quad (70)$$

if $\|\delta \eta_{ij}\| > 0$ or $\|\delta \zeta_{ij}\| > 0$.

Comparing Eq. (61) and Eq. (63) and enforcing the results in Eqs. (65)–(69) yields:

$$\left(Q_{ji}^* - \frac{\partial \psi}{\partial Q_{i,j}^*} - P_{ij} \right) \delta q_{i,j}^* + \left(M_{ji,j}^* - \frac{\partial \psi}{\partial m_i^*} + e_{ijk} P_{kj} \right) \delta m_i^* + \left(M_{ji}^* - \frac{\partial \psi}{\partial m_{i,j}^*} - N_{ij} \right) \delta m_{i,j}^* = 0. \quad (71)$$

Equation (71) must hold true for all arbitrary variations $\delta q_{i,j}^*$, δm_i^* and $\delta m_{i,j}^*$ satisfying the dissipation condition in Eq. (27). In addition, for all variations of $q_{i,j}^*$ and m_i^* where $\delta m_{i,j}^* = 0$ and

$$\delta \eta_{i,j} = \delta q_{i,j}^* + e_{ijk} \delta m_k^* = 0, \quad (72)$$

the following is true: $P_{ij} = 0$ and

$$\left(M_{ji,j}^* - \frac{\partial \psi}{\partial m_i^*} - e_{ijk} \left(Q_{kj}^* - \frac{\partial \psi}{\partial q_{j,k}^*} \right) \right) \delta m_i^* = 0. \quad (73)$$

As any number of $\delta q_{i,j}^*$ and δm_i^* can be chosen to satisfy Eq. (72), Eq. (73) can only be true if

$$M_{ji,j}^* - \frac{\partial \psi}{\partial m_i^*} = e_{ijk} \left(Q_{kj}^* - \frac{\partial \psi}{\partial q_{j,k}^*} \right), \quad (74)$$

in which case Eq. (71) becomes

$$\left(Q_{ji}^* - \frac{\partial \psi}{\partial Q_{i,j}^*} - P_{ij} \right) \delta \eta_{ij} + \left(M_{ji}^* - \frac{\partial \psi}{\partial m_{i,j}^*} - N_{ij} \right) \delta \zeta_{ij} = 0. \quad (75)$$

Equation (75) may be rewritten as

$$(\mathbf{Q} - \mathbf{P}) \cdot \delta \mathbf{q} = 0, \quad (76)$$

where \mathbf{Q} , \mathbf{P} and \mathbf{q} are 18-vectors defined as

$$\mathbf{Q} = \left[Q_{1i}^* - \frac{\partial\psi}{\partial m_{i,1}^*}, \dots, Q_{3i}^* - \frac{\partial\psi}{\partial m_{i,3}^*}, M_{1i}^* - \frac{\partial\psi}{\partial m_{i,1}^*}, \dots, M_{3i}^* - \frac{\partial\psi}{\partial m_{i,3}^*} \right]^T, \quad (77)$$

$$\mathbf{P} = [P_{i1}, \dots, P_{i3}, N_{i1}, \dots, N_{i3}]^T \quad (78)$$

and

$$\mathbf{q} = [\eta_{i1}, \dots, \eta_{i3}, \zeta_{i1}, \dots, \zeta_{i3}]^T. \quad (79)$$

Equation (76) is a statement that $(\mathbf{Q} - \mathbf{P})$ is orthogonal to the variation in \mathbf{q} . However, it would be more useful to show that $\mathbf{Q} = \mathbf{P}$. This result is often introduced by invoking Ziegler's orthogonality postulate (see, for example, Collins and Houlsby [18], Houlsby and Puzrin [20] and the discussion in Ziegler [17]). Here the use of virtual displacements makes it possible to show this result without referring to Ziegler's postulate. This was originally shown by Valanis [15], [19] for the classical continuum case. An alternative proof, applicable to both classical and micropolar continua, is given in Appendix A. Consequently, Eq. (75) can only be satisfied for all admissible $\delta\eta_{ij}$ and $\delta\zeta_{ij}$ if all of the following relations are satisfied:

$$Q_{ji}^* - \frac{\partial\psi}{\partial Q_{i,j}^*} - P_{ij} = 0, \quad (80)$$

$$M_{ji}^* - \frac{\partial\psi}{\partial m_{i,j}^*} - N_{ij} = 0, \quad (81)$$

$$M_{ji,j}^* - \frac{\partial\psi}{\partial m_i^*} + e_{ijk}P_{kj} = 0. \quad (82)$$

Up until this point no use has been made of the constraint in Eq. (55). When expressed in terms of the free energy it is equivalent to

$$\delta\psi = 0 \quad (83)$$

for all rigid body motions. Using this constraint Valanis [18] rederived the conservation laws for linear and angular momentum for a classical continuum. In Appendix B, the conservation laws for a micropolar material are rederived from the expression for the free energy in Eq. (61). By considering an infinitesimal rigid body displacement, the conservation of linear momentum is obtained, i.e.,

$$\bar{\sigma}_{ji,j} + f_i = 0, \quad (84)$$

while considering a rigid body rotation leads to the expression for conservation of angular momentum, i.e.,

$$\bar{\mu}_{ji,j} + g_i = e_{ijk}\bar{\sigma}_{kj}. \quad (85)$$

Note that, as a result, the stress tensor is in general asymmetric.

Both Eq. (84) and Eq. (85) place important constraints on the form of the free energy. Comparing Eq. (66) and Eq. (84), it is clear that

$$\frac{\partial\psi}{\partial u_i} = 0. \quad (86)$$

Hence, the free energy has no dependence on the displacement, answering the objections noted earlier.

Equations (65), (80) and (85) lead to the following:

$$\frac{\partial \psi}{\partial \bar{\omega}_i} = e_{ijk} \frac{\partial \psi}{\partial \bar{u}_{j,k}}. \quad (87)$$

Thus, in order to satisfy conservation of linear momentum the free energy must be a function of the average microstrain:

$$\psi(\bar{u}_{i,j}; \bar{\omega}_i) = \psi(\bar{\varepsilon}_{ij}). \quad (88)$$

This result has also been found to be true in micropolar elasticity (Eringen [24]).

At this point, the equations that describe the material behavior apply only on a local level. To proceed, these expressions are transformed into those that describe the material behavior in terms of global quantities, i.e., functions of the mesodomain's location X_i . This is achieved by introducing a weighting function ϕ in the manner described in Sect. 2. The notation $[\hat{\cdot}]$ is introduced to represent the weighted volume integral for a quantity $[\cdot]$:

$$[\hat{\cdot}] = \int_{V_\varnothing} [\cdot] \phi dV. \quad (89)$$

Accordingly Eqs. (66) – (70) and Eqs. (81) – (83) become:

$$\bar{\sigma}_{ji} = \frac{\partial \hat{\psi}}{\partial \bar{u}_{i,j}}, \quad (90)$$

$$\bar{\sigma}_{ji,j} + f_i = 0, \quad (91)$$

$$\hat{Q}_{ji}^* = \frac{\partial \hat{\psi}}{\partial q_i^*}, \quad (92)$$

$$\bar{\mu}_{ji} = \frac{\partial \hat{\psi}}{\partial \bar{\omega}_{i,j}}, \quad (93)$$

$$\bar{\mu}_{ji,j} + g_i = \frac{\partial \hat{\psi}}{\partial \bar{\omega}_i}, \quad (94)$$

$$\hat{Q}_{ji}^* - \hat{P}_{ij} = \frac{\partial \hat{\psi}}{\partial q_{i,j}^*}, \quad (95)$$

$$\hat{M}_{ji}^* - \hat{N}_{ij} = \frac{\partial \hat{\psi}}{\partial m_{i,j}^*}, \quad (96)$$

and

$$\hat{M}_{ji}^* + e_{ijk} \hat{P}_{kj} = \frac{\partial \hat{\psi}}{\partial m_i^*}. \quad (97)$$

Material models can be derived from the generalised constitutive relations by specifying the forms of two functions – the free energy ψ and the dissipation function D . In Sect. 4, these equations are used to develop a simple model of a two-dimensional granular material. An elastic micropolar theory, equivalent to that of Eringen [24] can be obtained by setting the internal variables q_i , m_i , Q_{ij} and M_{ij} to zero.

4 Thermomechanical model for a granular material

A simple model of a two-dimensional granular assembly (Schneebeli system) of equally sized circular particles is developed in this section. An expression is found for the free energy via a micromechanical analysis of a cluster consisting of a particle and its first ring of neighbors (Tordesillas and Walsh [8]). Stress-strain relations are then derived from the free energy using the generalized constitutive relations in Eqs. (90)–(97). These relations are then used to model a granular material undergoing a simple shear deformation.

The free energy inside a granular assembly is stored at the particle contacts. The free energy associated with a reference particle ψ^p is given by

$$\psi^p = \frac{1}{2} \sum_c \psi^c, \quad (98)$$

where ψ^c is the free energy of the particle contact and the sum is over all contacts around the particle. The factor of one-half is introduced as the energy at each contact is assumed to be distributed evenly between the two contacting particles.

Each particle is then assigned a void ratio by performing a Voronoi tessellation of the discrete assembly (see Fig. 3). As the assembly consists of equally sized disks of radius R , the free energy density ψ can be related to the free energy of each particle ψ^p via

$$\psi = \frac{1-v}{\pi R^2} \psi^p, \quad (99)$$

where v is the void ratio.

At this point a contact density distribution function Φ , equivalent to that used by Tordesillas and Walsh [8], is introduced. The contact density distribution function $\Phi = \Phi(\mathbf{n})$ is defined such that, given a unit vector \mathbf{n} pointing out from the centre of the particle, $\Phi d\mathbf{n}$ represents the probability of a particle contact occurring on the particle surface within a solid angle $d\mathbf{n}$ containing \mathbf{n} . With the introduction of the contact density distribution, Eq. (98) can be expressed as

$$\psi^p = \frac{1}{2} \int \psi^c \Phi(\mathbf{n}) d\mathbf{n}. \quad (100)$$

If the particle contacts undergo elastic deformation, the free energy of each contact ψ^c is given by

$$\psi^c = \frac{1}{2} k_n (\Delta u_i^{lc} n_i)^2 + \frac{1}{2} k_t (\Delta u_i^{lc} t_i)^2 + \frac{1}{2} k_r (\Delta \omega^{lc})^2, \quad (101)$$

where Δu_i^{lc} is the contact displacement, $\Delta \omega^{lc}$ is the contact rotation, n_i denotes the components of a unit vector normal to the contact surface, t_i denotes the components of a vector tangential

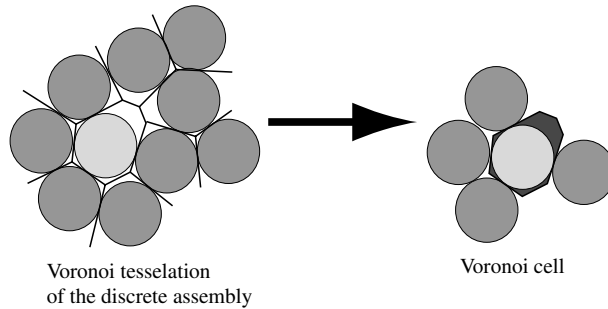


Fig. 3. A Voronoi tessellation of the discrete assembly assigns a Voronoi cell to each particle from which a void ratio can be determined

to the contact surface such that $e_{ij3}t_i n_j = 1$, k_n is the normal stiffness constant, k_t is the tangential stiffness constant and k_r is the rotational stiffness constant.

In a granular material, stored energy is lost by tangential slipping and rolling resistance at the contacts. In order to capture this behavior in a linear model the free energy is rewritten as

$$\begin{aligned} \psi^c = & \frac{1}{2} k_n (\Delta u_i^c n_i)^2 + \frac{1}{2} \left[k_a (\Delta u_i^c t_i)^2 + 2k_b \Delta u_i^c t_i \Delta q_j^c t_j + k_c (\Delta q_i^c t_i)^2 \right] \\ & + \frac{1}{2} \left[k_d (\Delta \omega)^2 + 2k_e \Delta \omega \Delta m + k_f (\Delta m)^2 \right], \end{aligned} \quad (102)$$

where k_a - k_f are material constants, with k_a - k_c being similar to the tangential stiffness constant k_t , while k_d - k_f are similar to the rotational stiffness constant k_r ; Δu_i^c and $\Delta \omega^c$ are the average contact displacement and contact rotation defined by

$$\Delta u_i^c = \frac{1}{V_{\mathcal{D}}} \int_{V_{\mathcal{D}}} \Delta u_i^c dV, \quad (104)$$

$$\Delta \omega^c = \frac{1}{V_{\mathcal{D}}} \int_{V_{\mathcal{D}}} \Delta \omega^c dV, \quad (105)$$

and $\Delta q_i^c = \Delta u_i^c - \Delta u_i^c$; $\Delta m^c = \Delta \omega^c - \Delta \omega^c$.

Thus

$$\begin{aligned} \psi = & \frac{1-\nu}{4\pi R^2} \int \left\{ k_n (\Delta u_i^c n_i)^2 + k_a (\Delta u_i^c t_i)^2 + 2k_b \Delta u_i^c t_i \Delta q_j^c t_j + k_c (\Delta q_i^c t_i)^2 \right. \\ & \left. + k_d (\Delta \omega)^2 + 2k_e \Delta \omega \Delta m + k_f (\Delta m)^2 \right\} \Phi(\mathbf{n}) d\mathbf{n}. \end{aligned} \quad (106)$$

To proceed the contact displacement and contact rotation must be linked with the kinematics of the micropolar media, which are described by the displacements and rotations of the centers of a reference particle and its contacting neighbors (see Fig. 4). The variables Δu_i^c , $\Delta \omega^c$ may be expressed in terms of the displacements u_i^a , u_i^b and rotations ω^a , ω^b of the reference particle “a” and its contacting neighbor “b” as follows:

$$\Delta u_i^c = u_i - u_i^a + e_{ij3} n_j R (\omega^{b_c} + \omega^a), \quad (107)$$

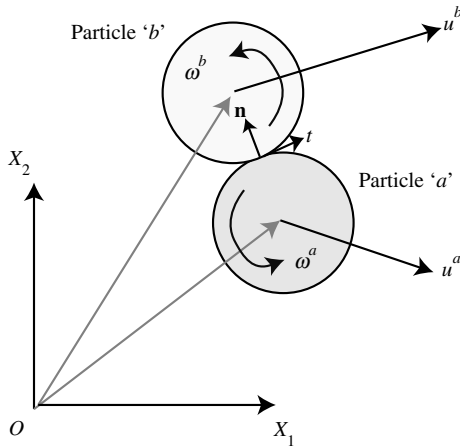


Fig. 4. The displacement and rotations of a reference particle “a” and one of its contacting neighbors “b”

and

$$\Delta\omega^{bc} = \omega^{b_c} - \omega^{a}. \quad (108)$$

As in Chang and Ma [10], it is assumed that the discrete quantities Δu_i^{bc} and $\Delta\omega^{bc}$ may be transformed into equivalent continuum expressions by introducing Taylor series expansions of the displacement and rotation of particle b_c in terms of the displacement and rotation of a contacting particle a , namely

$$u_i^{b_c} = u_i^a + 2R u_{i,j}^a n_j + \dots + \text{higher-order terms}, \quad (109)$$

$$\omega^{b_c} = \omega^a + 2R \omega_{,i}^a n_i + \dots + \text{higher-order terms}, \quad (110)$$

Thus the contact displacement and contact rotation can be expressed as

$$\Delta u_i^{bc} = 2R \left(u_{i,j}^a n_j + e_{ij3} n_j (\omega' + R \omega'_{,k} n_k) \right), \quad (111)$$

and

$$\Delta\omega^{bc} = 2R \omega'_{,i} n_i, \quad (112)$$

respectively. Likewise

$$\Delta \bar{u}_i^c = 2R \left(\bar{u}_{i,j} n_j + e_{ij3} n_j (\bar{\omega} + R \bar{\omega}_{,k} n_k) \right), \quad (113)$$

$$\Delta q_i^c = 2R \left(q_{i,j} n_j + e_{ij3} n_j (m^* + R m^*_{,k} n_k) \right), \quad (114)$$

and

$$\Delta \bar{\omega}^c = 2R \bar{\omega}_{,i} n_i, \quad (115)$$

$$\Delta m^c = 2R m^*_{,i} n_i. \quad (116)$$

With these relations, (106) becomes

$$\begin{aligned} \psi = & \frac{1-\nu}{\pi} \left\{ k_n \epsilon'_{ij} \epsilon'_{kl} \int n_i n_j n_k n_l \Phi d\mathbf{n} + (k_a \bar{e}_{ij} \bar{e}_{kl} + 2k_b \bar{e}_{ij} \eta_{kl} + k_c \eta_{ij} \eta_{kl}) \right. \\ & \times \int t_i n_j t_k n_l \Phi d\mathbf{n} + 2R (k_a \bar{e}_{ij} \bar{\omega}_{,k} + k_b (\bar{e}_{ij} m^*_{,k} + \eta_{ij} \bar{\omega}_{,k}) + k_c \eta_{ij} m^*_{,k}) \\ & \times \int t_i n_j n_k \Phi d\mathbf{n} + ((R^2 k_a + k_d) \bar{\omega}_{,i} \bar{\omega}_{,j} + (R^2 k_b + k_e) \bar{\omega}_{,i} m^*_{,j} + (R^2 k_a + k_d) m^*_{,i} m^*_{,j}) \\ & \left. \times \int n_i n_j \Phi d\mathbf{n} \right\}, \quad (117) \end{aligned}$$

where $\epsilon'_{ij} = u'_{i,j} + e_{ijk} \omega'_{,k}$, $\bar{e}_{ij} = \bar{u}_{i,j} + e_{ijk} \bar{\omega}_{,k}$ and $\eta_{ij} = q^*_{i,j} + e_{ij3} m^*$. Note that this expression for the free energy is a function of the microstrain $\bar{e}_{ij} = \bar{u}_{i,j}$ in accordance with Eq. (89).

For simplicity it is assumed that the void ratio and the contact density distribution function are constant throughout the deformation. An anisotropic contact density distribution function is assumed to be of the form:

$$\Phi = \frac{N}{2\pi} (1 + \alpha \cos(2\theta)), \quad (118)$$

where N is the number of particle contacts, α is a measure of the magnitude of the contact anisotropy ($0 \leq \alpha \leq 1$), and θ is defined as the angle between \mathbf{n} and the principle direction of

contact anisotropy \mathbf{r} (i.e., $\cos(\theta) = r_i n_i$). This contact density distribution function is illustrated in Fig. 5.

In this case, Eqs. (90)–(97) give the following relations:

$$\bar{\sigma}_{ji} = (k_n G_{ijkl} + k_a H_{ijkl}) \bar{e}_{kl} + (k_n G_{ijkl} + k_b H_{ijkl}) \hat{\eta}_{kl}, \quad (119)$$

$$\hat{Q}_{ji}^* - P_{ij} = (k_n G_{ijkl} + k_b H_{ijkl}) \bar{e}_{kl} + (k_n G_{ijkl} + k_c H_{ijkl}) \hat{\eta}_{kl}, \quad (120)$$

$$\bar{\sigma}_{ji,j} = 0, \quad (121)$$

$$\hat{Q}_{ji,j}^* = 0, \quad (122)$$

$$\bar{\mu}_i = (R^2 k_a + k_d) I_{ij} \bar{\omega}_j + (R^2 k_b + k_e) I_{ij} \hat{m}_j^*, \quad (123)$$

$$\hat{M}_i^* - \hat{N}_i = (R^2 k_b + k_e) I_{ij} \bar{\omega}_j + (R^2 k_c + k_f) I_{ij} \hat{m}_j^*, \quad (124)$$

$$\bar{\mu}_{i,i} = k_a J_{ij} \bar{e}_{ij} + k_b J_{ij} \hat{\eta}_{ij}, \quad (125)$$

and

$$\hat{M}_{ji,i}^* - e_{ij3} \hat{P}_{ij} = k_b J_{ij} \bar{e}_{ij} + k_c J_{ij} \hat{\eta}_{ij}, \quad (126)$$

where

$$G_{ijkl} = \frac{N(1-\nu)}{\pi} \left\{ \frac{1}{4} (\delta_{ij} \delta_{kl} + \delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) + \frac{\alpha}{2} (r_i r_j r_k r_l - s_i s_j s_k s_l) \right\}, \quad (127)$$

$$H_{ijkl} = \frac{N(1-\nu)}{\pi} \left\{ \frac{3}{4} \delta_{ik} \delta_{jl} - \frac{1}{4} \delta_{ij} \delta_{kl} - \frac{1}{4} \delta_{il} \delta_{jk} + \frac{\alpha}{2} (\delta_{ik} (r_j r_l + s_j s_l) - r_i r_j r_k r_l + s_i s_j s_k s_l) \right\}, \quad (128)$$

$$I_{ij} = \frac{N(1-\nu)}{\pi} \left\{ \delta_{ij} + \frac{\alpha}{2} (r_i r_j - s_i s_j) \right\}, \quad (129)$$

$$J_{ij} = \frac{N(1-\nu)}{\pi} \left\{ s_i r_j - r_i s_j + \frac{\alpha}{2} (r_i s_j - s_i r_j) \right\}, \quad (130)$$

δ_{ij} is the Kronecker delta symbol and s_i is a unit vector tangential to r_i such that $e_{ij3} s_i r_j = 1$. We note that a more sophisticated set of constitutive relations can be developed by adopting a contact density distribution function which evolves with strain. One example which allows both

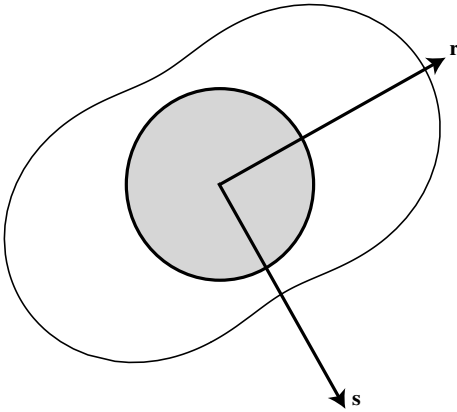


Fig. 5. The contact density distribution function $\Phi(\mathbf{n}, \mathbf{r}, \alpha, N) = (N/2\pi)(1 + \alpha \cos(2\theta))$ with the two vectors \mathbf{r} and \mathbf{s} representing the directions of maximum and minimum anisotropy, respectively

the degree and direction of the contact anisotropy to change with strain has been proposed recently by Gardiner and Tordesillas [27].

4.1 A simple shear example

We now consider a special case of a material body of infinite width and fixed height L undergoing a simple shear deformation (Fig. 6). Our intent here is not to provide the most comprehensive model of this system, but simply to demonstrate the application of the constitutive relations derived in the previous section. Toward this goal, we have adopted several assumptions to simplify the analysis. We allow no variation in the horizontal X_1 -direction and assume that $u'_{1,2}$ is constant in space. The material response is therefore a function of the vertical position y within the body. The normal stress on the boundaries σ'_{22} is held constant, and there are no body forces or moments.

The progress of the deformation is assumed to be solely a function of the macroscopic shear strain experienced by the sample. For this reason an intrinsic time t is introduced such that

$$dt^2 = du_{1,2}^2, \quad (131)$$

or, for this calculation where the shear strain is assumed to be strictly increasing from zero,

$$t = u_{1,2}. \quad (132)$$

The preferred direction of contact anisotropy r_i is assumed to lie along the X_2 axis. This is consistent with observations of contact distributions reported at the start of simple shear tests by Matsuoka [28] and Oda and Konishi [29]. In these experiments the distribution of contacts was observed to evolve as the shear test progressed. Recall that from Eq. (118) this evolution has not been accounted for in the present model. Therefore, only small strains are considered here.

It is assumed that the rolling resistance at the particle contacts is negligible. Consequently, the material parameters related to the rolling stiffnesses k_d , k_e and k_f , and the dissipative couple stress N_i are set to zero. This implies that the total dissipation function D is equal to D^n (Eq. (25)), which is due to the internal fluctuations in the microstrain η_{ij} . The dissipation inequality, Eq. (27), is satisfied by choosing $P_{ij} = b\partial\eta_{ij}/\partial t$ or

$$\hat{P}_{ij} = b \frac{\partial \hat{\eta}_{ij}}{\partial t}, \quad (133)$$

where b is a positive constant.

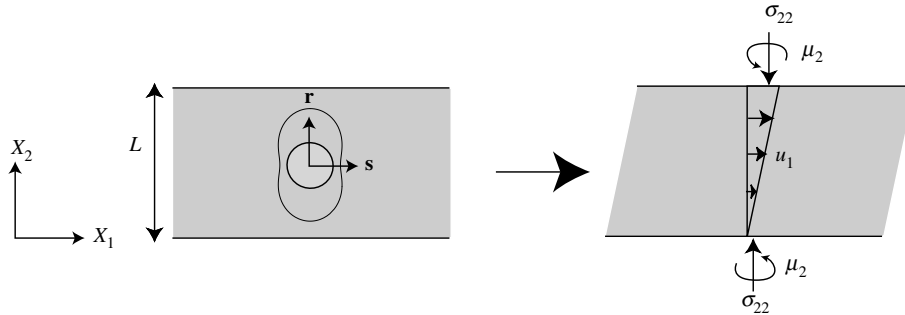


Fig. 6. An assembly undergoing a simple shear deformation

With these assumptions, Eqs. (119) to (126) can be rewritten as

$$\bar{\sigma}_{22} = (k_n G_{2222} + k_a H_{2222}) \bar{\epsilon}_{22} + (k_n G_{2222} + k_b H_{2222}) \hat{q}_{2,2}^*, \quad (134)$$

$$\hat{Q}_{22}^* - b \frac{\partial \hat{q}_{2,2}^*}{\partial t} = (k_n G_{2222} + k_b H_{2222}) \bar{\epsilon}_{22} + (k_n G_{2222} + k_c H_{2222}) \hat{q}_{2,2}^*, \quad (135)$$

$$\bar{\sigma}_{22,2} = 0, \quad (136)$$

$$\hat{Q}_{22,2}^* = 0, \quad (137)$$

$$\bar{\mu}_2 = (k_a \bar{\omega}_{,2} + k_b \hat{m}_{,2}^*) R^2 I_{22}, \quad (138)$$

$$\hat{M}_2^* = (k_b \bar{\omega}_{,2} + k_c \hat{m}_{,2}^*) R^2 I_{22}, \quad (139)$$

$$\bar{\mu}_{2,2} = k_a J_{12} \bar{u}_{1,2} + k_a (J_{12} - J_{21}) \bar{\omega} + k_b (J_{12} - J_{21}) \hat{m}^*, \quad (140)$$

$$\hat{M}_{2,2}^* - 2b \frac{\partial \hat{m}^*}{\partial t} = k_b J_{12} \bar{u}_{1,2} + k_b (J_{12} - J_{21}) \bar{\omega} + k_c (J_{12} - J_{21}) \hat{m}^*, \quad (141)$$

The initial and boundary conditions for this set of equations are as follows:

(i) At $t = 0$ it is assumed that

$$\hat{q}_2^* = \hat{m}^* = 0; \quad (142)$$

(ii) At $y = 0$ and $y = L$, the internal variation in the stress and moments are assumed to be zero,

$$\hat{Q}_{22}^* = \hat{M}_2^* = 0; \quad (143)$$

(iii) The stress normal to the boundary $\bar{\sigma}_{22}(0) = \bar{\sigma}_{22}(L) = 0$ is held constant throughout the deformation;

(iv) Once the deformation begins a couple stress is imposed on the material, which impedes the rotation at the boundaries: $\bar{\mu}_2(0) = -\bar{\mu}_2(L) = \mu$. The couple stress is assumed to increase linearly as the deformation progresses,

$$\mu = -\kappa t, \quad (144)$$

where κ is a positive constant.

Note that the equations describing the strain and the internal displacement Eqs. (134)–(137) are decoupled from those describing the rotations in Eqs. (138)–(141). This result is possible because of the particular form of the contact density distribution function (Eq. 118). The predicted material response is especially sensitive to the assumed form of the contact anisotropy and other micromechanical properties of the material. For example, the constant stress conditions at the boundaries and the absence of any evolution in the contact density distribution function lead to the following uniform distribution for the strain:

$$\bar{\epsilon}_{22} = \frac{\bar{\sigma}_{22}}{k_n G_{2222} + k_a H_{2222}}. \quad (145)$$

However, if the assumed form for Φ evolves with strain (as proposed in Gardiner and Tordellas [27]), the predicted strain may vary both in space and time.

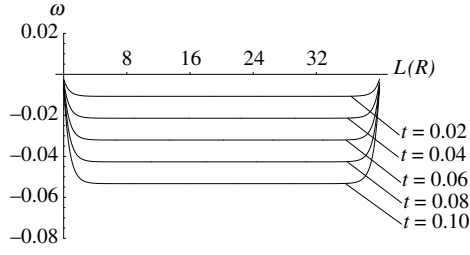


Fig. 7. Graphs of particle rotation at different times t : $N = 3.4$, $\nu = 0.2$, $\alpha = 0.2$, $L = 40R$, $\kappa = 0.05Rk_a$, $b = 100k_a$, $k_b = 0.8k_a$, $k_c = 0.8k_a$

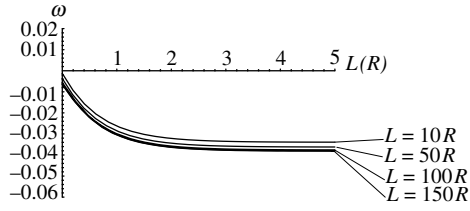


Fig. 8. Distribution of particle rotations near the boundary for different heights L : $t = 0.07$, $N = 3.4$, $\nu = 0.2$, $\alpha = 0.2$, $\kappa = 0.05Rk_a$, $b = 100k_a$, $k_b = 0.8k_a$, $k_c = 0.8k_a$

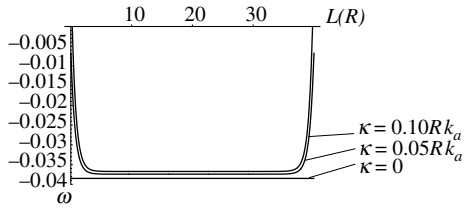


Fig. 9. The effects of κ on particle rotation: $t = 0.07$, $N = 3.4$, $\nu = 0.2$, $\alpha = 0.2$, $L = 40R$, $b = 100k_a$, $k_b = 0.8k_a$, $k_c = 0.8k_a$

The equations describing the rotations, Eqs. (138)–(141), lead to the following differential equations:

$$(k_a \bar{\omega}_{,22} + k_b \hat{m}_{,22}^*) R^2 I_{22} = k_a J_{12} \bar{u}_{1,2} + k_a (J_{12} - J_{21}) \bar{\omega} + k_b (J_{12} - J_{21}) \hat{m}^*, \quad (146)$$

$$(k_b \bar{\omega}_{,22} + k_c \hat{m}_{,22}^*) R^2 I_{22} = k_b J_{12} \bar{u}_{1,2} + k_b (J_{12} - J_{21}) \bar{\omega} + k_c (J_{12} - J_{21}) \hat{m}^* + 2b \frac{\partial \hat{m}^*}{\partial t}. \quad (147)$$

A solution for the macroscopic rotations $\bar{\omega}$ can be obtained from Eq. (146) and Eq. (147) using a finite Fourier cosine transform:

$$\bar{\omega} = -\frac{J_{12}}{J_{12} - J_{21}} - \frac{2}{L} \sum_n \left\{ \frac{((-1)^n + 1) \kappa \cos(n\pi y/L)}{k_a (J_{12} - J_{21} + I_{22} n^2 \pi^2 R^2 / L^2)} \times \left[t - \frac{k_b^2}{k_a k_c - k_b^2} \left(t - 2b \frac{1 - e^{-(k_c - k_b^2/k_a)(J_{12} - J_{21} + I_{22} n^2 \pi^2 R^2 / L^2)t/2b}}{(k_c - k_b^2/k_a)(J_{12} - J_{21} + I_{22} n^2 \pi^2 R^2 / L^2)} \right) \right] \right\}. \quad (148)$$

The evolution of the macroscopic particle rotation within the assembly is shown in Fig. 7. The model predicts the appearance of a region of decreased rotation next to the boundaries. As shown in Fig. 8, the distribution of rotations close to the boundaries becomes independent of the height of the assembly as the ratio R/L decreases.

The amount of rotation at the boundary is dependent upon the couple stress, the number of particle contacts N and the void ratio ν . As would be expected, increasing the couple stress causes an overall decrease in the rotation, particularly at the boundaries (Fig. 9). Increasing the packing density has the opposite effect, resulting in less of a discrepancy between the rotations

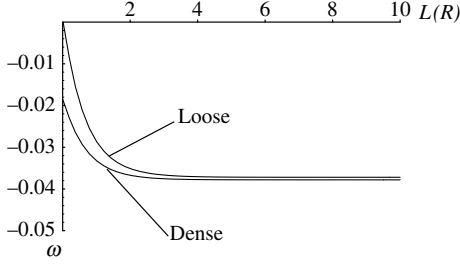


Fig. 10. Comparing the rotation close to the boundary: densely packed assembly ($N = 3.4$, $\nu = 0.2$) versus loosely packed assembly ($N = 2.2$, $\nu = 0.4$): $t = 0.07$, $\alpha = 0.2$, $L = 40R$, $\kappa = 0.03Rk_a$, $b = 100k_a$, $k_b = 0.8k_a$, $k_c = 0.8k_a$

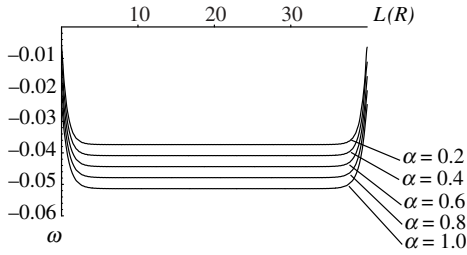


Fig. 11. Distribution of particle rotations for varying degrees of contact anisotropy α , $t = 0.07$, $N = 3.4$, $\nu = 0.2$, $L = 40R$, $\kappa = 0.05Rk_a$, $b = 100k_a$, $k_b = 0.8k_a$, $k_c = 0.8k_a$

at the boundaries and those at the centre (Fig. 10). As mentioned earlier, the form of the contact density distribution function has a particularly strong effect on the behaviour of the model. Varying the degree of contact anisotropy changes the rotations across the assembly. As demonstrated in Fig. 11, increasing the contact anisotropy resulted in a linear increase in the amount of rotation experienced by the material.

5 Conclusions

Using a thermomechanical approach, constitutive relations have been derived for a micropolar continuum undergoing isothermal deformation. The constitutive relations developed are expressed in terms of two sets of internal variables q_i and m_i and their material gradients. These variables are introduced to capture internal variations in the displacement and rotation fields, respectively. Specific material models can be derived from these generalised constitutive relations by specifying the form of the free energy and the dissipation function. The thermomechanical approach presented here guarantees that the resulting micropolar models are consistent with the laws of thermodynamics.

Two important constraints were introduced in the derivation of the generalised constitutive laws: (a) that the free energy is invariant under rigid body motions, and (b) that changes due to the microstrain and curvature on the local scale result in the dissipation of energy. Imposing the first constraint leads to the conservation of momentum laws for a micropolar continuum. This result in turn imposed a restriction on the form of the free energy, specifically that it must be a function of the microstrain. The second constraint was used in the variational approach to obtain the final set of constitutive laws without the use of Ziegler's orthogonality postulate.

Particular stress-strain relations for a granular assembly were developed from the generalised constitutive relations. These stress-strain relations were then used to model a special case of a granular assembly undergoing a simple shear deformation. For assemblies obeying the assumptions delineated in Sect. 4.1, the model predicts the appearance of two regions of

reduced rotation next to the boundaries. The packing density is seen to have a noticeable influence on the thickness of these regions. The nonuniform distribution of rotations close to the boundaries becomes independent of the height of the assembly as L becomes much larger than R . Future model refinements that account for the evolution of anisotropy (both force and contact), interparticle rolling resistance and more detailed dissipative effects are underway.

Appendix A

Equivalence of P and Q

In the main body of the text it was shown that if $\|\delta\mathbf{q}\| > 0$

$$(\mathbf{Q} - \mathbf{P}) \cdot \delta\mathbf{q} = 0 \quad (149)$$

holds for all arbitrary variations in the internal strain field and the internal curvature field satisfying the conditions that

$$\mathbf{Q} \cdot \delta\mathbf{q} = 0, \quad (150)$$

$$\mathbf{P} \cdot \delta\mathbf{q} = 0. \quad (151)$$

The aim of this Appendix is to show that under these conditions

$$\mathbf{Q} = \mathbf{P}. \quad (152)$$

To prove this result, a vector \mathbf{n} is introduced such that

$$\mathbf{n} = \alpha\hat{\mathbf{Q}} + (1 - \alpha)\hat{\mathbf{P}}, \quad (153)$$

where $\hat{\mathbf{Q}} = \mathbf{Q}/\|\mathbf{Q}\|$; $\hat{\mathbf{P}} = \mathbf{P}/\|\mathbf{P}\|$ and α is an as yet undetermined scalar. An arbitrary variation of \mathbf{q} in the direction of \mathbf{n} is denoted by $\delta\mathbf{n}$, i.e.,

$$\delta\mathbf{n} = \beta\mathbf{n}, \quad (154)$$

where $\beta > 0$.

If \mathbf{Q} and \mathbf{P} are not co-linear then $\delta\mathbf{n}$ satisfies both the conditions in Eq. (150) and Eq. (151) if

$$\frac{1}{1 - \gamma} > \alpha > \frac{-\gamma}{1 - \gamma}, \quad (155)$$

where

$$1 > \gamma = \hat{\mathbf{P}} \cdot \hat{\mathbf{Q}} > -1. \quad (156)$$

In this case, Eq. (149) only holds if

$$(\mathbf{Q} - \mathbf{P}) \cdot (\alpha\hat{\mathbf{Q}} + (1 - \alpha)\hat{\mathbf{P}}) = 0 \quad (157)$$

or

$$\alpha = \frac{\|\mathbf{P}\| - \|\mathbf{Q}\|\gamma}{(\|\mathbf{P}\| + \|\mathbf{Q}\|)(1 - \gamma)}. \quad (158)$$

However, any number of α 's can be chosen that violate this equation and yet satisfy the conditions in Eq. (155). Thus \mathbf{Q} and \mathbf{P} must be co-linear.

If \mathbf{Q} and \mathbf{P} are co-linear then the conditions in Eq. (150) and Eq. (151) cannot both be satisfied unless

$$\hat{\mathbf{Q}} = \hat{\mathbf{P}}, \quad (159)$$

in which case $\delta \mathbf{n} = \beta \hat{\mathbf{Q}}$ satisfies both inequalities, and Eq. (149) may be written

$$\|\mathbf{Q}\| - \|\mathbf{P}\| = 0. \quad (160)$$

This is only possible if $\mathbf{Q} = \mathbf{P}$.

Appendix B

Conservation of linear and angular momentum

By stipulating that the internal variables and the internal energy remain constant during rigid body rotations, Valanis [18] was able to rederive the conservation laws for linear and angular momentum for a classical continuum. Here the conservation laws for a Cosserat material are rederived from the expression for the free energy in Eq. (61).

In the case of a rigid body translation ($\delta u'_i = \delta \bar{u}_i$, $\delta \omega'_i = 0$), Eq. (61) becomes

$$(\bar{\sigma}_{ji,j} + f_i) \delta \bar{u}_i = 0 \quad (161)$$

or

$$\bar{\sigma}_{ji,j} + f_i = 0, \quad (162)$$

which can be recognised as the law of conservation of linear momentum.

For a rigid body rotation $\delta u'_i = e_{ijk} \delta \Gamma_j x_k$ and $\delta \omega'_i = \delta \Gamma_i$. In this case, Eq. (61) becomes

$$(\bar{\mu}_{ji,j} + g_i) \delta \Gamma_i + \bar{\sigma}_{ji} e_{ijk} \delta \Gamma_k = 0. \quad (163)$$

After rearranging Eq. (163) and factorising out $\delta \Gamma_i$, the following result is obtained:

$$\bar{\mu}_{ji,j} + g_i + e_{ijk} \bar{\sigma}_{jk} = 0. \quad (164)$$

It can be shown that this expression is equivalent to the conservation of angular momentum within the mesodomain. If angular momentum is conserved then the moments applied to the surface of the mesodomain (from either surface couples or an uneven distribution of the tractions) must be balanced by the body moments, i.e.,

$$\int_{S_{\mathcal{D}}} \{e_{ijk} T'_k x_j + \Omega'_i\} dS + \int_{V_{\mathcal{D}}} g_i dV = 0. \quad (165)$$

Note that

$$\begin{aligned} \int_{S_{\mathcal{D}}} \{e_{ijk} T'_k x_j + \Omega'_i\} dS + \int_{V_{\mathcal{D}}} g_i dV &= \int_{S_{\mathcal{D}}} \{e_{ijk} \sigma'_{ik} x_j + \mu'_{ii}\} n_i dS + \int_{V_{\mathcal{D}}} g_i dV \\ &= \int_{V_{\mathcal{D}}} \left\{ [e_{ijk} \sigma'_{ik} x_j + \mu'_{ii}]_{,i} + g_i \right\} dV \\ &= \int_{V_{\mathcal{D}}} \{e_{ijk} \bar{\sigma}_{jk} + \bar{\mu}_{ji,j} + g_i\} dV. \end{aligned} \quad (166)$$

As $\bar{\mu}_{ji,j}$, $\bar{\sigma}_{jk}$ and g_i are all constant within the mesodomain, Eq. (165) is only true if

$$\bar{\mu}_{ji,j} + e_{ijk} \bar{\sigma}_{jk} + g_i = 0, \quad (167)$$

which is equivalent to Eq. (164).

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References

- [1] Oda, M., Konishi, J., Nemat-Nasser, S.: Experimental micromechanical evaluation of strength of granular materials: effects of particle rolling. *Mech. Mater.* **1**, 269–283 (1982).
- [2] Oda, M., Kazama, H.: Microstructure of shear bands and its relation to the mechanisms of dilatancy and failure of dense granular soils. *Geotech.* **48**, 465–481 (1998).
- [3] Oda, M., Iwashita, K.: Study on couple stress and shear band development in granular media based on numerical simulation analyses. *Int. J. Engng. Sci.* **38**, 1713–1740 (2000).
- [4] Bardet, J. P., Proubet, J.: A numerical investigation of the structure of persistent shear bands in granular materials. *Geotech.* **41**, 159–182 (1991).
- [5] Rothenburg, L., Bathurst, R. J.: Influence of particle eccentricity on micromechanical behavior of granular materials. *Mech. Mater.* **16**, 141–152 (1993).
- [6] Howell, D. W., Behringer, R. P., Veje, C. T.: Fluctuations in granular media. *Chaos* **9**, 559–572 (1999).
- [7] Calvetti, F., Combe, G., Lanier, J.: Experimental micromechanical analysis of a 2D granular material: relation between structure evolution and loading path. *Mech. Cohesive Frict. Matter.* **2**, 121–163 (1997).
- [8] Tordesillas, A., Walsh, S. D. C.: Incorporating rolling resistance and contact anisotropy in micromechanical models of granular media. *Powder Technol.* **124**, 106–111 (2002).
- [9] Tordesillas, A., Peters, J. F., Gradiner, B.: Shear band evolution and accumulated microstructural development in Cosserat media. *Geotech.* (submitted).
- [10] Chang, C. S., Ma, L.: A micromechanically-based micropolar theory for deformation of granular solids. *Int. J. Solids Struct.* **28**, 67–86 (1991).
- [11] Kuhn, M. R.: Structured deformation in granular materials. *Mech. Matter.* **31**, 407–429 (1999).
- [12] Kuhn, M. R., Bagi, K.: Particle rotations in granular materials. In: (CD-ROM) 15th ASCE Engng Mech. Conf. (Smyth, A., ed.), New York: Columbia University, 2002.
- [13] Radjai, F., Roux, S.: Turbulentlike fluctuations in quasistatic flow of granular media. *Phys. Rev. Lett.* **89**, Art. No. 064302 (2002).
- [14] Didwania, A. K.: Kinematic diffusion in Quasi-static granular deformation. *Quart. J. Mech. Appl. Math.* **54**, 413–429 (2001).
- [15] Valanis, K. C.: A gradient theory of finite viscoelasticity. *Arch. Mech.* **49**, 589–609 (1997).
- [16] Peters, J. F., Horner, D. A.: Development of a continuum representation of a discrete granular medium. In: (CD-ROM) 15th ASCE Engng Mech. Conf. (Smyth, A., ed.), New York: Columbia University, 2002.
- [17] Ziegler, H.: An introduction to thermomechanics, 2nd ed. Amsterdam: North Holland, 1983.
- [18] Collins, I. F., Housby, G. T.: Applications of thermomechanical principles to the modeling of geotechnical materials. *Proc. R. Soc. London, Ser. A* **453**, 1975–2001 (1997).
- [19] Valanis, K. C.: A gradient theory of internal variables. *Acta Mech.* **116**, 1–14 (1996).
- [20] Housby, G. T., Puzrin, A. M.: A thermomechanical framework for constitutive models for rate-independent dissipative materials. *Int. J. Plasticity* **16**, 1017–1047 (2000).
- [21] Collins, I. F., Kelly, P. A.: A thermomechanical analysis of a family of soil models. *Geotech.* **52**, 507–518 (2002).
- [22] Collins, I. F., Hilder, T.: A theoretical framework for constructing elastic/plastic constitutive models of triaxial tests. *Int. J. Numer. Anal. Meth. Geomech.* **26**, 1313–1347 (2002).
- [23] Read, H. E., Hegemeier, G. A.: Strain softening of rock, soil and concrete; a review article. *Mech. Mater.* **3**, 271–294 (1984).
- [24] Wolf, D. E., Radjai, F., Dippel, S.: Dissipation in granular materials. *Phil. Mag. Ser. B*, **77**, 1413–1425 (1998).

- [25] Lubliner, J.: Plasticity theory, p. 43. New York: Macmillan 1990.
- [26] Eringen, A. C.: Theory of micropolar elasticity. In: Fracture – an advanced treatise, vol. II (Liebowitz, H., ed.), pp. 621–693. New York: Academic Press, 1968.
- [27] Gardiner, B. S., Tordesillas, A.: Micromechanical constitutive modelling of granular material: a focus on the evolution and loss of contacts in particle clusters. *J. Engng Math.* (submitted).
- [28] Matsuoka, H.: A microscopic study on shear mechanism of granular materials. *Soils and Foundations* **14**, 29–43 (1974).
- [29] Oda, M., Konishi, J.: Microscopic deformation mechanism of granular material in simple shear. *Soils and Foundations* **14**, 25–38 (1974).

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