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Micromorphic modeling of granular dynamics

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Abstract

This paper provides micromorphic modeling of a granular material. Micromorphic modeling treats an individual particle as a microelement and the particle composition in a representative volume element as a macroelement. By specifying the volume of a macroelement, continuum volume-type quantities such as mass density, body force, body couple, kinetic energy density, internal energy density, specific heat supply, etc., are determined by taking the averages of their discrete counterparts in a macroelement. The discrete expressions for the divergence of surface-type quantities (fluxes) are obtained with the help of discretecontinuum analogy for the discrete balance equations. We demonstrate that the discrete formulation of stress tensor in the dynamic condition, which involves both contributions from body forces and relative particle accelerations in a macroelement, can be simply expressed in terms of contact forces and branch vectors. This study constructs complete discrete-type and continuum-type balance equations for a granular material in a macroelement and at a macroscopic point, using the discrete-continuum correspondence for these field quantities.

Keywords: Granular materials; Microcontinuum; Continuum mechanics

1 Introduction

Microcontinuum field theory has been developed by Eringen and Suhubi (1964) and Eringen (1964; 1999; 2001) to characterize detailed behaviors of materials with internal degrees of freedom. A microcontinuum can be categorized into micromorphic, microstretch, and micropolar continua according to different macroelement internal deformations. The success of this theory over the past four decades has been justified in applications describing peculiar responses of liquid crystals, polymers, suspensions, and many kinds of materials. The purpose of this study is to discuss the feasibility and applicability of the microcontinuum theory

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to characterize the dynamics of a single-phase granular material.

A granular material is an aggregate of a large number of discrete solid grains. Two different approaches model the mechanical behaviors of granular materials: the microscopic discrete-particle approach and the macroscopic continuum mechanical approach. The discrete element method and the molecular dynamics method are usually employed to depict individual particle motion in a granular system (Goldhirsch and Goldenberg, 2004). Homogenization helps to formulate granular material macro fields in terms of corresponding micro-fields, such as contact forces and displacements between particles (Chang and Liao, 1994). The continuum theory provides another useful approach to dealing with the mechanics of granular materials, contrary to discrete treatments. This approach has been successfully applied to analyze the motion of avalanches, debris, and mud flows of granular matters (Takahashi, 1991; Hutter *et al.*, 1996).

A complete understanding of the mechanics of granular materials under the continuum mechanical approach is currently still lacking. This lack is due to the internal structural complexity of these materials and a lack of considering macroscopic influence contributed by the characteristic length of these materials. Specifically, in addition to standard balance equations in continuum mechanics, another equation is necessary to account for the effects caused by internal relative motion of particles. Recognizing that pore space plays an important role in granular material behavior, Goodman and Cowin (1972) developed a continuum theory for these materials which treats the solid volume fraction as an internal variable and then proposes an equilibrated force balance equation for this variable. Other internal variables for a granular material have also been investigated, among which particle rotation has received much attention. Treating particle rotation as an internal variable is partly responsible for driving the development of micropolar continuum studies on granular materials. Early treatments of the mechanics of materials with internal rotation trace back to Voigt and Cosserat brothers. Later studies concentrate on developing micropolar continuum theories (Toupin, 1964; Eringen, 1964; Green, 1965; Mindlin, 1965; Nowacki, 1986).

The significant effect of microrotation in metals has so far not received experimental support to date, even though micropolar theories have predicted several interesting phenomena in materials. However, micropolar effect might be taken into account in other materials, such as human compact bones, for which some experimental observations suggest that a micropolar solid seems to be a more accurate model (Yang and Lakes, 1982). Moreover, experimental evidence (Oda, 1997) showing the important role of discrete granular particle rotation in the development of shear band reinforces the viability of micropolar theory

applicability to granular media, especially in a loosely packed state. As for theoretical treatments, researchers have used micropolar theories to analyze the deformation and flow of granular materials (Kanatani, 1979; Chang and Ma, 1991). Recently, Goddard (2005) proposed an energy-based homogenization method to derive the quasi-static continuum models of discrete granular media, obtaining the higher-order stresses for micropolar continua by expanding particle displacements and forces in terms of their polynomial representations. Froiio *et al.* (2006) established a mathematical framework to develop linear-momentum and angular-momentum balance laws for granular materials by introducing the concepts of "part", "granular surface", "separately additive function", and "flux". Other excellent works also investigate micropolar continuum applicability to granular materials (Chang and Ma, 1990; Ehlers and Volk,1998; Bardet and Vardoulakis, 2001; Tordesillas and Walsh, 2002; Kruyt, 2003; Ehlers *et al.*, 2003; Chang and Kuhn, 2005).

This study proposes a micromorphic model, accounting for both microstructural motions of granular media – the bulk motion due to arrangement and compressibility of grains (Goodman-Cowin treatment) and the rotational motion of grains (micropolar treatment). The current work links a representative volume element (RVE) and a macroelement (Eringen, 1999), treating a macroelement as a region for averaging discrete quantities. By specifying a macroelement volume, we obtain micromorphic continuum quantities in terms of discrete quantities. Special emphasis is paid to the general discrete formulation of the stress tensor, in which contact forces between grains, volumetrical forces of grains, and grain accelerations relative to the macroelement's center of mass (COM) are taken into account. The six discrete balance equations – mass, microinertia, linear momentum, angular momentum, energy, and entropy are formulated within a macroelement, and then transformed to their continuum correspondences. In the past, Babic (1997) and Zhu and Yu (2002) have proposed a space-time averaging technique to link discrete balance equations to the standard continuum balance equations mentioned above. Besides the five equations, micromorphic modeling in the current study helps to provide a new balance equation – the microinertia balance equation, which describes the evolution of second-order moment of mass density. This equation can be used to characterize grain arrangement in a macroelement.

This paper is organized as follows. Section 2 briefly reviews the background of a microcontinuum. Section 3 presents the micromorphic model by proposing a macroelement-particle treatment. Proposing a macroelement correlates the volume-type and surface-type continuum quantities for a granular material with their discrete counterparts. Section 4 provides discrete macroelement-particle-based balance equations and derives their corresponding con-

tinuum balance equations. Section 5 states conclusions and final remarks.

2 Formulation of field equations for a microcontinuum

A material body \mathcal{B} in the microcontinuum theory is treated as a collection of deformable macroelements { $\Delta \mathcal{B}$ }. A macroelement, whose mass, volume, and mass density are respectively denoted by dm, dV, and $\rho(=dm/dV)$, contains many microelements, having mass dm', volume dV', and mass density $\rho' = dm'/dV'$, such that $\rho dV = \int_{\Delta \mathcal{B}} \rho' dV'$ and $dV = \int_{\Delta \mathcal{B}} dV'$, where the quantities with "prime" above indicate those of a microelement. A macroelement $\Delta \mathcal{B}(\mathbf{X}, \boldsymbol{\Xi})$ can be characterized by its center of mass \mathcal{C} and vectors $\boldsymbol{\Xi}$'s relative to \mathcal{C} , where the vector \mathbf{X} represents the position vector of \mathcal{C} and the vector $\boldsymbol{\Xi}$ describes the intrinsic structure of the macroelement. This vector $\boldsymbol{\Xi}$ measures the position vector of a microelement relative to the macroelement's COM.

The kinematics of a macroelement $\Delta \mathcal{B}$ can be described by the two mappings:

$$\mathbf{X} \to \mathbf{x} = \hat{\mathbf{x}}(\mathbf{X}, t), \tag{1}$$

$$\boldsymbol{\Xi} \to \boldsymbol{\xi} = \hat{\boldsymbol{\xi}}(\mathbf{X}, \boldsymbol{\Xi}, t), \tag{2}$$

where **X** and **\Xi** are measured in the reference configuration, and **x** and $\boldsymbol{\xi}$ are the corresponding vectors of **X** and **\Xi** in the current configuration. The first mapping is the macromotion and the second one is the micromotion. The macromotion is mathematically described by the deformation gradient **F**, and under a linear approximation the micromotion can be characterized by the deformable directors $\boldsymbol{\chi}$ such that we have the two relations:

$$d\mathbf{x} = \mathbf{F} \cdot d\mathbf{X}, \qquad \boldsymbol{\xi} = \boldsymbol{\chi} \cdot \boldsymbol{\Xi}.$$
 (3)

The complete set of balance equations in the microcontinuum field theory is (Eringen, 1999)

$$\frac{d\rho}{dt} + \rho \nabla \cdot \mathbf{v} = 0, \tag{4}$$

$$\frac{d\mathbf{i}}{dt} - \boldsymbol{\nu} \cdot \mathbf{i} - \mathbf{i} \cdot \boldsymbol{\nu}^T = \mathbf{0},\tag{5}$$

$$\rho \frac{d\mathbf{v}}{dt} - \nabla \cdot \mathbf{t} - \rho \mathbf{f} = \mathbf{0},\tag{6}$$

$$\rho \boldsymbol{\sigma} - \nabla \cdot \boldsymbol{\mu} - (\mathbf{t} - \boldsymbol{\tau})^T - \rho \mathbf{l} = \mathbf{0}, \tag{7}$$

$$\rho \frac{d\varepsilon}{dt} - \mathbf{t}^T : (\nabla \mathbf{v} - \boldsymbol{\nu}) - \boldsymbol{\tau}^T : \boldsymbol{\nu} - \boldsymbol{\mu} \stackrel{!}{:} \nabla \boldsymbol{\nu} + \nabla \cdot \mathbf{q} - \rho r = 0,$$
(8)

$$\rho \frac{d\eta}{dt} + \nabla \cdot \mathbf{\Phi} - \gamma = 0. \tag{9}$$

These equations represent the balance of mass, microinertia, linear momentum, momentum moment, internal energy, and entropy, respectively. Here, d/dt is the total time derivative and the superscript "T" means the transpose. The operators ":" and ":" stand for the double and triple contractions in the last two and three indices such that for a (k + 2)-order tensor **a** and a (l+2)-order tensor **b** with components $a_{i_1i_2...i_{k+2}}$ and $b_{i_1i_2...i_{l+2}}$, we have $(\mathbf{a}:\mathbf{b}) = a_{i_1i_2...i_kmn}b_{i_1i_2...i_lmn}$ and $(\mathbf{a}:\mathbf{b}) = a_{i_1i_2...i_{k-1}mnp}b_{i_1i_2...i_{l-1}mnp}$. The sixteen quantities $\rho, \mathbf{v}, \mathbf{i}, \boldsymbol{\nu}, \mathbf{t}, \mathbf{f}, \boldsymbol{\sigma}, \boldsymbol{\mu}, \boldsymbol{\tau}, \mathbf{l}, \varepsilon, \mathbf{q}, r, \eta, \boldsymbol{\Phi}$, and γ are respectively the mass density, the velocity field, the microinertia tensor, the microgyration tensor, the stress tensor, the body force, the spin inertia per unit mass, the stress momentum tensor, the microstress, the body couple per unit mass, the internal energy density, the heat flux vector, the heat source, the entropy density, the entropy flux, and the entropy production.

The success of the macroscopic field theory of a microcontinuum can be found not only in its application to modeling the behavior of a lot of substances but also in its support from a microscopic derivation (Oevel and Schröter, 1981; Chen and Lee, 2003). Whether or not the microcontinuum equations can be applied to a discrete granular system heavily depends on the interpretation and formulation of continuum quantities in terms of corresponding discrete quantities. The next section discusses an approach to modeling a granular system as a microcontinuum.

3 Micromorphic modeling

Producing macroscopic quantities of a granular assembly requires choosing a suitable spatial domain, over which those quantities can be obtained by taking the average of their corresponding microscopic counterparts. Tordesillas and Walsh (2002) treated a particle and its contact particles as a domain to link discrete mechanical quantities with micropolar continuum quantities. This treatment recognizes that homogenizing a large number of particles cannot delineate the evolution of shear bands, only a few particles wide. Thus, a fundamental problem in presenting a good macroscopic description of a granular system is to determine the size of an RVE, or how many grains should be contained in an RVE? Researchers to date have not reached a consensus on determining the extent of an RVE. Basically, a good macroscopic description requires the following condition

$$\lambda_P < \lambda_R < \lambda_D, \tag{10}$$

where λ_P , λ_R , and λ_D denote the characteristic lengths of a granular particle, an RVE, and the whole granular system, respectively. The following derivation follows this constraint



Figure 1: A spherical RVE containing N particles is adopted. In the center-of-mass coordinate system, the position of a particle is decomposed into the position vector of the COM of all particles in the RVE and the position relative to the COM. For convenience of expression, the particles are symbolically represented in a spherical form.

condition.

3.1 RVE, macroelement, and macroscopic point

In the reference configuration, let's consider a spherical RVE with radius r_R and denote the number of particles in the RVE by N. For the sake of simplicity, we assume that particles are spherical because the effect of particle shape does not explicitly enter into the formulation of our modeling. This does not contradict with the fact that the geometric shape of particles has a great influence on the response of granular materials such as shear bands induced by biaxial forces (Powrie *et al.*, 2005). Indeed, particle shape will indirectly contribute to the granular dynamics by influencing the distributions of particle mass and contact forces, which in turn determine the related continuum quantities, such as the microinertia tensor and stress tensor.

Figure 1 shows that the position vector of a particle *i* in the RVE, \mathbf{x}^{i} , can be represented by the position of the COM of all particles in the RVE, \mathbf{x} , and the position relative to the COM, $\boldsymbol{\xi}^{i}$. To be explicit, we set

$$\mathbf{x}^i = \mathbf{x} + \boldsymbol{\xi}^i. \tag{11}$$

Introducing the coordinate system $(\mathbf{x}, \boldsymbol{\xi}^i)$ provides (3N + 3) translational degrees of freedom (DOFs) for all particles in the RVE, greater than the original 3N translational DOFs, described by the N vectors \mathbf{x}^i . However, this center-of-mass coordinate system implicitly

imposes three additional constraint conditions $\sum_{i=1}^{N} \boldsymbol{\xi}^{i} = \mathbf{0}$. Together with the other 3N DOFs for N-particle spins, there are 6N numbers of independent DOFs for the RVE.

The construction of continuum field quantities from discrete quantities requires the specification of the volume of domain for averaging. Using the notion of macroelement in microcontinuum field theory, an RVE is inappropriately viewed as a macroelement because an RVE is usually treated as a fixed domain in the reference configuration and a macroelement is a moving material element. This study accordingly defines a macroelement in this micromorphic modeling as a moving domain composed of those particles in an RVE. A microelement in this modeling is meanwhile adopted as a single particle. Furthermore, we adopt the cell volume of the Dirichlet tessellation (Dirichlet, 1850; Oda and Iwashita, 1999) as the basic volume unit, which includes the volume of a single particle and partial spatial volume of surrounding void. Let ΔV^i be the cell volume of particle *i* in the Dirichlet tessellation, and the macroelement volume be the sum of the cell volumes of all particles in the macroelement, i.e., $\Delta V = \sum_{i=1}^{N} \Delta V^i$. Macroelement volume ΔV is notably time-dependent.

This work images and assumes a macroelement as a macroscopic "point", and assigns the position of this macroscopic point as the macroelement's COM, in order to have a continuum description of the discrete system. In this manner, all related macroscopic quantities at a macroscopic point \mathbf{x} are given as the average of their corresponding discrete counterparts over the macroelement. With the definition of a macroscopic point, the relative position vectors $\boldsymbol{\xi}^i$ are treated as internal DOFs at point \mathbf{x} and these internal DOFs evidently characterize the particle arrangement in an RVE.

Similar to the decomposition of the position vector in Eq. (11), the velocity of particle i in a macroelement measured at the origin of a Cartesian coordinate can be written as

$$\mathbf{v}^i = \mathbf{v} + \dot{\boldsymbol{\xi}}^i, \tag{12}$$

where \mathbf{v} is the velocity of the macroelement's COM, and $\dot{\boldsymbol{\xi}}^{i}$ represents the velocity of particle i measured from the COM.

3.2 Discrete-continuum relations for volume-type quantities

As soon as specifying the volume of a macroelement, one can readily construct the relations between the other macroscopic field quantities and their discrete counterparts. These macroscopic quantities can be separated into two categories: (i) volume-type quantities such as mass density, specific body force, specific body couple, entropy density, kinetic energy density, and internal energy density, and (ii) surface-type quantities, including stress tensor, couple stress, and heat flux.

With the volume ΔV of a macroelement, the discrete-continuum correspondences for the mass density ρ , body force density \mathbf{f} , body couple tensor \mathbf{l} , spin density \mathbf{s} , total angular momentum density \mathbf{S} , kinetic energy density T, internal energy density ε , and entropy density η of a granular assembly can be readily found as

$$\frac{1}{\Delta V} \sum_{i=1}^{N} m^{i} = \frac{m}{\Delta V} = \langle \rho \rangle \to \rho(\mathbf{x}, t), \tag{13}$$

$$\frac{1}{\Delta V} \sum_{i=1}^{N} m^{i} \mathbf{f}^{i} = \langle \rho \mathbf{f} \rangle \to \rho(\mathbf{x}, t) \mathbf{f}(\mathbf{x}, t), \tag{14}$$

$$\frac{1}{\Delta V} \sum_{i=1}^{N} m^{i} \mathbf{f}^{i} \otimes \boldsymbol{\xi}^{i} = \langle \rho \mathbf{l} \rangle \to \rho(\mathbf{x}, t) \mathbf{l}(\mathbf{x}, t), \qquad (15)$$

$$\frac{1}{\Delta V} \sum_{i=1}^{N} m^{i} \mathbf{s}^{i} = \langle \rho \mathbf{s} \rangle \to \rho(\mathbf{x}, t) \mathbf{s}(\mathbf{x}, t),$$
(16)

$$\frac{1}{\Delta V} \sum_{i=1}^{N} m^{i} \left(\mathbf{x}^{i} \times \mathbf{v}^{i} + \mathbf{s}^{i} \right) = \langle \rho \mathbf{S} \rangle \to \rho(\mathbf{x}, t) \mathbf{S}(\mathbf{x}, t),$$
(17)

$$\frac{1}{\Delta V} \left[\frac{1}{2} m \mathbf{v} \cdot \mathbf{v} + \frac{1}{2} \sum_{i=1}^{N} m^{i} (\dot{\boldsymbol{\xi}}^{i} \cdot \dot{\boldsymbol{\xi}}^{i} + \mathbf{s}^{i} \cdot \boldsymbol{\theta}^{i^{-1}} \cdot \mathbf{s}^{i}) \right] = \langle T \rangle \to T(\mathbf{x}, t), \tag{18}$$

$$\frac{1}{\Delta V} \sum_{i=1}^{N} m^{i} \varepsilon^{i} = \langle \rho \varepsilon \rangle \to \rho(\mathbf{x}, t) \varepsilon(\mathbf{x}, t),$$
(19)

$$\frac{1}{\Delta V} \sum_{i=1}^{N} m^{i} \eta^{i} = \langle \rho \eta \rangle \to \rho(\mathbf{x}, t) \eta(\mathbf{x}, t), \qquad (20)$$

where the quantities between left and right angles indicate the discrete averages in a macroelement and they are assigned to the point \mathbf{x} , which is the COM for the macroelement. Here, \mathbf{f}^i , \mathbf{s}^i , $\boldsymbol{\theta}^i$, ε^i , and η^i are the specific body force, spin density, tensor of moment of inertia, specific internal energy, and specific entropy for particle *i* in a macroelement. The operator " \otimes " is referred to the tensor product and *m* stands for the total mass of the macroelement.

It is straightforward to express the linear momentum at the point \mathbf{x} as

$$\frac{1}{\Delta V} \sum_{i=1}^{N} m^{i} \mathbf{v}^{i} = \langle \rho \mathbf{v} \rangle \to \rho(\mathbf{x}, t) \mathbf{v}(\mathbf{x}, t).$$
(21)

Substituting Eq. (12) into Eq. (21) yields

$$\sum_{i=1}^{N} m^i \dot{\boldsymbol{\xi}}^i = \mathbf{0},\tag{22}$$

which reflects the fact that the momentum measured at the macroelement's COM is zero.

The total angular momentum at the point \mathbf{x} is composed of the "spin" angular momentum in a macroelement characterizing particle spin and the "orbital" angular momentum of particles about the origin of the coordinate system. The orbital angular momentum is expressed by $\sum_{i=1}^{N} m^i (\mathbf{x}^i \times \mathbf{v}^i)$, and, using Eqs. (11), (12) and (22), it can be transformed to a simple form:

$$m\left(\mathbf{x}\times\mathbf{v}\right)+\sum_{i=1}^{N}m^{i}\left(\boldsymbol{\xi}^{i}\times\dot{\boldsymbol{\xi}}^{i}\right).$$

The kinetic energy at the point **x** contains three parts: (i) the kinetic energy of macroelement's COM with velocity **v**, (ii) the relative kinetic energy of particle *i* with relative velocity $\dot{\boldsymbol{\xi}}^{i}$, and (iii) the spin energy of particle *i* with angular velocity $\boldsymbol{\theta}^{i^{-1}} \cdot \mathbf{s}^{i}$.

In addition to the general quantities in standard continuum mechanics, microcontinuum field theory introduces a new quantity, called microinertia density **i**, to account for the second-moment of inertia of a macroelement. The importance of the symmetric second-order microinertia tensor, $\mathbf{i} = (1/\rho dV) \int_{\Delta B} \rho' \boldsymbol{\xi} \otimes \boldsymbol{\xi} dV'$, lies in the manifestation of mass distribution in a macroelement. This is the very reason why microcontinuum theory is a suitable candidate for describing a granular material, since the particle arrangement is crucial to determining several physical quantities of this material. With reference to the definition of the microinertia density, this study proposes the discrete-continuum correspondence for $\rho \mathbf{i}$ to be

$$\frac{1}{\Delta V} \sum_{i=1}^{N} m^{i} \boldsymbol{\xi}^{i} \otimes \boldsymbol{\xi}^{i} = \langle \rho \mathbf{i} \rangle \to \rho(\mathbf{x}, t) \mathbf{i}(\mathbf{x}, t), \qquad (23)$$

for a micromorphic modeling of a granular material.

3.3 Discrete-continuum relation for surface-type quantities-stress tensor

Consider the proposition of the macroscopic definition of stress tensor. For a microcontinuum the stress tensor \mathbf{t} at a point \mathbf{x} is formulated as

$$(\mathbf{n} \cdot \mathbf{t}) \, dS = \int \mathbf{T}^{(\mathbf{n}_{\zeta}')} dS',\tag{24}$$

where $\mathbf{T}^{(\mathbf{n}_{\zeta}')}$ is the traction exerting on the surface of a microelement with surface element dS'and its unit normal \mathbf{n}_{ζ}' . The surface element dS and its unit normal \mathbf{n} of the macroelement satisfy the relation: $\mathbf{n}dS = \int \mathbf{n}_{\zeta}' dS'$.

For a granular material, due to its discrete nature, various definitions of stress tensor in terms of discrete contact forces and related quantities have been proposed (Bagi, 1996).

Two approaches to this end can be found. The first approach adopts the basic definition of stress tensor by finding the average force on an arbitrary plane that cuts the packing (Jagota *et al.*, 1988). The second approach defines the volume-average stress within a finitesize domain that contains several particles (Rothenburg and Selvadurai, 1981; Kanatani, 1981; Christoffersen *et al.*, 1981). In a static condition, the second approach suggests that the definition of stress tensor should be

$$\langle \mathbf{t} \rangle = \frac{1}{V} \sum_{c} \mathbf{b}^{c} \otimes \mathbf{F}^{c}, \tag{25}$$

where V, \mathbf{F}^c , and \mathbf{b}^c are the volume of the domain in question, the contact force, and the branch vector connecting the centers of two particles in contact, respectively. The summation \sum_c is performed over all internal contacts within the domain of interest. Note that the definition (25) is also valid when both the volumetric loads and the contacting forces are taken into account (Bagi, 1999). This study will apply the definition (25) to dynamic cases by treating the inertia term as a volumetric load. The analysis is as follows.

From the continuum point of view, the linear momentum balance equation helps to express the stress tensor \mathbf{t} and its spatial gradient $\nabla \cdot \mathbf{t}$ as

$$t_{ji} = (x_j t_{ki})_{,k} - x_j t_{ki,k} = (x_j t_{ki})_{,k} - x_j (\rho \dot{v}_i - \rho f_i), \quad t_{ji,j} = (t_{ji})_{,j}, \quad (26)$$

with mass density ρ , acceleration \dot{v}_i , and specific body force f_i . Choosing a suitable domain V, the volume-average stress tensor $\langle t_{ji} \rangle$ and the volume-average stress gradient $\langle t_{ji,j} \rangle$ in this domain are

$$\langle t_{ji} \rangle = \frac{1}{V} \int_{V} \left(\left(x_j t_{ki} \right)_{,k} - x_j t_{ki,k} \right) dV = \frac{1}{V} \oint_{\partial V} n_k x_j t_{ki} dS - \frac{1}{V} \int_{V} x_j (\dot{v}_i - f_i) \rho dV, \quad (27)$$

$$\langle t_{ji,j} \rangle = \frac{1}{V} \int_{V} t_{ji,j} dV = \frac{1}{V} \oint_{\partial V} n_j t_{ji} dS.$$
(28)

For a granular assembly, if $(\mathbf{n} \cdot \mathbf{t} dS)$ corresponds to contact force \mathbf{F}^c , then, analogous to the expressions (27) and (28), the stress tensor \mathbf{t} and its divergence of a granular assembly are

$$\frac{1}{\Delta V} \sum_{(b)c} \mathbf{x}^{c} \otimes \mathbf{F}^{c} - \frac{1}{\Delta V} \sum_{i=1}^{N} m^{i} \mathbf{x}^{i} \otimes (\dot{\mathbf{v}}^{i} - \mathbf{f}^{i})$$

$$= \frac{1}{\Delta V} \left[\mathbf{x} \otimes (\mathbf{F}_{t}^{c} + m\mathbf{f}_{b} - m\dot{\mathbf{v}}) + \sum_{(b)c} \mathbf{r}^{c} \otimes \mathbf{F}^{c} - \sum_{i=1}^{N} m^{i} \boldsymbol{\xi}^{i} \otimes (\ddot{\boldsymbol{\xi}}^{i} - \mathbf{f}^{i}) \right] \rightarrow \mathbf{t}(\mathbf{x}, t), \quad (29)$$

$$\frac{1}{\Delta V} \sum_{(b)c} \mathbf{F}^c \to \nabla \cdot \mathbf{t},\tag{30}$$



Figure 2: The position of a contact point c can be decomposed by $\mathbf{x}^c = \mathbf{x} + \mathbf{r}^c$. The vector \mathbf{r}^c is the position of contact point measured from the macroelement's COM, \mathbf{x} . Two particles interact each other through a contact force \mathbf{F}^c and a possible contact couple moment \mathbf{m}^c .

where the kinematic relations (11) and (12) are employed and \mathbf{x}^c represents the contact point position. As Fig. 2 illustrates, the position of a contact point c can be decomposed through the relation: $\mathbf{x}^c = \mathbf{x} + \mathbf{r}^c$, where \mathbf{r}^c is the contact point position measured from the macroelement's COM, i.e., \mathbf{x} . In Eq. (29), $\mathbf{F}_t^c (= \sum_{(b)c} \mathbf{F}^c)$ is the total contact force acting on the macroelement and $\sum_{(b)c}$ denotes the summation over points of contacts with the boundary of the macroelement. The equivalent body force per unit mass \mathbf{f}_b is defined as

$$m\mathbf{f}_b = \sum_{i=1}^N m^i \mathbf{f}^i$$

Thus, the balance of linear momentum for a macroelement implies

$$\mathbf{F}_t^c + m\mathbf{f}_b - m\dot{\mathbf{v}} = \mathbf{0},\tag{31}$$

which helps to reduce Eq. (29) to

$$\sum_{i=1}^{N} \frac{1}{\Delta V} \left[\sum_{(b)c} \mathbf{r}^{c} \otimes \mathbf{F}^{c} - \sum_{i=1}^{N} m^{i} \boldsymbol{\xi}^{i} \otimes (\ddot{\boldsymbol{\xi}}^{i} - \mathbf{f}^{i}) \right] \to \mathbf{t}(\mathbf{x}, t).$$
(32)

In the absence of acceleration and volumetric (body) forces, the discrete-continuum correspondence (32) for the stress tensor becomes

$$\frac{1}{\Delta V} \sum_{(b)c} \mathbf{r}^c \otimes \mathbf{F}^c \to \mathbf{t}(\mathbf{x}, t).$$
(33)

If the volumetric forces \mathbf{f}^i are the same for all particles *i* such as gravity force, the discrete formulation of the stress tensor in Eq. (33) still holds for static conditions (Bagi, 1999). However, in dynamic conditions, Eq. (32) shows that the discrete formulation of stress tensor for a granular assembly involves a contribution due to relative accelerations of particles in a macroelement. It should be emphasized that, since relative accelerations rather than absolute accelerations of particles are involved in the general expression of the stress tensor, the form of (32) is not changed when we alter the coordinate system, i.e., the stress expression satisfies the objectivity condition.

In addition, the discrete formulation of stress tensor in Eq. (32) can be further modified by taking into account the balance of linear momentum for a single particle *i*, i.e., $m^i \dot{\mathbf{v}}^i = m^i \mathbf{f}^i + \sum_{(i)c} \mathbf{F}^{(i)c}$. Accordingly, Eq. (29) can be transformed into

$$\frac{1}{\Delta V} \sum_{(b)c} \mathbf{x}^{c} \otimes \mathbf{F}^{c} - \frac{1}{\Delta V} \sum_{i=1}^{N} m^{i} \mathbf{x}^{i} \otimes (\dot{\mathbf{v}}^{i} - \mathbf{f}^{i})$$
$$= \frac{1}{\Delta V} \left[\sum_{(b)c} \mathbf{x}^{c} \otimes \mathbf{F}^{c} - \sum_{i}^{N} \mathbf{x}^{i} \otimes \left(\sum_{(i)c} \mathbf{F}^{(i)c} \right) \right] \to \mathbf{t}(\mathbf{x}, t),$$

where $\sum_{(i)c}$ denotes the summation over contact points for the particle *i*, and $\mathbf{F}^{(i)c}$ stands for the contact forces on the *i*-particle. Bagi's (1999) definition of the branch vector is $\mathbf{b}^c = \mathbf{x}^i - \mathbf{x}^j$ in the inside of the macroelement, and is $\mathbf{b}^c = \boldsymbol{\kappa}^c$ for those faces on the boundary, where $\boldsymbol{\kappa}^c$ refers to those position vectors measured from the centers of mass of boundary particles to their contact points with boundary. With the aid of this definition, the standard expression of stress tensor $(1/\Delta V) \sum_c \mathbf{b}^c \otimes \mathbf{F}^c$ is readily recovered, where it should be noted that the sum is over all contacts, i.e., internal and boundary. This derivation manifests that in terms of the branch vector the discrete formulation of stress tensor does not involve body forces and particle accelerations.

It is evident that the balance equation of linear momentum helps to determine the discrete formulation of stress tensor for a granular material. Similarly, other balance equations will help to formulate the continuum expressions of surface-type related quantities, such as the divergences of couple stress tensor and heat flux. The following section continues this discussion.

4 Macroelement-particle-based balance equations

This study uses an RVE in the reference configuration to identify a macroelement, then proposes the macroelement-particle treatment to define macroscopic quantities, which are

assigned to the macroelement's COM. With this modeling, various mechanical balance equations in a macroelement can be transformed into their corresponding continuum limits through the following analysis.

4.1 Mass balance equation

Since a macroelement is a material element, the total mass of a macroelement should be conserved. Using the definition of mass density in Eq. (13), we calculate

$$\frac{d}{dt}\left(\frac{m}{\Delta V}\right) = m\frac{d}{dt}\left(\frac{1}{\Delta V}\right).$$
(34)

The volume change of a macroelement can be caused by particle rearrangement and particle compressibility in this macroelement. Because the continuum limit of the time rate of change of ΔV can be found to be $\Delta V(\nabla \cdot \mathbf{v})$, the continuum counterpart of Eq. (34) is reduced to the standard continuum expression of the mass balance equation:

$$\frac{d\rho}{dt} + \rho \nabla \cdot \mathbf{v} = 0. \tag{35}$$

4.2 Microinertia balance equation

In the micromorphic modeling of a granular material, the microinertia density $\rho \mathbf{i}$ characterizes particle arrangement in a macroelement. Taking the total time derivative of the discrete analogy of $\rho \mathbf{i} dV$, given in Eq. (23), yields

$$\frac{d}{dt}\left(\sum_{i=1}^{N}m^{i}\boldsymbol{\xi}^{i}\otimes\boldsymbol{\xi}^{i}\right)=\sum_{i=1}^{N}m^{i}\boldsymbol{\xi}^{i}\otimes\dot{\boldsymbol{\xi}}^{i}+\left(\sum_{i=1}^{N}m^{i}\boldsymbol{\xi}^{i}\otimes\dot{\boldsymbol{\xi}}^{i}\right)^{T}.$$
(36)

To describe the motion of particles relative to the macroelement's COM, this study denotes by α the orbital angular momentum tensor per unit volume, i.e.,

$$\frac{1}{\Delta V} \sum_{i=1}^{N} m^{i} \boldsymbol{\xi}^{i} \otimes \dot{\boldsymbol{\xi}}^{i} = \langle \rho \boldsymbol{\alpha} \rangle \to \rho(\mathbf{x}, t) \boldsymbol{\alpha}(\mathbf{x}, t).$$
(37)

Thus, it follows from Eq. (36) that the continuum counterpart of microinertia balance equation is

$$\frac{d\mathbf{i}}{dt} - \boldsymbol{\alpha} - \boldsymbol{\alpha}^T = \mathbf{0}.$$
(38)

4.3 Linear momentum balance equation

While deriving the discrete expression of stress tensor in the previous section, the discrete balance equation of linear momentum for a macroelement has been proposed, i.e., Eq. (31).

By means of the discrete-continuum correspondences in Eqs. (13) and (30), the linear momentum balance equation at a macroscopic point is directly obtained from the continuum limit of Eq. (31):

$$\rho \frac{d\mathbf{v}}{dt} - \nabla \cdot \mathbf{t} - \rho \mathbf{f}_b = \mathbf{0}. \tag{39}$$

4.4 Angular momentum balance equation (without particle spin)

In classical dynamics, it is well-known that the Euler equation governs angular momentum evolution of a system, and its vectorial form reads

$$\frac{d\mathbf{H}_p}{dt} = \mathbf{M}_p,\tag{40}$$

with the angular momentum \mathbf{H}_p and moment \mathbf{M}_p relative to a point p. This equation is valid only when one of the following conditions is satisfied: (i) the point p is the system's COM; (ii) the point p is fixed in space or moves with a constant velocity; and (iii) the point p is accelerating toward or away from the COM. Let the point p be the fixed origin o of the Cartesian coordinate and choose the system as a macroelement. Without taking particle spin and contact couple moment into account, the angular momentum balance equation of a macroelement should be

$$\frac{d\mathbf{H}_o}{dt} = \mathbf{M}_o^{body} + \mathbf{M}_o^{sur},\tag{41}$$

where \mathbf{H}_o , \mathbf{M}_o^{body} , and \mathbf{M}_o^{sur} are respectively the angular momentum and two moments contributed from body and surface forces. They are expressed as

$$\mathbf{H}_{o} = \sum_{i=1}^{N} m^{i} \mathbf{x}^{i} \times \mathbf{v}^{i}, \tag{42}$$

$$\mathbf{M}_{o}^{body} = \sum_{i=1}^{N} m^{i} \mathbf{x}^{i} \times \mathbf{f}^{i}, \tag{43}$$

$$\mathbf{M}_{o}^{sur} = \sum_{(b)c} \mathbf{x}^{c} \times \mathbf{F}^{c}.$$
(44)

Substituting Eqs. (42), (43), and (44) into (41) leads to the discrete formulation of angular momentum balance equation:

$$\frac{d}{dt} \left(\sum_{i=1}^{N} m^{i} \boldsymbol{\xi}^{i} \times \dot{\boldsymbol{\xi}}^{i} \right) = \sum_{i=1}^{N} m^{i} \boldsymbol{\xi}^{i} \times \mathbf{f}^{i} + m \mathbf{x} \times (\mathbf{f}_{b} - \dot{\mathbf{v}}) + \sum_{(b)c} \mathbf{x}^{c} \times \mathbf{F}^{c}.$$
(45)

In this derivation, the angular momentum (42) is simplified by the two identities

$$\sum_{i=1}^{N} m^{i} \mathbf{x} \times \dot{\boldsymbol{\xi}}^{i} = \mathbf{0}, \tag{46}$$

$$\sum_{i=1}^{N} m^{i} \boldsymbol{\xi}^{i} \times \mathbf{v} = \mathbf{0}, \tag{47}$$

which are derived by accounting for the macroelement's COM coordinate system and by using Eqs. (11) and (12).

To obtain the continuum counterpart of the discrete angular momentum balance equation, we transform each term in Eq. (45) from the discrete expression to its continuum analogy. First, with the help of mass conservation and Eq. (37), we can find that

$$\frac{1}{\Delta V}\frac{d}{dt}\left(\sum_{i=1}^{N}m^{i}\boldsymbol{\xi}^{i}\times\dot{\boldsymbol{\xi}}^{i}\right) = \frac{d}{dt}\left(\frac{1}{\Delta V}\sum_{i=1}^{N}m^{i}\boldsymbol{\xi}^{i}\times\dot{\boldsymbol{\xi}}^{i}\right) - \frac{d}{dt}\left(\frac{1}{\Delta V}\right)\sum_{i=1}^{N}m^{i}\boldsymbol{\xi}^{i}\times\dot{\boldsymbol{\xi}}^{i} \to \rho\mathbf{e}\cdot\dot{\boldsymbol{\alpha}},\tag{48}$$

where \mathbf{e} is the third-order permutation symbol. Second, recalling Eq. (15), we arrive at

$$\frac{1}{\Delta V} \sum_{i=1}^{N} m^{i} \boldsymbol{\xi}^{i} \times \mathbf{f}^{i} \to -\rho \mathbf{e} \cdot \mathbf{l}.$$
(49)

Third, from Eqs. (30) and (31), we obtain the correspondence:

$$\frac{m}{\Delta V} \mathbf{x} \times (\mathbf{f}_b - \dot{\mathbf{v}}) \to -\mathbf{x} \times (\nabla \cdot \mathbf{t}).$$
(50)

Fourth, expressing the continuum limit of the moment from surface force and using the Cauchy first principle $\mathbf{T}^{(n)} = \mathbf{n} \cdot \mathbf{t}$ and the divergence theorem leads to

$$\frac{1}{\Delta V} \sum_{(b)c} \mathbf{x}^{c} \times \mathbf{F}^{c} \to \frac{1}{V} \oint_{\partial V} \mathbf{y} \times \mathbf{T}^{(n)} dS_{y} = \frac{1}{V} \oint_{\partial V} (\mathbf{x} + \boldsymbol{\zeta}) \times \mathbf{T}^{(n)} dS_{y}$$
$$= \frac{1}{V} \mathbf{x} \times \oint_{\partial V} \mathbf{T}^{(n)} dS_{y} - \frac{1}{V} \mathbf{e} : \int_{V} \nabla_{y} \cdot (\mathbf{t} \otimes \boldsymbol{\zeta}) dV_{y}, \tag{51}$$

where \mathbf{y} is a dummy coordinate and $\mathbf{T}^{(n)}$ is the traction on the surface element dS_y . The position vector of a point, \mathbf{y} , within the volume V can be expressed by $\mathbf{y} = \mathbf{x} + \boldsymbol{\zeta}$, where \mathbf{x} is the position of the center of mass of V, and $\boldsymbol{\zeta}$ is the coordinate relative to the mass center. The first term on the right hand side of Eq. (51) represents the moment produced by the total outer contact forces of the macroelement, and the expression of the second term suggests that the definitions of the volume-averages of the couple stress $\boldsymbol{\mu}$ and its divergence can be

$$\langle \mu_{ijk} \rangle = \frac{1}{V} \int_{V} t_{ij} \zeta_k \, dV, \tag{52}$$

$$\langle \mu_{ijk,i} \rangle = \frac{1}{V} \int_{V} (t_{ij}\zeta_k)_{,i} \, dV.$$
(53)

Unlike the discrete formulation of stress tensor (32), couple stress μ is a higher-order stress and is defined under the continuum framework. Equations (52) and (53) show that the definition of μ involves stress tensor **t**, so the discrete formulation of couple stress tensor, if it is strongly required, is still undetermined in this study.

Now, by virtue of Eqs. (48), (49), (50), (51), and (53), the continuum counterpart of the discrete angular momentum balance equation (45):

$$\mathbf{e}: \left(\rho \frac{d\boldsymbol{\alpha}}{dt} + \rho \mathbf{l} + \nabla \cdot \boldsymbol{\mu}\right) = \mathbf{0},\tag{54}$$

is readily obtained. In order to be compatible with Eq. (7) in the microcontinuum field theory, we introduce a symmetric tensor $\boldsymbol{\tau}$, called microstress tensor, which helps to extend the vectorial balance equation of angular momentum (54) to a tensorial equation (Eringen, 1999; Chen, 2007)

$$\rho \frac{d\boldsymbol{\alpha}}{dt} + \rho \mathbf{l} + \nabla \cdot \boldsymbol{\mu} = \boldsymbol{\tau}.$$
(55)

This microstress tensor, or called microstress average, is a result of the stresses averaged over all particles in the inner structure of the macroelement from the microscopic atomic viewpoint (Chen *et al.*, 2004). The issue of finding the discrete formulation of the microstress tensor, however, awaits further study.

In addition, two differences can be observed when we compare Eq. (55) with the balance equation of momentum moment (7). The first difference is that there is no stress tensor term in Eq. (55), and the second is that the spin inertia per unit mass $\boldsymbol{\sigma}$ in Eq. (7), defined as $(1/\Delta V) \sum_{i=1}^{N} m^i \ddot{\boldsymbol{\xi}}^i \otimes \boldsymbol{\xi}^i \to \rho \boldsymbol{\sigma}$, is replaced by the rate of orbital angular momentum tensor $\dot{\boldsymbol{\alpha}}$. The reason for the first difference lies in the fact that the stress tensor in our micromorphic modeling is symmetric, leading to its vanishing in Eq. (54). The symmetry can be readily verified by performing the operation " \mathbf{e} :" on the discrete formulation of stress tensor (32), i.e.,

$$\frac{1}{\Delta V} \left[\sum_{(b)c} \mathbf{r}^c \times \mathbf{F}^c - \sum_{i=1}^N m^i \boldsymbol{\xi}^i \times (\ddot{\boldsymbol{\xi}}^i - \mathbf{f}^i) \right] \to \mathbf{e} : \mathbf{t}$$

from which we obtain $\mathbf{e} : \mathbf{t} = \mathbf{0}$ by using the angular momentum balance equation (45). This fact is also compatible with Bagi's (1999) conclusion that the stress tensor in the volume-average expression is symmetric when grains are in moment equilibrium. As for the second difference, we notice that

$$\frac{1}{\Delta V} \sum_{i=1}^{N} m^{i} \dot{\boldsymbol{\xi}}^{i} \otimes \dot{\boldsymbol{\xi}}^{i} = \left\{ \frac{d}{dt} \left(\frac{1}{\Delta V} \sum_{i=1}^{N} m^{i} \boldsymbol{\xi}^{i} \otimes \dot{\boldsymbol{\xi}}^{i} \right) - \frac{d}{dt} \left(\frac{1}{\Delta V} \right) \sum_{i=1}^{N} m^{i} \boldsymbol{\xi}^{i} \otimes \dot{\boldsymbol{\xi}}^{i} \right\} - \frac{1}{\Delta V} \sum_{i=1}^{N} m^{i} \boldsymbol{\xi}^{i} \otimes \ddot{\boldsymbol{\xi}}^{i}$$

which yields the following correspondence:

$$\frac{1}{\Delta V} \sum_{i=1}^{N} m^{i} \dot{\boldsymbol{\xi}}^{i} \otimes \dot{\boldsymbol{\xi}}^{i} \to \rho \dot{\boldsymbol{\alpha}} - \rho \boldsymbol{\sigma}^{T}.$$
(56)

The symmetry of the left-hand side indicates that $\mathbf{e} : \dot{\boldsymbol{\alpha}} = \mathbf{e} : \boldsymbol{\sigma}^T$, which explains the second difference.

4.5 Angular momentum balance equation (with particle spin)

The total angular momentum in a macroelement is composed of two parts: the orbital and spin angular momenta. The spin angular momentum describes particle rotation and the orbital angular momentum depicts particle motion relative to the macroelement's COM. The original derivation of the microcontinuum field theory does not provide the possibility of the latter part. Taking the spin contribution into account, the total angular momentum per unit mass is

$$\mathbf{S} = \mathbf{s} + \mathbf{e} : \boldsymbol{\alpha}. \tag{57}$$

Then, analogous to Eq. (45), the total discrete formulation of angular momentum balance equation (41) becomes

$$\frac{d}{dt} \left(\sum_{i=1}^{N} m^{i} (\boldsymbol{\xi}^{i} \times \dot{\boldsymbol{\xi}}^{i} + \mathbf{s}^{i}) \right) - \sum_{(b)c} \mathbf{x}^{c} \times \mathbf{F}^{c} - \sum_{(b)c} \mathbf{m}^{c} = \sum_{i=1}^{N} m^{i} (\boldsymbol{\xi}^{i} \times \mathbf{f}^{i} + \mathbf{g}^{i}) + m\mathbf{x} \times (\mathbf{f}_{b} - \dot{\mathbf{v}}), \quad (58)$$

where the newly introduced spin-related quantities \mathbf{m}^{c} and $m^{i}\mathbf{g}^{i}$ represent the local surface couple moment acting on contact point c and the body couple for the particle i, respectively. Equation (16) and the following two correspondences:

$$\frac{1}{\Delta V} \sum_{i=1}^{N} m^{i} \mathbf{g}^{i} \to \rho \mathbf{g}(\mathbf{x}, t), \tag{59}$$

$$\frac{1}{\Delta V} \sum_{(b)c} \mathbf{m}^c \to \frac{1}{V} \oint_{\partial V} \mathbf{m} dS = \frac{1}{V} \int_V \nabla \cdot \mathbf{c} dV, \tag{60}$$

present the discrete-continuum relations for the three additional spin contributions, where the continuum counterpart of \mathbf{m}^c is denoted by $\mathbf{m}dS$. This study further assumes that the local surface couple moment \mathbf{m} plays a role similar to the traction in continuum mechanics such that the analogous Cauchy first principle is satisfied. To be explicit, the relation $\mathbf{m} = \mathbf{n} \cdot \mathbf{c}$ holds, in which \mathbf{c} is the local couple stress tensor. Equations (59) and (60) express the two discrete-continuum correspondences for the local body couple per unit mass \mathbf{g} and the divergence of local couple stress $\nabla \cdot \mathbf{c}$. Setting the volume V as a macroelement

and assigning the volume-average of $\nabla \cdot \mathbf{c}$ at the point \mathbf{x} , the continuum counterpart of the balance equation of angular momentum with particle spin being included can be deduced from Eq. (58) to be

$$\mathbf{e}: \left(\rho \frac{d\boldsymbol{\alpha}}{dt} + \rho \mathbf{l} + \nabla \cdot \boldsymbol{\mu}\right) + \mathbf{k} = \mathbf{0},\tag{61}$$

where

$$\mathbf{k} = \rho \frac{d\mathbf{s}}{dt} - \rho \mathbf{g} - \nabla \cdot \mathbf{c}, \tag{62}$$

is a spin-related quantity. Using the two abbreviated notations $\mathbf{C} = \mathbf{c} - \boldsymbol{\mu} : \mathbf{e}$ and $\mathbf{G} = \mathbf{g} - \mathbf{l} : \mathbf{e}$, Eq. (61) can be written as

$$\rho \frac{d\mathbf{S}}{dt} - \nabla \cdot \mathbf{C} - \rho \mathbf{G} = \mathbf{0}.$$
(63)

4.6 Energy balance equation

The total energy at a point \mathbf{x} in this macroelement-particle treatment is comprised of the kinetic energy of the macroelement's COM, the kinetic energy relative to the macroelement's COM, the spin energy, and the internal energy. Equations (18) and (19) show the discrete formulation of the total energy of a macroelement. The energy balance law states that the change of a system's total energy is balanced by mechanical work and heat input to the system. Applying this law to a macroelement immediately leads to

$$\frac{d}{dt} \left[\frac{1}{2} m \mathbf{v} \cdot \mathbf{v} + \sum_{i=1}^{N} m^{i} (\varepsilon^{i} + \frac{1}{2} \dot{\boldsymbol{\xi}}^{i} \cdot \dot{\boldsymbol{\xi}}^{i} + \frac{1}{2} \mathbf{s}^{i} \cdot \boldsymbol{\theta}^{i^{-1}} \cdot \mathbf{s}^{i}) \right]$$

$$= W_{1} + W_{2} + W_{3} + W_{4} + Q_{1} + Q_{2},$$
(64)

where W_1 , W_2 , W_3 , and W_4 are the four types of mechanical powers done by body force, surface force, body couple, and surface couple, respectively. Q_1 and Q_2 are the energy supply rates due to radiation and heat conduction. The discrete formulations of the four mechanical powers are

$$W_1 = \sum_{i=1}^N m^i \mathbf{f}^i \cdot \mathbf{v}^i = m\mathbf{f}_b \cdot \mathbf{v} + \sum_{i=1}^N m^i \mathbf{f}^i \cdot \dot{\boldsymbol{\xi}}^i, \tag{65}$$

$$W_2 = \sum_{(b)c} \mathbf{F}^c \cdot \mathbf{v}^c, \tag{66}$$

$$W_3 = \sum_{i=1}^{N} m^i \mathbf{g}^i \cdot \hat{\mathbf{s}}^i = m \mathbf{g} \cdot \hat{\mathbf{s}} + \sum_{i=1}^{N} m^i \mathbf{g}^i \cdot \Delta(\hat{\mathbf{s}}^i),$$
(67)

$$W_4 = \sum_{i,c} \mathbf{m}^{i,c} \cdot \hat{\mathbf{s}}^i.$$
(68)

Here, $\hat{\mathbf{s}}^{i} (= \boldsymbol{\theta}^{i^{-1}} \cdot \mathbf{s}^{i})$ is the angular velocity of particle *i*, with the moment of inertia $\boldsymbol{\theta}^{i^{-1}}$ $\hat{\mathbf{s}}$ is the average angular velocity of the macroelement. The difference of angular velocity $\Delta(\hat{\mathbf{s}}^i)$ is defined by $\Delta(\hat{\mathbf{s}}^i) = \hat{\mathbf{s}}^i - \hat{\mathbf{s}}$. $\mathbf{m}^{i,c}$ represents the local couple moment exerting on the contact point c of particle i. To obtain the continuum limit of the four mechanical powers, this study finds the following two correspondences:

$$\frac{1}{\Delta V} \sum_{(b)c} \mathbf{F}^c \cdot \mathbf{v}^c \to \frac{1}{V} \oint_{\partial V} (\mathbf{n} \cdot \mathbf{t}) \cdot \mathbf{v} \, dS = \frac{1}{V} \int_V \left(\mathbf{t}^T : \nabla \mathbf{v} + (\nabla \cdot \mathbf{t}) \cdot \mathbf{v} \right) \, dV, \tag{69}$$

$$\frac{1}{\Delta V} \sum_{i,c} \mathbf{m}^{i,c} \cdot \hat{\mathbf{s}}^i \to \frac{1}{V} \oint_{\partial V} (\mathbf{n} \cdot \mathbf{c}) \cdot \hat{\mathbf{s}} \, dS = \frac{1}{V} \int_{V} \left(\mathbf{c}^T : \nabla \hat{\mathbf{s}} + (\nabla \cdot \mathbf{c}) \cdot \hat{\mathbf{s}} \right) \, dV, \tag{70}$$

where use has made of the divergence theorem and Eq. (62).

Moreover, the discrete expressions of the two energy supply rates are

$$Q_1 = \sum_{i=1}^N m^i r^i, \tag{71}$$

$$Q_2 = -\sum_{(b)c} q^c, \tag{72}$$

where r^i is the energy radiation rate per unit mass for particle *i*. Here, it is assumed that heat only conducts through contact point between two particles, and q^c represents the heat outflow through the contact point c per unit time. The continuum limits of the two energy supply rates, i.e., the specific heat supply r and the divergence of heat flux $\nabla \cdot \mathbf{q}$, are found to be

$$\frac{1}{\Delta V} \sum_{i=1}^{N} m^{i} r^{i} = \langle \rho r \rangle \to \rho(\mathbf{x}, t) r(\mathbf{x}, t),$$
(73)

$$\frac{1}{\Delta V} \sum_{(b)c} q^c \to \frac{1}{V} \oint_{\partial V} n_k q_k dS = \frac{1}{V} \int_V q_{k,k} dV = \langle q_{k,k} \rangle \to q_{k,k}(\mathbf{x},t).$$
(74)

It is worthwhile to mention that the discrete formulation of heat flux q (Babic, 1997) can be suggested to be

$$\langle q_k \rangle = \frac{1}{V} \int_V \left((x_k q_l)_{,l} - x_k q_{l,l} \right) dV = \frac{1}{V} \left(\oint_{\partial V} x_k n_l q_l dS - \int_V x_k q_{l,l} dV \right)$$
$$\rightarrow \frac{1}{\Delta V} \left(\sum_{(b)c} x_k^c q^c - \sum_{i=1}^N x_k^i q^{ic} \right) = \frac{1}{\Delta V} \sum_c b_k^c q^c, \tag{75}$$

where \mathbf{b}^{c} is the branch vector as mentioned in Sec. 3. In this derivation we have assumed that Eq. (74) holds for a single particle, i.e., $q_{k,k}^i \Delta V_i \to \sum q^{ic}$, with q^{ic} being the rate of heat outflow through the contact point c of the particle i.

Finally, the balance equation of internal energy, which is obtained from Eq. (64) by accounting for Eqs. (39), (62), (69), (70), (73), and (74), is written as

$$\rho \dot{\varepsilon}_e - \mathbf{t}^T : \nabla \mathbf{v} - \mathbf{c}^T : \nabla \hat{\mathbf{s}} + \mathbf{k} \cdot \hat{\mathbf{s}} + \nabla \cdot \mathbf{q} - \rho r_e = 0,$$
(76)

where ε_e and r_e are the equivalent internal energy and the equivalent energy supply, respectively, and their discrete counterparts are

$$\frac{1}{\Delta V} \sum_{i=1}^{N} m^{i} (\varepsilon^{i} + \frac{1}{2} \dot{\boldsymbol{\xi}}^{i} \cdot \dot{\boldsymbol{\xi}}^{i} + \frac{1}{2} \Delta \mathbf{s}^{i} \cdot \theta^{i^{-1}} \cdot \Delta \mathbf{s}^{i}) = \langle \rho \varepsilon_{e} \rangle \to \rho(\mathbf{x}, t) \varepsilon_{e}(\mathbf{x}, t),$$
(77)

$$\frac{1}{\Delta V} \sum_{i=1}^{N} m^{i} \left(r^{i} + \mathbf{f}^{i} \cdot \dot{\boldsymbol{\xi}}^{i} + \mathbf{g}^{i} \cdot \Delta(\hat{\mathbf{s}}^{i}) \right) = \langle \rho r_{e} \rangle \to \rho(\mathbf{x}, t) r_{e}(\mathbf{x}, t).$$
(78)

Comparing Eq. (76) and the energy balance equation in the microcontinuum field theory shown in Section 2 reveals that the macroelement-particle-based equation is more general in describing the evolution of a granular material within a continuum framework. Two reasons for this are as follows. (i) This modeling does not introduce the gyration tensor $\boldsymbol{\nu}$, which describes the motion of a microelement relative to the macroelement's COM. Therefore, the condition $\dot{\boldsymbol{\xi}} = \boldsymbol{\nu} \cdot \boldsymbol{\xi}$, which is the requirement for a micromorphic continuum of grade one, is not necessary. (ii) This modeling takes into account particle spin represented by local spin, which is missing in the original microcontinuum theory. The macroelement-particle-based balance equation can reduce to Eq. (8) if the two requirements are satisfied: (i) the particle spin is discarded, and (ii) the condition $\dot{\boldsymbol{\xi}} = \boldsymbol{\nu} \cdot \boldsymbol{\xi}$ is adopted, i.e., every $\boldsymbol{\xi}$ in a macroelement has the same gyration. This reduction involves the following two operations:

$$\frac{d}{dt}\left(\sum_{i=1}^{N} (\frac{1}{2}m^{i}\dot{\boldsymbol{\xi}}^{i} \cdot \dot{\boldsymbol{\xi}}^{i})\right) = \left[(\boldsymbol{\nu} \cdot \boldsymbol{\nu} + \dot{\boldsymbol{\nu}}) \cdot \left(\sum_{i=1}^{N} (m^{i}\boldsymbol{\xi}^{i} \otimes \boldsymbol{\xi}^{i})\right) \right] : \boldsymbol{\nu}, \tag{79}$$

$$\sum_{i=1}^{N} m^{i} \mathbf{f}^{i} \cdot \dot{\boldsymbol{\xi}}^{i} = \left(\sum_{i=1}^{N} m^{i} \mathbf{f}^{i} \otimes \boldsymbol{\xi}^{i}\right) : \boldsymbol{\nu}, \tag{80}$$

and the definitions of energy supply r and equivalent heat flux \mathbf{q}_e in the form of

$$r = r_e - \mathbf{l} : \boldsymbol{\nu},\tag{81}$$

$$\mathbf{q}_e = \mathbf{q} + \boldsymbol{\mu} : \boldsymbol{\nu}. \tag{82}$$

Hence, Eq. (76) is simplified to

$$\rho \frac{d\varepsilon}{dt} - \mathbf{t}^T : \nabla \mathbf{v} - \boldsymbol{\tau} : \boldsymbol{\nu} - \boldsymbol{\mu} : \nabla \boldsymbol{\nu} + \nabla \cdot \mathbf{q}_e - \rho r = 0,$$
(83)

which is in the form of the internal energy equation (8) of a micromorphic continuum of grade one.

4.7 Entropy balance equation

For a complete description of thermodynamical phenomena, one should introduce the entropy as an additional variable to account for the irreversibility of a system (Jou *et al.*, 2001). Let the entropy Λ be an extensive quantity and its time rate of change be written as

$$\frac{d\Lambda}{dt} = \frac{d^e\Lambda}{dt} + \frac{d^i\Lambda}{dt},\tag{84}$$

where $d^e \Lambda/dt$ represents the rate of entropy exchanged from the system boundary. If we disregard the entropy supply, then $d^i \Lambda/dt$ denotes the entropy production generated inside the system. According to the second law of thermodynamics, $d^i \Lambda/dt$ must be a non-negative quantity if the second law also holds at any macroscopic point. For a macroelement, the explicit form of Eq. (84) gives

$$\frac{d}{dt}\left(\sum_{i=1}^{N}m^{i}\eta^{i}\right) = -\sum_{(b)c}\Phi^{c} + \sum_{i=1}^{N}\gamma^{i},$$
(85)

where η^i , Φ^c , and γ^i are the specific entropy for particle *i*, the entropy outflow through the contact point *c* per unit time, and the entropy production, respectively. Given that the continuum limits of the two macroscopic fields, namely, the entropy flux Φ and the entropy production per unit volume γ , can be obtained from their corresponding discrete counterparts:

$$\frac{1}{\Delta V} \sum_{(b)c} \Phi^c \to \frac{1}{V} \oint_{\partial V} n_k \Phi_k dS = \frac{1}{V} \int_V \Phi_{k,k} dV = \langle \Phi_{k,k} \rangle \to \Phi_{k,k}(\mathbf{x},t), \tag{86}$$

$$\frac{1}{\Delta V} \sum_{i=1}^{N} \gamma^{i} = \langle \gamma \rangle \to \gamma(\mathbf{x}, t), \tag{87}$$

the continuum correspondence of Eq. (85) takes the form

$$\rho \frac{d\eta}{dt} + \nabla \cdot \mathbf{\Phi} - \gamma = 0, \tag{88}$$

which is exactly the balance equation of entropy (9).

5 Concluding remarks

This paper discusses the modeling of a discrete granular system as a micromorphic continuum by using an RVE to identify a macroelement and treating a single particle as a microelement. The relative position vectors of particles in a macroelement are interpreted as internal degrees of freedom at a macroscopic point. Proposing the macroelement-particle treatment

helps to construct a bridge between the discrete and continuum quantities for a granular material. After specifying the volume of a macroelement to determine the continuum field quantities from their discrete counterparts, this study formulates the discrete expressions of balance equations in a macroelement. The derived discrete balance equations are Eqs. (34), (36), (31), (58), (64), and (85). Then these equations are transformed into their continuum counterparts, i.e., Eqs. (35), (38), (39), (63), (76), and (88), which govern the time evolutions for the field quantities (ρ , **i**, **v**, α , **s**, ϵ_e , η). Disregarding the entropy equation, the external sources in these equations are (\mathbf{f}_b , \mathbf{l} , \mathbf{g} , r_e), and other quantities (\mathbf{t} , $\boldsymbol{\mu}$, \mathbf{c} , \mathbf{q}) should be determined by proposing additional constitutive relations. A slight difference between our derived continuum equations and those in the microcontinuum theory can be found. That is, our system rotation consists of two parts. The reason for this is that choosing a granular particle as a microelement leads to microelement spins.

The volume-type field quantities are readily constructed by performing the discretecontinuum analogy. However, surface-type quantities can not be obtained in such a straightforward manner. The general discrete expression for stress tensor of granular materials is obtained with the help of linear momentum balance equation, and we show that this expression involves not only the standard expression in a static condition, $(1/\Delta V) \sum_{(b)c} \mathbf{r}^c \otimes \mathbf{F}^c$, but also the contributions due to specific body forces and particle differences in acceleration. Furthermore, we show that the stress formulation can be expressed as $(1/\Delta V) \sum_c \mathbf{b}^c \otimes \mathbf{F}^c$ while introducing the branch vector \mathbf{b}^c , and the stress tensor is symmetric by accounting for the balance of angular momentum.

This macroelement-particle treatment has three major advantages, listed as follows. First, this modeling presents detailed information on particle arrangement at a macroscopic point that other continuum mechanical approaches cannot reach. Second, this modeling connects the theory of micromechanics (Nemat-Nasser and Hori, 1993) and the microcontinuum field theory in two ways. On the one hand, it drives the study of micromechanics to dynamic applications and, on the other hand, it extends the study of a microcontinuum to a discrete system. The third advantage of this modeling is that it offers a convenient way to link discrete and continuum quantities of a granular material. It finds continuum field quantities by taking continuum analogies of corresponding discrete quantities. Based on this modeling, we can formulate the local form of balance equations for a granular continuum, i.e., balance equations of mass, microinertia, linear momentum, angular momentum, energy, and entropy, from their discrete balance equations for a macroelement.

Furthermore, it has been shown that a micromorphic continuum is endowed with three

types of internal deformation at every macroscopic point, namely, rotational, dilatancy, and shearing. The three types of deformation can be mathematically characterized by the antisymmetric part, the bulk symmetric part, and the deviatoric symmetric part of microcontinuum field quantities (Chen and Lan, 2008). This micromorphic modeling provides a more general understanding of granular dynamics in that it can not only be reduced to the micropolar modeling of a granular assembly (Kanatani, 1979; Chang and Ma, 1991) by just considering the rotational degree of freedom, but it can also be simplified to the Goodman-Cowin theory (1972), where the dilatant effect at a macropoint for granular materials is taken into account (Chen and Lan, 2008).

Finally, we discuss some issues which remain unresolved. First, kinematic variables used in this dynamic study of a discrete granular system are position vector, velocity vector, acceleration vector, and angular velocity vector. However, this study does not discuss strain measure, which is the dominant kinematic variable in a quasi-static case and an essential quantity in constitutive analysis. This topic requires further investigation. Second, this study presents a simple derivation of continuum quantities for a granular assembly using discrete-continuum correspondence. The detailed discussion on space and time continuity for these continuum quantities is not addressed here. Our ensuing study will account for the weighting function around the space point \mathbf{x} and time t (Zhu and Yu, 2002) to provide a more precise micromorphic continuum description. Third, As for a real application of the micromorphic model to granular materials, thorough studies on the specification of suitable boundary conditions and the determination of constitutive relations are urgently required.

Introducing this macroelement-particle treatment, an advanced perspective on a granular material might be proposed: this material could be conceived as a micromorphic medium of multi-grade N. The number N is the particle number in a macroelement, and is not a constant in space and time. Although the general theory for a micromorphic medium of grade N is yet to be developed, a simplification has been made of the grade one theory and serves to present valuable information about mechanical properties of a granular medium.

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