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On virtual work and stress in granular media

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Abstract

A granular medium can be treated as an equivalent continuum. Appropriate representative stresses can be derived from the virtual work principle. However, the expression of virtual work is not unique and therefore may lead to different results of stress expressions in terms of discrete quantities—contact forces, contact moments, and branch vectors. In this paper, we introduced a generalized expression of virtual work that includes the restriction of boundary conditions. To show the advantages of the current expression, the virtual work expression is applied to derive expressions for stress, couple stress, a higher-order stress, and the stress moment. A distinction is made between the average stress within a granular volume and the representative stress that is conjugate with the representative strain of the volume. The current work is compared with that of [International Journal of Solids and Structures 38 (2) (2001) 353–367], and the current stress expressions are shown to satisfy three essential conditions of a stress measure.

Keywords: Granular material; Virtual work; Stress; Couple stress

1. Introduction

Stress at a material point is a continuum concept associated with infinitesimal regions. Because a granular material is highly heterogeneous, consisting of particles and voids, the stress field based on infinitesimal regions is not only highly non-uniform but also discontinuous across the boundaries of solid particles and voids. In order to preserve the notion of a continuum, we alter the viewing scale. Instead of an infinitesimal region, the stress at a material point is now defined as the representative stress of a finite volume of material

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associated with the material point. The finite volume should contain a sufficient number of particles such that the material is statistically homogeneous and that the stress defined in this manner is continuous in this medium. The study and modeling of granular materials require, therefore, a means of determining the representative stress of a finite volume through a homogenizing process, preferably in terms of the discrete forces and moments between contacting particles within the volume. We develop two notions of stress: a macro stress and an average stress, based on two different homogenization processes. The *macro stress* is derived from the principle of energy balance, i.e. it is conjugate with the macro strain defined for the representative volume. Because they are conjugate, the macro stress and macro strain can be used in a generalized continuum representation of a granular medium. The *average stress* is the volume-average of the local stress within the representative volume. The average stress is not necessarily conjugate with the average strain.

We treat a granular medium as a discrete system and use the virtual work principle to obtain definitions of the macro and average Cauchy stress, couple stress, and higher-order stress. Virtual work has already been used to derive stress expressions for granular materials. However, the results can differ due to hypotheses of the particular virtual work expression, selection of reference points, and other assumptions used in the process. For example, derivations can lead to an average stress that differs from that found by the direct integration of stress within a region (Bardet and Vardoulakis, 2001). A virtual work approach can also lead to a non-unique average that depends upon the selection of reference points assigned to individual particles (Kuhn, 2003). Other derivations also exist for average stress, but subtle differences can arise in the treatment of peripheral particles along a region's boundary (Christoffersen et al., 1981; Rothenburg and Selvadurai, 1981; Bagi, 1999; Kruyt, 2003). In this paper, we suggest a generalized virtual work expression and discuss the effects of associated assumptions. We also show that the definition of an average stress may depend upon the continuum description with which the discrete material is expected to comply. For example, different micromorphic settings can involve different stress quantities and, perhaps, lead to different definitions of a particular stress quantity. It is imperative that consistent definitions of the macro and average stress be resolved for small subregions of a granular media, since analytical studies and numerical simulations are increasingly focusing on the localized behavior of these discrete systems.

We seek expressions of the macro and average stress quantities (stress, couple stress, and higher-order stress) of a representative volume that properly account for the contact forces and contact moments among particles. The expressions should satisfy three conditions:

(1) We must usually assign a reference material point to each particle and express the macro or average stress in terms of the inter-particle forces and the relative vectors (branch vectors) that connect the reference points of adjacent particles. *The expression of a macro or average stress quantity must not depend upon the choice of these particle reference points*.
(2) *A stress quantity should be objective: two independent observers should measure the same stress after an appropriate tensor transformation of the observed stress components.* Because we consider only the stress and not its rate, the observers can be stationary, although their frames may differ by a finite rotation and translation (Truesdell and Noll, 1960, §17).
(3) The virtual work principle is a statement of equilibrium. Moment equilibrium necessarily involves the first moment of force about a central point (or points). *The expression of a macro or average stress quantity must not depend upon the choice of the central point.*

We restrict our study, however, to the following situations: we assume static conditions in which external forces are applied at the boundaries, and we exclude body forces and body moments on the particles themselves.

In Section 2 we introduce the essential notation and review the equilibrium condition for individual grains. In Section 3, we suggest a generalized expression of virtual work and use the expression to derive equilibrium relationships among the external and internal contact forces. We then employ these equilibrium relations to develop definitions for the macro stress quantities. We also derive average stress quantities in the context of three continuum settings: a classical continuum, a Cosserat continuum, and a higher-order continuum. We then determine whether the macro and average stress quantities satisfy the three conditions that were prescribed above. Many of the derivation details are placed in Appendices A and B. Appendix C evaluates the results of Bardet and Vardoulakis (2001) and shows that these results violate two of the three conditions that were prescribed above.

2. Equilibrium equations of particles

A *representative volume* of granular material is a contiguous collection of particles (Fig. 1a). The particles could be a sub-region of a larger particle assembly, or the representative volume could simply be a cluster of particles that are meant to emulate the micro-scale discrete behavior within a macro-scale continuum setting. The particles within a representative volume are either interior or peripheral, with the latter possibly interacting with material outside the representative volume. Forces and moments, both applied and internal, are discrete: they are either associated with pairs of particles inside the representative volume (i.e., at contacts) or with the externally applied forces on individual particles. The set V of internal contacts includes contacts between interior–interior particle pairs and between interior–peripheral pairs. Externally applied forces include contact forces and moments within the set of external (boundary) contacts B of peripheral particles as well as body forces and moments applied to interior and peripheral particles. We will soon exclude, however, such body forces and body moments in our analysis. That is, only contact forces and moments will be considered: contact forces and contact moments at the internal contacts V and at the external contacts B. A volume V is associated with the representative volume, and this volume encompasses both interior and peripheral particles and voids, although several approaches could be used in assigning peripheral void space to this volume. We refer to two unambiguous approaches to volume partitioning: the material cell partition of Bagi (1996) for particles of arbitrary shape, and the Dirichlet partition of Satake (2004) for circular or spherical particles.

The location of X_i^0 is defined in a global coordinate system $\mathbf{X}$. The stress at X_i^0 is evaluated from an auxiliary representative volume associated with this point. For points within the representative volume, a relative, local coordinate system $\mathbf{x}$ is used whose origin is at the point X_i^0, such that

$$x_i = X_i - X_i^0 \tag{1}$$

The point X_i^0 is usually at the centroid of the representative volume (Section 3.6).

A reference particle point $\mathbf{x}^n$ with Cartesian coordinates x_i^n is assigned to each nth particle in the relative system $\mathbf{x}$ (Fig. 1b). These particle points will serve in two roles: (a) as points of constraint when virtual particle movements must conform to a continuum field, and (b) as the central points for applying the moment equilibrium conditions for individual particles. We denote f_i^{nm} and m_i^{nm} as the interior contact force and moment exerted on particle n by another particle "m"; whereas, f_i^{nb} and m_i^{nb} will denote the force and moment at an external contact "b" of a peripheral particle n (Fig. 1b and c). For the moment, we use f_i^n and m_i^n to denote the resultant external body force and body moment acting at the reference point $\mathbf{x}^n$ of a particle n, although these forces will soon be excluded. We exclude particle inertia, so that the static equilibrium of particle n requires

$$\begin{aligned} &f_i^n + \sum_{b\in B} f_i^{nb} + \sum_{m\in V} f_i^{nm} = 0; \\ &m_i^n + \sum_{b\in B}\left(m_i^{nb} + e_{ijk} r_j^{nb} f_k^{nb}\right) + \sum_{m\in V}\left(m_i^{nm} + e_{ijk} r_j^{nm} f_k^{nm}\right) = 0 \end{aligned} \tag{2}$$

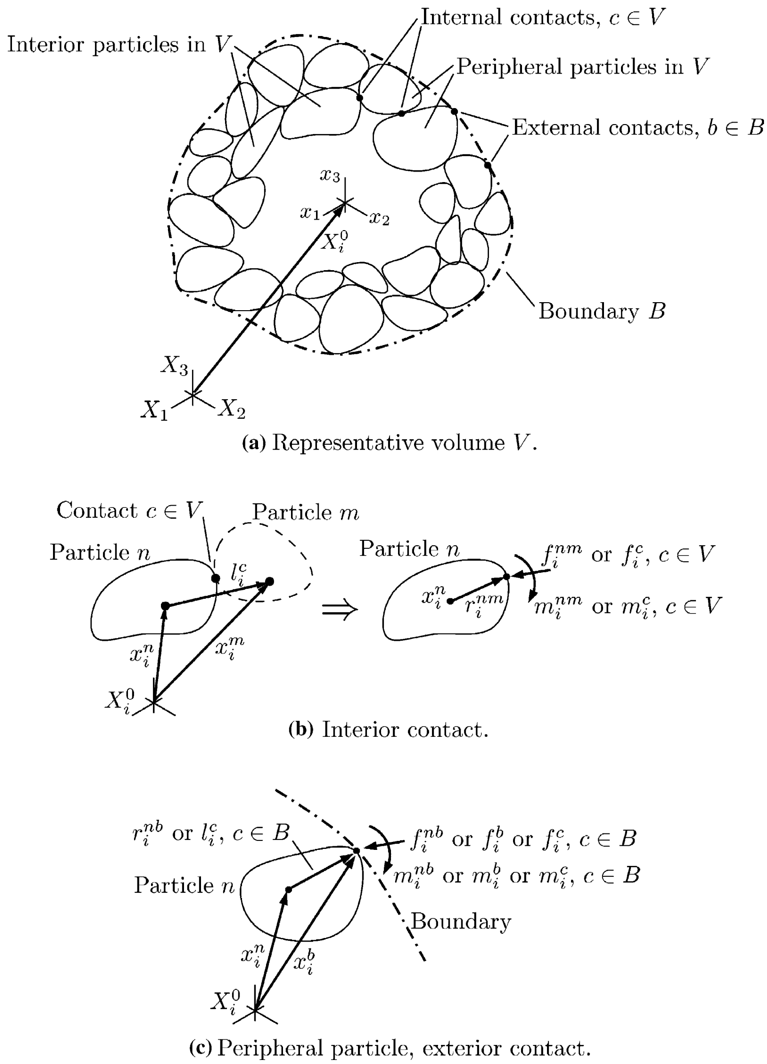

Fig. 1. A representative volume and the notation for discrete quantities.

The interior radial vector r_j^{nm} joins the particle reference point $\mathbf{x}^n$ to the mth interior contact point (Fig. 1b); whereas, the peripheral radial vector r_i^{nb} is from the particle reference point $\mathbf{x}^n$ to the bth external contact point (Fig. 1c). The permutation tensor e_{ijk} effects the cross product $\mathbf{r} \times \mathbf{f}$ of radial and force vectors. Each summation in Eq. (2) is for the contacts of any single particle n. In the remainder of the paper, we assume that the externally applied body force and body moment are zero for each particle: $f_i^n = 0$ and $m_i^n = 0$. The particles in an assembly interact at their contacts and we must supplement Eqs. (2) with the equilibrium constraints

$$f_i^{nm} = -f_i^{mn}; \quad m_i^{nm} = -m_i^{mn} \tag{3}$$

so that the internal contacts forces are self-equilibrating. We also note that the moment equilibrium of a particle in Eq. (3) is taken about the reference point $\mathbf{x}^n$ of that particle, although we will later shift these multiple reference points to a single point as a test of the Condition 3 of Section 1 (see Section 3.9 and Appendix B).

3. Derivations of macro and average stress

3.1. Virtual work of the discrete system

Rather than introduce the principle of virtual work as a postulate of equilibrium, we use the principle as an extension of the classical (strong) equilibrium equations (2), by multiplying each, nth equation by six arbitrary coefficients δu_i^n and $\delta\omega_i^n$ and then summing over all particles:

$$\delta W^{d,1} = \frac{1}{V}\sum_n\left(\sum_{b\in B} f_i^{nb} + \sum_{m\in V} f_i^{nm}\right)\delta u_i^n + \frac{1}{V}\sum_n\left(\sum_{b\in B}\left(m_i^{nb} + e_{ijk}r_j^{nb}f_k^{nb}\right) + \sum_{m\in V}\left(m_i^{nm} + e_{ijk}r_j^{nm}f_k^{nm}\right)\right)\delta\omega_i^n = 0 \tag{4}$$

noting that we have now removed the body forces f_i^n and body moments m_i^n. In this equilibrium equation, each, nth particle undergoes its own arbitrary and possibly finite virtual displacement δu_i^n and virtual rotation $\delta\omega_i^n$ at its reference point $\mathbf{x}^n$, and the outer summations are carried over all particles in the representative volume. The "discrete" virtual work $\delta W^{d,1}$ must be zero for any values of the δu_i^n and $\delta\omega_i^n$. In Eq. (4) we have divided by the volume V to give the virtual work $\delta W^{\mathrm{d},1}$ per unit volume.

The superscript "d" in $\delta W^{d,1}$ refers to the virtual work of a discrete system. The superscript "1" designates the first of two virtual work expressions that will be discussed in the paper. Bardet and Vardoulakis (2001) used the virtual work of Eq. (4) to derive an average stress for the discrete system. In Appendix C, we show, however, that Eq. (4) leads to an average stress that violates Conditions 1 and 3 of Section 1. We depart from Eq. (4) by introducing the supplementary independent virtual displacements δu_i^b and $\delta\omega_i^b$ of the boundary contact points themselves. Because of deformation and rotation of peripheral particles, these boundary displacements may differ from the displacements δu_i^n and $\delta\omega_i^n$ of the peripheral particles' interior reference points $\mathbf{x}^n$. The virtual work in Eq. (4) can now be written as

$$\delta W^{d,2} = \frac{1}{V}\sum_n\left(\sum_{b\in B} f_i^{nb} + \sum_{m\in V} f_i^{nm}\right)\delta u_i^n + \frac{1}{V}\sum_n\left(\sum_{b\in B}\left(m_i^{nb} + e_{ijk}r_j^{nb}f_k^{nb}\right) + \sum_{m\in V}\left(m_i^{nm} + e_{ijk}r_j^{nm}f_k^{nm}\right)\right)\delta\omega_i^n + \frac{1}{V}\sum_{b\in B}\left(f_i^b - f_i^b\right)\delta u_i^b + \frac{1}{V}\sum_{b\in B}\left(m_i^b - m_i^b\right)\delta\omega_i^b = 0 \tag{5}$$

In the final two sums, we have replaced the notation f_i^{nb} and m_i^{nb} with the simpler f_i^b and m_i^b to represent the external forces and moments, which are multiplied by the boundary displacements δu_i^b and $\delta\omega_i^b$. No work is done by the final two sums, and the two work expressions $\delta W^{d,1}$ and $\delta W^{d,2}$ are equivalent. We will see, however, that the work $\delta W^{d,2}$ leads to superior stress expressions. We refer to Eq. (5) as the generalized expression of virtual work, which is analogous to generalized variational statements that include their own boundary restrictions.

We return briefly to the work $\delta W^{d,1}$ in Eq. (4) can be separated into two parts: an external virtual work $\delta W_E^{d,1}$ associated with the boundary displacements and an internal virtual work $\delta W_I^{d,1}$ associated with internal deformation, which we write as

$$\delta W^{d,1} = \delta W_E^{d,1} - \delta W_I^{d,1} = 0 \tag{6}$$

The external and internal virtual works per unit of volume are

$$\delta W_E^{d,1} = \frac{1}{V}\sum_n \sum_{b\in B} f_i^{nb}\delta u_i^n + \frac{1}{V}\sum_n \sum_{b\in B}\left(m_i^{nb} + e_{ijk}r_j^{nb}f_k^{nb}\right)\delta\omega_i^n \tag{7}$$

$$\delta W_I^{d,1} = -\frac{1}{V}\sum_n \sum_{m\in V} f_i^{nm}\delta u_i^n - \frac{1}{V}\sum_n \sum_{m\in V}\left(m_i^{nm} + e_{ijk}r_j^{nm}f_k^{nm}\right)\delta\omega_i^n \tag{8}$$

where the sums for each, nth particle are either for its external or its interior contacts, $b \in B$ and $m \in V$, respectively. Eq. (6) is a standard statement of equilibrium: for a deformable structure in equilibrium under the action of a system of applied forces, the external virtual work due to an admissible virtual displacement state is equal to the internal virtual work due to the same virtual displacements.

With Eqs. (7) and (8), internal deformation is permitted throughout some, but not all, of the representative volume. Here, an external force f_i^{nb} moves and rotates with its peripheral particle about the particle's interior reference point $\mathbf{x}^n$, which implies that the peripheral particles are rigid between their interior reference points and their external contact points. Indeed, the term "external work" may not be entirely appropriate with Eq. (7), since $\delta W_E^{d,1}$ involves the products of external forces (f_i^{nb} and m_i^{nb}) and internal displacements (δu_i^n and $\delta\omega_i^n$).

Both issues are resolved by using the second virtual work $\delta W^{d,2}$ of Eq. (5), which can also be separated into external and internal parts:

$$\delta W_E^{d,2} = \frac{1}{V}\sum_{b\in B} f_i^b\delta u_i^b + \frac{1}{V}\sum_{b\in B} m_i^b\delta\omega_i^b \tag{9}$$

$$\begin{aligned}\delta W_I^{d,2} = &-\frac{1}{V}\sum_n \sum_{m\in V} f_i^{nm}\delta u_i^n - \frac{1}{V}\sum_n \sum_{m\in V}\left(m_i^{nm} + e_{ijk}r_j^{nm}f_k^{nm}\right)\delta\omega_i^n + \frac{1}{V}\sum_{b\in B} f_i^b\left(\delta u_i^b - \delta u_i^n\right)\\ &+\frac{1}{V}\sum_{b\in B} m_i^b\left(\delta\omega_i^b - \delta\omega_i^n\right) - \frac{1}{V}\sum_{b\in B} e_{ijk}r_j^{nb}f_k^b\delta\omega_i^n\end{aligned} \tag{10}$$

With these two expressions, the external work $\delta W_E^{d,2}$ is entirely associated with boundary displacements, and the internal work $\delta W_I^{d,2}$ is entirely due to internal deformation of the grains. The internal work $\delta W_I^{d,2}$ in Eq. (10) can also be arranged as

$$\begin{aligned}\delta W_I^{d,2} = &-\frac{1}{V}\sum_n \sum_{m\in V}\left[f_i^{nm}\left(\delta u_i^n - e_{ijk}r_j^{nm}\delta\omega_i^n\right) + m_i^{nm}\delta\omega_i^n\right]\\ &+\frac{1}{V}\sum_{b\in B}\left[f_i^b\left(\delta u_i^b - \left(\delta u_i^n - e_{ijk}r_j^{nb}\delta\omega_i^n\right)\right) + m_i^b\left(\delta\omega_i^b - \delta\omega_i^n\right)\right]\end{aligned} \tag{11}$$

By examining each term in this alternative form, we see that the granular material can be conceptually treated as an assembly of rigid particles with compliant or sliding contacts. The displacement at a contact of nth particle is produced by the translation and rotation of this particle by $\delta u_i^n - e_{ijk}r_j^{nb}\delta\omega_i^n$. The contact forces generate internal work on the relative translations of the two rigid grains at their contact points, and, similarly, the contact moments produce internal work on the relative rotations of the contacting rigid particles. In the case of peripheral particles, the deformations due to the compliance of external contacts produce the relative movements $\delta u_i^b - (\delta u_i^n - e_{ijk}r_j^{nb}\delta\omega_i^n)$ and $\delta\omega_i^b - \delta\omega_i^n$. This deformation occurs within the peripheral particles and thus contributes to the internal work of the representative volume. Therefore, the internal work $\delta W_I^{d,2}$ is a better measure than $\delta W_I^{d,1}$ because it accounts for the work done throughout the entire representative volume, both within its interior and within its peripheral particles.

When separating virtual work into external and internal parts, the work expressions $\delta W^{d,1}$ and $\delta W^{d,2}$ have led to different values for the two parts. Some work that would be considered external in $\delta W^{d,1}$ is instead considered as internal in $\delta W^{d,2}$, and vice versa. The work $\delta W^{d,2}$ in Eq. (5), leads to different (and superior) stress expressions. Eq. (5) is developed in the body of the paper; whereas an analysis of Eq. (4) is deferred to Appendix C.

3.2. Continuum field for the discrete particle system

Stress is a continuum concept, and to make a link between the discrete force system and its continuum equivalent, we adopt the approach of Chang and Liao (1990), Chang and Gao (1996), and Bardet and Vardoulakis (2001). We restrict the virtual displacement fields $\delta u_i(\mathbf{x})$ and $\delta\omega_i(\mathbf{x})$ to a continuous virtual displacement field $\delta\hat{u}_i(\mathbf{x})$ and virtual rotation field $\delta\hat{\omega}_i(\mathbf{x})$. Instead of applying the usual linear displacement field to an infinitesimal element, we approximate the displacement field of the representative volume (associated with the material point X_i^0 as shown in Fig. 1) with a polynomial series containing quadratic terms. A linear field of particle rotations is also considered:

$$\begin{aligned}\delta\hat{u}_i(\mathbf{x}) &= \delta u_i^0 + \delta u_{ij}^0 x_j + \frac{1}{2}\delta u_{ijk}^0 x_j x_k \\ \delta\hat{\omega}_i(\mathbf{x}) &= \delta\omega_i^0 + \delta\omega_{ij}^0 x_j\end{aligned} \tag{12}$$

The coordinates x_i in Eq. (12) are measured relative to the point X_i^0, as in Eq. (1). The scalar coefficients δu_i^0, δu_{ij}^0, δu_{ijk}^0, $\delta\omega_i^0$ and $\delta\omega_{ij}^0$ fully describe the deformation of the representative volume. Thus, these scalar coefficients are used as strain measures of the material point X_i^0. The conventional strain at the same material point (associated with an infinitesimal element) is different from the strains δu_{ij}^0. We note that the conventional strain at a point is defined as the derivatives of $\delta u_i(\mathbf{x})$ and $\delta\omega_i(\mathbf{x})$ at the point; whereas δu_{ij}^0 are characteristic strains of the representative volume. To distinguish the two notions, the strain at a point within the representative volume is called the *local strain*, and the scalar coefficients in Eq. (12) are called *macro strains*. The macro strains may differ from the volume average of local strains within the representative volume. The second rank matrices δu_{ij}^0 and $\delta\omega_{ij}^0$ each have 9 elements, and the third rank matrix δu_{ijk}^0 has 27 elements. After considering symmetry with respect to indices jk, δu_{ijk}^0 has 18 terms.

To develop expressions for stress, couple stress, and higher-order stress, we will restrict the discrete virtual displacements and rotations, δu_i^n, $\delta\omega_i^n$, δu_i^b and $\delta\omega_i^b$, to the continuous fields (12) applied at the particle reference points $\mathbf{x}^n$ and at the external contact points $\mathbf{x}^b$:

$$\delta u_i^n = \delta\hat{u}_i(\mathbf{x}^n); \quad \delta\omega_i^n = \delta\hat{\omega}_i(\mathbf{x}^n); \quad \delta u_i^b = \delta\hat{u}_i(\mathbf{x}^b); \quad \delta\omega_i^b = \delta\hat{\omega}_i(\mathbf{x}^b) \tag{13}$$

That is, we will replace the many (perhaps thousands) of arbitrary virtual displacements δu_i^n, $\delta\omega_i^n$, δu_i^b and $\delta\omega_i^b$ with the 42 virtual macro strains δu_i^0, δu_{ij}^0, δu_{ijk}^0, $\delta\omega_i^0$ and $\delta\omega_{ij}^0$ of Eq. (12).

3.3. Equilibrium of the discrete force system

We now restrict the displacements δu_i^n, $\delta\omega_i^n$, δu_i^b and $\delta\omega_i^b$ in Eqs. (9) and (10) to the continuum field Eq. (12). In terms of the macro strains, the external work $\delta W_E^{d,2}$ of Eq. (9) is

$$\delta W_E^{d,2} = \delta u_i^0 \frac{1}{V}\sum_{b\in B} f_i^b + \delta u_{ij}^0 \frac{1}{V}\sum_{b\in B} f_i^b x_j^b + \delta u_{ijk}^0 \frac{1}{2V}\sum_{b\in B} f_i^b x_j^b x_k^b + \delta\omega_i^0 \frac{1}{V}\sum_{b\in B} m_i^b + \delta\omega_{ij}^0 \frac{1}{V}\sum_{b\in B} m_i^b x_j^b \tag{14}$$

although the first sum is zero, due to equilibrium of the external contact forces f_i^b. The internal work $\delta W_I^{d,2}$ of Eq. (9) is

$$\delta W_I^{d,2} = \delta u_{ij}^0 \frac{1}{V} \sum_{c \in V \cup B} f_i^c l_j^c + \delta u_{ijk}^0 \frac{1}{2V} \sum_{c \in V \cup B} f_i^c J_{jk}^c - \delta\omega_i^0 \frac{1}{V} \sum_{c \in V \cup B} e_{ijk} f_k^c l_j^c + \delta\omega_{ij}^0 \frac{1}{V} \sum_{c \in V \cup B} \left[m_i^c l_j^c + e_{ik\ell} f_k^c \left(J_{\ell j}^c - x_\ell^c l_j^c \right) \right] \tag{15}$$

as derived in Appendix A. Eq. (15) regroups the sums in Eq. (10) by combining them over the full set of interior and exterior contacts ($c \in V \cup B$). As such, the quantities l_i^c, J_{ij}^c, f_i^c and m_i^c depend upon whether a contact "c" is interior or exterior:

$$l_i^c = \begin{cases} x_i^m - x_i^n; & c \in V \\ x_i^b - x_i^n; & c \in B \end{cases}; \quad J_{ij}^c = \begin{cases} x_i^m x_j^m - x_i^n x_j^n; & c \in V \\ x_i^b x_j^b - x_i^n x_j^n; & c \in B \end{cases} \tag{16}$$

$$f_i^c = \begin{cases} f_i^{nm} = -f_i^{mn}; & c \in V \\ f_i^b = f_i^{nb}; & c \in B \end{cases}; \quad m_i^c = \begin{cases} m_i^{nm} = -m_i^{mn}; & c \in V \\ m_i^b = m_i^{nb}; & c \in B \end{cases} \tag{17}$$

For an interior contact, the branch vector l_i^c connects the reference points $\mathbf{x}^n$ and $\mathbf{x}^m$ of the particle pair, and the interior contact force and moment on particle n are simply denoted as f_i^c and m_i^c. For an exterior contact, the branch vector l_i^c connects the reference point of the peripheral particle with its boundary contact point x_i^b, and the external contact force and moment are denoted as $f_i^c = f_i^b = f_i^{nb}$ and $m_i^c = m_i^b = m_i^{nb}$. Note that boundary forces are denoted as f_i^b and m_i^b in the external sums of Eq. (14), but they are also included as interior forces f_i^c and m_i^c in Eq. (15). The position x_ℓ^c is of the contact point, $x_\ell^c = x_\ell^n + r_\ell^{nm} = x_\ell^m + r_\ell^{mn}$. The derivation of Eq. (15) is given in Appendix A. The terms in Eq. (15) can also be rearranged into an alternative form that will be useful in examining the stress definitions:

$$\delta W_I^{d,2} = \left(\delta u_{ij}^0 + e_{ijk} \delta\omega_k^0 \right) \frac{1}{V} \sum_{c \in V \cup B} f_i^c l_j^c + \left(\delta u_{ijk}^0 + e_{ij\ell} \delta\omega_{\ell k}^0 \right) \frac{1}{2V} \sum_{c \in V \cup B} f_i^c J_{jk}^c + \delta\omega_{ij}^0 \frac{1}{V} \sum_{c \in V \cup B} \left[m_i^c l_j^c + e_{ik\ell} f_k^c \left(\frac{1}{2} J_{\ell j}^c - x_\ell^c l_j^c \right) \right] \tag{18}$$

The interior and exterior virtual works must be equal for an arbitrary choice of the macro strains $\delta u_{ij}^0, \delta u_{ijk}^0, \delta\omega_i^0$ and $\delta\omega_{ij}^0$, as in Eq. (6). The equivalence of $\delta W_E^{d,2}$ and $\delta W_I^{d,2}$ in Eqs. (14) and (15) leads to the following equivalences among the force sums:

$$\frac{1}{V} \sum_{b \in B} f_i^b x_j^b = \frac{1}{V} \sum_{c \in V \cup B} f_i^c l_j^c \tag{19}$$

$$\frac{1}{V} \sum_{b \in B} f_i^b x_j^b x_k^b = \frac{1}{V} \sum_{c \in V \cup B} f_i^c J_{jk}^c \tag{20}$$

$$\frac{1}{V} \sum_{b \in B} m_i^b = -\frac{1}{V} \sum_{c \in V \cup B} e_{ijk} f_k^c l_j^c \tag{21}$$

$$\frac{1}{V} \sum_{b \in B} m_i^b x_j^b = \frac{1}{V} \sum_{c \in V \cup B} \left[m_i^c l_j^c + e_{ik\ell} f_k^c \left(J_{\ell j}^c - x_\ell^c l_j^c \right) \right] \tag{22}$$

These sums will be used in constructing stress quantities in the following two sections.

3.4. Macro stress

In this section, we consider the virtual work done due to the virtual macro strain of a representative volume. The macro stress is defined to be conjugate with the macro strain. However, the macro stress quantities are not necessarily equal to their average stress counterparts, a distinction that is elaborated in Section 3.5, where we derive average stress quantities. To derive the macro stress quantities, we will consider two forms of the internal virtual work per unit volume. The first form is

$$\delta W_I^a = \sigma_{ji}^0 \delta u_{ij}^0 + \sigma_{jki}^0 \delta u_{ijk}^0 + T_i^0 \delta\omega_i^0 + T_{ji}^0 \delta\omega_{ij}^0 \tag{23}$$

where the superscript "a" denotes the first form; δu_{ij}^0, δu_{ijk}^0, $\delta\omega_i^0$ and $\delta\omega_{ij}^0$ are the macro strains of Eq. (12); and σ_{ji}^0, σ_{jki}^0, T_i^0 and T_{ji}^0 are the stress measures of the representative volume: the macro stress, macro higher-order stress, macro internal torque, and macro torque stress, respectively. Unlike the discrete work $\delta W_I^{d,2}$ in Eq. (15), the work δW_I^a is for an equivalent continuum that approximates the discrete system. The correspondence of terms in Eqs. (15) and (23) implies the following definitions of the macro stresses:

$$\sigma_{ji}^0 = \frac{1}{V}\sum_{b\in B} f_i^b x_j^b = \frac{1}{V}\sum_{c\in V\cup B} f_i^c l_j^c \tag{24}$$

$$\sigma_{jki}^0 = \frac{1}{2V}\sum_{b\in B} f_i^b x_j^b x_k^b = \frac{1}{2V}\sum_{c\in V\cup B} f_i^c J_{jk}^c \tag{25}$$

$$T_i^0 = \frac{1}{V}\sum_{b\in B} m_i^b = -\frac{1}{V}\sum_{c\in V\cup B} e_{ijk} f_k^c l_j^c \tag{26}$$

$$T_{ji}^0 = \frac{1}{V}\sum_{b\in B} m_i^b x_j^b = \frac{1}{V}\sum_{c\in V\cup B}\left[m_i^c l_j^c + e_{ik\ell} f_k^c \left(J_{\ell j}^c - x_\ell^c l_j^c\right)\right] \tag{27}$$

in which we have used the equivalences among internal and external sums given in Eqs. (19)–(22).

Eq. (18) suggests a second, "b", form of internal virtual work of the equivalent continuum:

$$\delta W_I^b = \sigma_{ji}^0\left(\delta u_{ij}^0 + e_{ijk}\delta\omega_k^0\right) + \sigma_{jki}^0\left(\delta u_{ijk}^0 + e_{ij\ell}\delta\omega_{\ell k}^0\right) + \mu_{ji}^0 \delta\omega_{ij}^0 \tag{28}$$

In this form, the macro strain measure $\delta u_{ij}^0 + e_{ijk}\delta\omega_k^0$ is analogous to the micropolar strain of a Cosserat continuum, and μ_{ji}^0 is the macro couple stress. The term $\delta u_{ijk}^0 + e_{ij\ell}\delta\omega_{\ell k}^0$ is not encountered in standard micropolar theory, but it can be regarded as a higher-order macro strain. The macro torque stress T_{ji}^0 in Eq. (23) is related to the macro couple stress and higher-order stress by

$$T_{ji}^0 = \mu_{ji}^0 + e_{k\ell i}\sigma_{\ell jk}^0 \tag{29}$$

The internal macro torque, $T_k^0 = e_{ijk}\sigma_{ji}^0$, is the anti-symmetric part of stress, which does not produce work in a classical continuum. The correspondence of terms in Eqs. (18) and (28) implies the following definition of the macro couple stress:

$$\mu_{ji}^0 = \frac{1}{V}\sum_{b\in B}\left(m_i^b x_j^b - \frac{1}{2} e_{ik\ell} f_k^b x_\ell^b x_j^b\right) = \frac{1}{V}\sum_{c\in V\cup B}\left[m_i^c l_j^c + e_{ik\ell} f_k^c \left(\frac{1}{2} J_{\ell j}^c - x_\ell^c l_j^c\right)\right] \tag{30}$$

in which we have also applied Eqs. (20) and (22) to derive the internal and external sums. The macro stresses σ_{ji}^0 and σ_{jki}^0 derived from the "b" form in Eq. (28) are the same as those in Eqs. (24) and (25).

3.5. Average stress

In the previous section, we equated the internal work of the representative volume with the product of macro stress and macro strain, which led to the expressions of macro stresses in Eqs. (24)–(27) and (30). In deriving the macro stresses, we considered representative volume as discrete particles with compliant contacts. Local stresses were not explicitly used within the representative volume; we instead derived the internal work done by the contact forces and moments within the volume. We now consider the representative volume as an equivalent continuum. The internal work is generated by the local stresses at points within the representative volume and we then integrate these local stresses throughout the representative volume to find expressions of average stress within the volume. The internal work of the representative volume is then determined by integrating the work at points within the volume. The specific expression of internal work at a point within the representative volume depends upon the type of continuum assumed for the material. The simplest form of internal work is the product $\sigma_{ji}\delta u_{i,j}$ for a classical continuum, but the work is more complex for micropolar continua. We consider the following three continua, having different forms of internal work.

(a) Continuum A—Classical continuum

$$\delta W_I^{\mathrm{A}} = \frac{1}{V}\int_V \sigma_{ji}\delta u_{i,j}\,\mathrm{d}V \tag{31}$$

(b) Continuum B—Micropolar Cosserat continuum

$$\delta W_I^{\mathrm{B}} = \frac{1}{V}\int_V \left[\sigma_{ji}\left(\delta u_{i,j} + e_{ijk}\delta\omega_k\right) + \mu_{ji}\delta\omega_{i,j}\right]\mathrm{d}V \tag{32}$$

(c) Continuum C—Higher-order Cosserat continuum

$$\delta W_I^{\mathrm{C}} = \frac{1}{V}\int_V \left[\sigma_{ji}\left(\delta u_{i,j} + e_{ijk}\delta\omega_k\right) + \sigma_{jki}\left(\delta u_{i,jk} + e_{ij\ell}\delta\omega_{\ell,k}\right) + \mu_{ji}\delta\omega_{i,j}\right]\mathrm{d}V \tag{33}$$

where σ_{ji}, σ_{jki}, and μ_{ji} are local stresses measured at points within the representative volume. In what follows, we will use these three equations to derive the average stresses $\bar{\sigma}_{ji}$, $\bar{\mu}_{ji}$, and $\bar{\sigma}_{jki}$ over the representative volume V.

3.5.1. Average stress in a classical continuum (Continuum A)

With the work δW_I^{A} of Continuum A in Eq. (31), we restrict the virtual displacements to the fields $\delta\hat{u}_i$ and $\delta\hat{\omega}_i$ given in Eqs. (12) and (13). For a classical continuum (Continuum A), the internal virtual work under the restricted displacements is

$$\delta W_I^{\mathrm{A}} = \frac{1}{V}\int_V \sigma_{ji}\delta u_{i,j}\,\mathrm{d}V = \delta u_{ij}^0\frac{1}{V}\int_V \sigma_{ji}\,\mathrm{d}V + \delta u_{ijk}^0\frac{1}{V}\int_V \sigma_{ji}x_k\,\mathrm{d}V \tag{34}$$

noting that the coefficients δu_{ijk}^0 are symmetric in the final indices jk. We define the volume average stress $\bar{\sigma}_{ji}^{\mathrm{A}}$ and stress moment $\bar{\Sigma}_{kji}^{\mathrm{A}}$ as

$$\bar{\sigma}_{ji}^{\mathrm{A}} = \frac{1}{V}\int_V \sigma_{ji}\,\mathrm{d}V; \quad \bar{\Sigma}_{kji}^{\mathrm{A}} = \frac{1}{V}\int_V \sigma_{ji}x_k\,\mathrm{d}V \tag{35}$$

The internal work δW_I^{A} in Eq. (34) must equal the work $\delta W_I^{d,2}$ in Eq. (15) for an arbitrary choice of the 48 macro strains δu_{ij}^0, δu_{ijk}^0, $\delta\omega_i^0$ and $\delta\omega_{ij}^0$. This equivalence and the four equilibrium Eqs. (19)–(22) imply the following average stress quantities for a classical continuum:

$$\bar{\sigma}^{\mathrm{A}}_{ji} = \frac{1}{V}\sum_{b\in B} f_i^b x_j^b = \frac{1}{V}\sum_{c\in V\cup B} f_i^c l_j^c \tag{36}$$

$$\bar{\Sigma}^{\mathrm{A}}_{kji} = \frac{1}{2V}\sum_{b\in B} f_i^b x_j^b x_k^b = \frac{1}{2V}\sum_{c\in V\cup B} f_i^c J_{jk}^c \tag{37}$$

provided that

$$\frac{1}{V}\sum_{b\in B} m_i^b = -\frac{1}{V}\sum_{b\in B\cup V} e_{ijk} f_k^c l_j^c = 0 \tag{38}$$

$$\frac{1}{V}\sum_{b\in B} m_i^b x_j^b = \frac{1}{V}\sum_{b\in B\cup V}\left[m_i^c l_j^c + e_{ik\ell} f_k^c \left(J_{\ell j}^c - x_\ell^c l_j^c\right)\right] = 0 \tag{39}$$

Because the sums in Eqs. (24) and (36) coincide, the macro stress and the average Cauchy stress are equal: $\sigma^0_{ji} = \bar{\sigma}^{\mathrm{A}}_{ji}$. A similar comparison of Eqs. (25) and (37) shows that the macro higher-order stress is equal to the average stress moment, $\sigma^0_{kji} = \bar{\Sigma}^{\mathrm{A}}_{kji}$, and that both stresses are symmetric in the initial indices kj. Eq. (34) reveals that the internal work of the representative volume is $\bar{\sigma}_{ji}\delta u^0_{ij} + \bar{\sigma}_{jki}\delta u^0_{ijk}$. Thus, the representative volume behaves as a higher-order continuum even though each point within the representative volume is a classical continuum. The relations in Eq. (38) imply that the average stress $\bar{\sigma}^{\mathrm{A}}_{ji}$ is symmetric for the classical continuum. Equations (38) and (39) also imply that contact moments m_i^c are disallowed in a classical continuum setting, since the two equations must apply to an arbitrary choice of granular region. The contact moments m_i do not contribute work in a classical continuum.

3.5.2. Average stress in a Cosserat continuum (Continuum B)

We now restrict the virtual work δW_I^{B} of a Cosserat continuum (Eq. (32)) to the displacement fields $\delta\hat{u}_i$ and $\delta\hat{\omega}_i$ in Eqs. (12) and (13). We will equate this continuum work with the internal work $\delta W_I^{d,2}$ of the discrete system in Eq. (18). For the Cosserat continuum (Continuum B), the virtual work is

$$\begin{aligned}\delta W_I^{\mathrm{B}} &= \frac{1}{V}\int_V \left[\sigma_{ji}\left(\delta\hat{u}_{i,j} + e_{ijk}\delta\hat{\omega}_k\right) + \mu_{ji}\delta\hat{\omega}_{i,j}\right]\mathrm{d}V \\ &= \left(\delta u^0_{ij} + e_{ijk}\delta\omega^0_k\right)\frac{1}{V}\int_V \sigma_{ji}\,\mathrm{d}V + \left(\delta u^0_{ijk} + e_{ij\ell}\delta\omega^0_{\ell k}\right)\frac{1}{V}\int_V \Sigma_{(kj)i}\,\mathrm{d}V + \delta\omega^0_{ij}\frac{1}{V} \\ &\quad\times\int_V \left(\mu_{ji} + e_{ik\ell}\Sigma_{[j\ell]k}\right)\mathrm{d}V\end{aligned} \tag{40}$$

where the micro-scale stress moment Σ_{kji} is the product $\sigma_{ji}x_k$, and the enclosures $(\cdot)$ and $[\cdot]$ refer to symmetric and skew-symmetric parts, respectively. The terms in Eq. (40) have been arranged to coincide with those in Eq. (18). The virtual works δW_I^{B} and $\delta W_I^{d,2}$ in Eqs. (40) and (18) must be equal for arbitrary values of the coefficients $\delta u^0_{ij}, \delta u^0_{ijk}, \delta\omega^0_i$ and $\delta\omega^0_{ij}$. This equivalence implies that the average Cauchy stress for a Cosserat continuum, $\bar{\sigma}^{\mathrm{B}}_{ji}$, is equal to that of a classical continuum $\bar{\sigma}^{\mathrm{A}}_{ji}$ and to the macro stress σ^0_{ji}, or $\sigma^0_{ji} = \bar{\sigma}^{\mathrm{A}}_{ji} = \bar{\sigma}^{\mathrm{B}}_{ji}$, although the average stress $\bar{\sigma}^{\mathrm{A}}_{ji}$ must be symmetric. The equivalence of the $(\delta u^0_{ijk} + e_{ij\ell}\delta\omega^0_{\ell k})$ terms in Eqs. (18) and (40) implies that the symmetric part of the average stress moment, $\bar{\Sigma}^{\mathrm{B}}_{(kj)i}$ is

$$\bar{\Sigma}^{\mathrm{B}}_{(kj)i} = \frac{1}{2V}\sum_{b\in B} f_i^b x_j^b x_k^b = \frac{1}{2V}\sum_{c\in V\cup B} f_i^c J_{jk}^c \tag{41}$$

and the equivalence of the final terms in Eqs. (40) and (18) implies that

$$\bar{\mu}^{\mathrm{B}}_{ji} + e_{ik\ell}\bar{\Sigma}^{\mathrm{B}}_{[j\ell]k} = \frac{1}{V}\sum_{b\in B}\left(m^b_i x^b_j - e_{ik\ell}\frac{1}{2}f^b_k x^b_\ell x^b_j\right) = \frac{1}{V}\sum_{c\in V\cup B}\left[m^c_i l^c_j + e_{ik\ell}f^c_k\left(\frac{1}{2}J^c_{\ell j} - x^c_\ell l^c_j\right)\right] \tag{42}$$

where the average couple stress $\bar{\mu}^{\mathrm{B}}_{ji}$ and average stress moment $\bar{\Sigma}^{\mathrm{B}}_{ijk}$ are defined as

$$\bar{\mu}^{\mathrm{B}}_{ji} = \frac{1}{V}\int_V \mu_{ji}\,\mathrm{d}V; \quad \bar{\Sigma}^{\mathrm{B}}_{ijk} = \frac{1}{V}\int_V x_i\sigma_{jk}\,\mathrm{d}V \tag{43}$$

We note that the average stress moment and couple stress, $\bar{\Sigma}^{\mathrm{B}}_{(kj)i}$ and $\bar{\mu}^{\mathrm{B}}_{ji}$, cannot be independently computed from the contact forces and moments: only the combinations $\bar{\Sigma}^{\mathrm{B}}_{(kj)i}$ and $\bar{\mu}^{\mathrm{B}}_{ji} + e_{ik\ell}\bar{\Sigma}^{\mathrm{B}}_{[j\ell]k}$ can be computed. Bardet and Vardoulakis (2001) reached a similar conclusion.

The macro couple stress $\bar{\mu}^{\mathrm{B}}_{ji}$ in Eq. (30) is not that same as the average couple stress, but instead

$$\mu^0_{ji} = \bar{\mu}^{\mathrm{B}}_{ji} + e_{ik\ell}\bar{\Sigma}^{\mathrm{B}}_{[j\ell]k} \tag{44}$$

That is, the average stress moment also contributes to the macro couple stress. Eq. (40) reveals that the internal work of the representative volume resembles that of a higher-order micropolar continuum (Section 3.5.3) even though each point within the representative volume is a standard micropolar continuum.

3.5.3. Average stress in a higher-order continuum (Continuum C)

We proceed as in the previous section, restricting the virtual displacements of the higher-order Continuum C (Eq. (33)) to the continuous fields in Eqs. (12) and (13):

$$\begin{aligned}\delta W^{\mathrm{C}}_I &= \frac{1}{V}\int_V \left[\sigma_{ji}\left(\delta\hat{u}_{i,j} + e_{ijk}\delta\hat{\omega}_k\right) + \sigma_{jki}\left(\delta\hat{u}_{i,jk} + e_{ij\ell}\delta\hat{\omega}_{\ell,k}\right) + \mu_{ji}\delta\hat{\omega}_{i,j}\right]\mathrm{d}V \\ &= \left(\delta u^0_{ij} + e_{ijk}\delta\omega^0_k\right)\frac{1}{V}\int_V \sigma_{ji}\,\mathrm{d}V + \left(\delta u^0_{ijk} + e_{ij\ell}\delta\omega^0_{\ell k}\right)\frac{1}{V}\int_V\left(\Sigma_{(kj)i} + \sigma_{(kj)i}\right)\mathrm{d}V \\ &\quad + \delta\omega^0_{ij}\frac{1}{V}\int_V\left(\mu_{ji} + e_{ik\ell}\left(\sigma_{[\ell j]k} - \Sigma_{[\ell j]k}\right)\right)\mathrm{d}V\end{aligned} \tag{45}$$

By comparing the terms in Eqs. (18), (28) and (33) on a coefficient-by-coefficient basis, we again reach the conclusion that the representative macro stress is equal to the average stress, $\sigma^0_{ji} = \bar{\sigma}^{\mathrm{C}}_{ji}$, with both stresses given by the sums in Eq. (24). The macro higher-order stress σ^0_{jki} and macro couple stress μ^0_{ji}, however, are equal to combinations of the average stress quantities: $\sigma^0_{jki} = \bar{\sigma}^{\mathrm{C}}_{(kj)i} + \bar{\Sigma}^{\mathrm{C}}_{(kj)i}$ and $\mu^0_{ji} = \bar{\mu}^{\mathrm{C}}_{ji} + e_{ik\ell}(\bar{\sigma}^{\mathrm{C}}_{[\ell j]k} + \bar{\Sigma}^{\mathrm{C}}_{[\ell j]k})$.

The average Cauchy stress $\bar{\sigma}^{\mathrm{C}}_{ji}$ has an explicit definition in terms of contact forces and contact moments (Eq. (24), noting that $\bar{\sigma}^{\mathrm{C}}_{ji} = \sigma^0_{ji}$). Because the couple stress, stress moment and higher-order stress appear together in combined forms in Eq. (45), we can not independently determine the averages, $\bar{\mu}^{\mathrm{C}}_{ji}$, $\bar{\Sigma}^{\mathrm{C}}_{kji}$, and $\bar{\sigma}^{\mathrm{C}}_{kji}$.

3.6. Discussion

The average Cauchy stresses, $\bar{\sigma}^{\mathrm{A}}_{ji}$, $\bar{\sigma}^{\mathrm{B}}_{ji}$, and $\bar{\sigma}^{\mathrm{C}}_{ji}$, for the three continua are identical to each other and to the macro stress σ^0_{ji}, which has a unique definition in terms of contact forces (Eq. (24)). Rothenburg and Selvadurai (1981) derived the same expressions for the average stress: the external and internal sums in Eq. (24) are the same as their Eqs. (2.4) and (3.5). The external sum for σ^0_{ji} in Eq. (24) is also the same as that of Drescher and de Josselin de Jong (1972) and Christoffersen et al. (1981). The latter investigators also gave a similar definition using an internal sum, although they did not explicitly account for peripheral particles. Both parts of σ^0_{ji} in Eq. (24) are identical to the definitions of Bagi (1999) in her Eqs. (12) and (15), and of Kruyt (2003) in his Eqs. (33) and (34). The average stress in Eq. (24) differs, however, from that of Bardet and Vardoulakis (2001), who treated peripheral particles differently than in the current work. Their expressions were derived from the virtual work $\delta W^{d,1}$ of Eq. (4) instead of the work $\delta W^{d,2}$ of Eq. (5), and their results are investigated in Appendix C. Kruyt (2003) derived an expression for the average couple stress $\bar{\mu}_{ji}$ that differs from Eq. (42). His definition is an internal sum that only includes the products $m^c_i l^c_j$ (compare with the final sum in Eq. (42)). He had assumed a smoothness condition for σ_{ji} at the micro-scale stress so that the force terms f^c_i make no contribution to $\bar{\mu}_{ji}$, an assumption not made in the current work.

The average stress $\bar{\sigma}^{\mathrm{A}}_{ji}$ is always symmetric in a classical continuum, but the average stresses in Cosserat and higher-order continua ($\bar{\sigma}^{\mathrm{B}}_{ji}$ and $\bar{\sigma}^{\mathrm{C}}_{ji}$) are, in general, asymmetric. In the absence of external contact moments m^b_i, however, these average stresses are also symmetric. This possible symmetry of the average stress $\bar{\sigma}_{ji}$ contrasts with the conclusion of Bardet and Vardoulakis (2001), which is analyzed in Appendix C.

We now consider the three conditions that were prescribed in Section 1 and whether the various stress quantities satisfy these conditions. The first condition is satisfied by all of the macro and average stress quantities derived in Sections 3.3 and 3.4: each stress quantity is independent of the choice of the internal reference points $\mathbf{x}^n$ assigned to the particles. These stress quantities are constructed from the contact sums in Eqs. (24)–(27), which are all independent of the choice of $\mathbf{x}^n$. This result is most apparent in the external sums, which only depend upon the locations x^b_i of the external contacts and not upon the internal reference points. This characteristic is not shared by the contact sums that would be derived from the alternative work expression $\delta W^{d,1}$ of Eq. (3) (see Appendix C).

As for the Condition 2 of objectivity, all of the stress quantities transform appropriately with a finite observer rotation, since the sums from which they are constructed transform as tensors upon a rotation of the coordinate basis vectors (i.e., the sums in Eqs. (19)–(22)). The coordinates x_i in these sums are relative vectors, $x_i = X_i - X^0_i$, and are also unchanged by an observer translation. The stress quantities, which are constructed from these sums, are therefore, objective. We note, however, that the average stresses $\bar{\mu}_{ji}$, $\bar{\sigma}_{jki}$, and $\bar{\Sigma}_{jki}$ depend upon the region selected as the representative volume. Condition 3 is investigated in the next section.

3.7. Changing the central point of moment equilibrium

We now determine whether the various averaged stress quantities satisfy Condition 3, which requires that a stress quantity derived from the virtual work principle should not depend upon the central point that is chosen for moment equilibrium. We will reformulate the virtual work expressions of Section 3.1, using the single, common central point X^0_i for moment equilibrium instead of the multiple reference points, x^n_i. Our purpose is to demonstrate that the stress quantities in Sections 3.3 and 3.4 are independent of the choice of the central point and, hence, satisfy Condition 3. As before, we allow virtual deformations within peripheral particles by including the virtual displacements δu^b_i and $\delta\omega^b_i$ of the boundary contact points $b \in B$. The moment equilibrium Eq. $(2)_2$ is now replaced with

$$m^n_i + \sum_{b\in B}\left(m^{nb}_i + e_{ijk}x^{nb}_j f^{nb}_k\right) + \sum_{m\in V}\left(m^{nm}_i + e_{ijk}x^{nm}_j f^{nm}_k\right) = 0 \tag{46}$$

for each, nth particle. The position vector x^{nm}_i replaces the radial vector r^{nm}_i in Eq. $(2)_2$ and is measured from the common central point X^0_i to the contact between particles n and m ; vector x^{nb}_i is measured from the common central point to the external contact point b of particle n (Fig. 1b and c). Neglecting the body forces and moments, f_i^n and m_i^n, the principle of virtual work can again be formulated by multiplying the sums in Eqs. (2)$_1$ and (46) by arbitrary virtual displacements, δu_i^n and $\delta\omega_i^n$:

$$\delta W^{d,2-\text{alt}} = \frac{1}{V}\sum_n\left(\sum_{b\in B} f_i^{nb} + \sum_{m\in V} f_i^{nm}\right)\delta u_i^n + \frac{1}{V}\sum_n\left(\sum_{b\in B}\left(m_i^{nb} + e_{ijk}x_j^{nb}f_k^{nb}\right)\right.$$
$$\left. + \sum_{m\in V}\left(m_i^{nm} + e_{ijk}x_j^{nm}f_k^{nm}\right)\right)\delta\omega_i^n + \frac{1}{V}\sum_{b\in B}\left(f_i^b - f_i^b\right)\delta u_i^b + \frac{1}{V}\sum_{b\in B}\left(m_i^b - m_i^b\right)\delta\omega_i^b = 0 \tag{47}$$

This alternative "alt" virtual work replaces that in Eq. (5). The work $\delta W^{d,2-\text{alt}}$ is partitioned into the following external and internal parts:

$$\delta W_E^{d,2-\text{alt}} = \frac{1}{V}\sum_{b\in B} f_i^b\delta u_i^b + \frac{1}{V}\sum_{b\in B} m_i^b\delta\omega_i^b \tag{48}$$

$$\delta W_I^{d,2-\text{alt}} = -\frac{1}{V}\sum_n\sum_{m\in V} f_i^{nm}\delta u_i^n - \frac{1}{V}\sum_n\sum_{m\in V}\left(m_i^{nm} + e_{ijk}x_j^{nm}f_k^{nm}\right)\delta\omega_i^n + \frac{1}{V}\sum_{b\in B} f_i^b\left(\delta u_i^b - \delta u_i^n\right)$$
$$+ \frac{1}{V}\sum_{b\in B} m_i^b\left(\delta\omega_i^b - \delta\omega_i^n\right) - \frac{1}{V}\sum_{b\in B} e_{ijk}x_j^{nb}f_k^b\delta\omega_i^n \tag{49}$$

The external work $\delta W_E^{d,2-\text{alt}}$ in Eq. (48) is identical to $\delta W_E^{d,2}$ in Eq. (9), so that the same external work expression, expressed in terms of macro strains, applies to both $\delta W_E^{d,2-\text{alt}}$ and $\delta W_E^{d,2}$ (see Eq. (14)). The internal work $\delta W_I^{d,2-\text{alt}}$ can also be expressed in terms of the macro strains δu_i^0, δu_{ij}^0, δu_{ijk}^0, $\delta\omega_i^0$ and $\delta\omega_{ij}^0$, and the resulting expression is identical to $\delta W_I^{d,2}$ in Eq. (15) (see Appendix B). That is,

$$\delta W_E^{d,2} = \delta W_E^{d,2-\text{alt}}; \quad \delta W_I^{d,2} = \delta W_I^{d,2-\text{alt}} \tag{50}$$

Therefore, the sums in Eqs. (19)–(22) are unaffected by shifting the central point for moment equilibrium, and the sums satisfy Condition 3. Since all of the macro and average stress quantities in Sections 3.3 and 3.4 were constructed from these sums, they, too, will satisfy Condition 3. The average stress proposed by Bardet and Vardoulakis (2001) does not satisfy this condition, as shown in Appendix C.

4. Conclusion

In the paper, we have introduced an expression of generalized virtual work, which accounts for the virtual work to deform the boundary of peripheral particles. We have shown that such peripheral deformation must be considered, otherwise the resulting stress expressions will violate two essential requirements of a stress measure.

We have made a distinction between macro stress and average stress, and we have derived expressions for both stresses. Because the macro stress is conjugate with the macro strain, the macro stress would be appropriate in approximating a discrete system as a continuum or in using representative particle clusters to derive constitutive relationships between the macro-scale stress and strain. The average stress, however, would be more useful in averaging the micro-scale stresses measured in physical or simulation experiments.

We have shown that the macro and average Cauchy stresses are equal but that subtle differences arise in the corresponding couple stresses and higher-order stresses. Moreover, different micro-scale continuum settings (e.g., classical or Cosserat) can lead to different averages of the couples stress, higher-order stress, and stress moment.

Appendix A. Simplifying the internal virtual work expression

In this appendix, we express the internal work $\delta W_I^{d,2}$ of Eq. (10) in terms of the macro strains δu_{ij}^0, δu_{ijk}^0, $\delta\omega_i^0$ and $\delta\omega_{ij}^0$ of the continuum fields $\delta\hat{u}_i$ and $\delta\hat{\omega}_i$ in Eq. (12). To simplify $\delta W_I^{d,2}$, we split Eq. (10) into several parts, express each part in terms of the continuum coefficients, and then reassemble the parts. We first consider the two "δu_i" terms in Eq. (10):

$$\delta W_I^{d,2,\delta u} = -\frac{1}{V}\sum_n \sum_{m\in V} f_i^{nm}\delta u_i^n + \frac{1}{V}\sum_{b\in B} f_i^b\left(\delta u_i^b - \delta u_i^n\right) \tag{A.1}$$

By constraining displacements δu_i^n (at the particle reference points $\mathbf{x}^n$) and δu_i^b (at the external contact points) to the continuum field $\delta\hat{u}_i$ in Eq. (12), the two terms in Eq. (A.1) become

$$\delta W_I^{d,2,\delta u} = \frac{1}{V}\sum_{c\in V} f_i^c\left(x_j^m - x_j^n\right)\delta u_{ij}^0 + \frac{1}{2V}\sum_{c\in V} f_i^c\left(x_j^m x_k^m - x_j^n x_k^n\right)\delta u_{ijk}^0 + \frac{1}{V}\sum_{c\in B} f_i^b\left(x_j^b - x_j^n\right)\delta u_{ij}^0$$
$$+\frac{1}{2V}\sum_{c\in V} f_i^b\left(x_j^b x_k^b - x_j^n x_k^n\right)\delta u_{ijk}^0 \tag{A.2}$$

where we use the notation $f_i^c = f_i^{nm} = -f_i^{mn}$ and $f_i^b = f_i^{nb}$. By combining summations over the interior and exterior contacts, we obtain

$$\delta W_I^{d,2,\delta u} = \frac{1}{V}\sum_{c\in V\cup B} f_i^c l_j^c \delta u_{ij}^0 + \frac{1}{2V}\sum_{c\in V\cup B} f_i^c J_{jk}^c \delta u_{ijk}^0 \tag{A.3}$$

with the terms l_i^c, J_{ij}^c, f_i^c, and m_i^c defined in Eqs. (16) and (17).

We now consider the three $\delta\omega_i$ (rotation) terms of Eq. (10):

$$\delta W_I^{d,2,\delta\omega} = -\frac{1}{V}\sum_n \sum_{m\in V}\left(m_i^{nm} + e_{ijk}r_j^{nc}f_k^{nm}\right)\delta\omega_i^n + \frac{1}{V}\sum_{b\in B} m_i^b\left(\delta\omega_i^b - \delta\omega_i^n\right) - \frac{1}{V}\sum_{b\in B} e_{ijk}r_j^{nb}f_k^{nb}\delta\omega_i^n \tag{A.4}$$

and constrain the rotations $\delta\omega_i^n$ and $\delta\omega_i^b$ to the continuum field $\delta\hat{\omega}_i$ in Eq. (12),

$$\delta W_I^{d,2,\delta\omega} = \left[-\frac{1}{V}\sum_n \sum_{m\in V}\left(m_i^{nm} + e_{ijk}r_j^{nc}f_k^{nm}\right)\delta\omega_i^0 - \frac{1}{V}\sum_{b\in B} e_{ijk}r_j^{nb}f_k^{nb}\delta\omega_i^0\right]$$
$$+\left[-\frac{1}{V}\sum_n \sum_{m\in V}\left(m_i^{nm} + e_{ijk}r_j^{nc}f_k^{nm}\right)x_\ell^n\delta\omega_{i\ell}^0 + \frac{1}{V}\sum_{b\in B} m_i^b\left(x_\ell^b - x_\ell^n\right)\delta\omega_{i\ell}^0 - \frac{1}{V}\sum_{b\in B} e_{ijk}r_j^{nb}f_k^{nb}x_\ell^n\delta\omega_{i\ell}^0\right] \tag{A.5}$$

Because the internal contact forces are self-equilibrating (as in Eq. (3)), we can combine terms in the first brackets as

$$\delta W_I^{d,2,\delta\omega,[1]} = -\frac{1}{V}\sum_n \sum_{m\in V} m_i^{nm}\delta\omega_i^0 - \frac{1}{V}\sum_{c\in V\cup B} e_{ijk}f_k^c l_j^c\delta\omega_i^0 \tag{A.6}$$

denoting this part with the superscript "[1]" and using the notations f_k^c and l_j^c defined in Eqs. (16) and (17). The first term in Eq. (A.6) is zero, since the internal contact moments are self-equilibrating, so that

$$\delta W_I^{d,2,\delta\omega,[1]} = -\frac{1}{V}\sum_{c\in V\cup B} e_{ijk}f_k^c l_j^c\delta\omega_i^0 \tag{A.7}$$

We now combine terms associated with the rotation gradient $\delta\omega_{i\ell}^0$ (i.e., terms in the second brackets "[2]" of Eq. (A.5)),

$$\delta W_I^{d,2,\delta\omega,[2]} = \frac{1}{V}\sum_{c\in V} m_i^c\left(x_\ell^m - x_\ell^n\right)\delta\omega_{i\ell}^0 + \frac{1}{V}\sum_{c\in V} e_{ijk}f_k^c\left(r_j^{mc}x_\ell^m - r_j^{nc}x_\ell^n\right)\delta\omega_{i\ell}^0 + \frac{1}{V}\sum_{b\in B} m_i^b\left(x_\ell^b - x_\ell^n\right)\delta\omega_{i\ell}^0 - \frac{1}{V}\sum_{b\in B} e_{ijk}r_j^{nb}f_k^b x_\ell^n\delta\omega_{i\ell}^0 \tag{A.8}$$

and after substituting l_ℓ^c, as defined in Eq. (16),

$$\delta W_I^{d,2,\delta\omega,[2]} = \frac{1}{V}\sum_{c\in V\cup B} m_i^c l_\ell^c\delta\omega_{i\ell}^0 + \frac{1}{V}\sum_{c\in V} e_{ijk}f_k^c\left(r_j^{mc}x_\ell^m - r_j^{nc}x_\ell^n\right)\delta\omega_{i\ell}^0 + \frac{1}{V}\sum_{b\in B} e_{ijk}f_k^b\left(0 - r_j^{nb}x_\ell^n\right)\delta\omega_{i\ell}^0 \tag{A.9}$$

The last two terms of Eq. (A.9) can be written in the form

$$\frac{1}{V}\sum_{c\in V} e_{ijk}f_k^c\left(\left(x_j^c - x_j^m\right)x_\ell^m - \left(x_j^c - x_j^n\right)x_\ell^n\right)\delta\omega_{i\ell}^0 + \frac{1}{V}\sum_{b\in B} e_{ijk}f_k^b\left(0 - \left(x_j^b - x_j^n\right)x_\ell^n\right)\delta\omega_{i\ell}^0 \tag{A.10}$$

which can be expanded to

$$\frac{1}{V}\sum_{c\in V} e_{ijk}f_k^c\left(x_j^c x_\ell^m - x_j^c x_\ell^n\right)\delta\omega_{i\ell}^0 - \frac{1}{V}\sum_{c\in V} e_{ijk}f_k^c\left(x_j^m x_\ell^m - x_j^n x_\ell^n\right)\delta\omega_{i\ell}^0 + \frac{1}{V}\sum_{b\in B} e_{ijk}f_k^b\left(0 - x_j^b x_\ell^n\right)\delta\omega_{i\ell}^0 - \frac{1}{V}\sum_{b\in B} e_{ijk}f_k^b\left(0 - x_j^n x_\ell^n\right)\delta\omega_{i\ell}^0 \tag{A.11}$$

We can add and subtract equivalent values in the last two terms,

$$\frac{1}{V}\sum_{c\in V} e_{ijk}f_k^c\left(x_j^c x_\ell^m - x_j^c x_\ell^n\right)\delta\omega_{i\ell}^0 - \frac{1}{V}\sum_{c\in V} e_{ijk}f_k^c\left(x_j^m x_\ell^m - x_j^n x_\ell^n\right)\delta\omega_{i\ell}^0 + \frac{1}{V}\sum_{b\in B} e_{ijk}f_k^b\left(x_j^b x_\ell^b - x_j^b x_\ell^n\right)\delta\omega_{i\ell}^0 - \frac{1}{V}\sum_{b\in B} e_{ijk}f_k^b\left(x_j^b x_\ell^b - x_j^n x_\ell^n\right)\delta\omega_{i\ell}^0 \tag{A.12}$$

and combine the summation ranges,

$$\frac{1}{V}\sum_{c\in V\cup B} e_{ijk}f_k^c l_\ell^c x_j^c\delta\omega_{i\ell}^0 - \frac{1}{V}\sum_{c\in V\cup B} e_{ijk}f_k^c J_{j\ell}^c\delta\omega_{i\ell}^0 \tag{A.13}$$

The total internal work $\delta W_I^{d,2}$ in Eq. (5) is the sum of the following parts: $\delta W_I^{d,2,\delta\omega,[1]}$ in Eq. (A.7), the first term of $\delta W_I^{d,2,\delta\omega,[2]}$ in Eq. (A.9), and expression (A.13) for the final two terms of $\delta W_I^{d,2,\delta\omega,[2]}$:

$$\delta W_I^{d,2} = \frac{1}{V}\sum_{c\in V\cup B} f_i^c l_j^c\delta u_{ij}^0 + \frac{1}{2V}\sum_{c\in V\cup B} f_i^c J_{jk}^c\delta u_{ijk}^0 - \frac{1}{V}\sum_{c\in V\cup B} e_{ijk}f_k^c l_j^c\delta\omega_i^0 + \frac{1}{V}\sum_{c\in V\cup B}\left(m_i^c l_\ell^c + e_{ijk}f_k^c l_\ell^c x_j^c\right)\delta\omega_{i\ell}^0 - \frac{1}{V}\sum_{c\in V\cup B} e_{ijk}f_k^c J_{j\ell}^c\delta\omega_{i\ell}^0 \tag{A.14}$$

This result is shown in Eq. (15) of Section 3.3 and used in finding the relations among the contact sums in Eqs. (19)–(22).

Appendix B. Internal virtual work with a single central point of moment equilibrium

Eq. (49) gives the virtual work $\delta W_E^{d,2-\text{alt}}$ that results from using a single central point in the moment equilibrium equations of each particle. In this appendix, we constrain the displacements δu_i^n, $\delta\omega_i^n$, δu_i^b and $\delta\omega_i^b$ to the continuum fields $\delta\hat{u}_i$ and $\delta\hat{\omega}_i$ of Eqs. (12) and (13), which are applied at the many particle reference points $\mathbf{x}^n$.

The first and third terms of Eq. (49) are identical to those of Eq. (10) and after introducing the continuum variables δu^0_{ij} and δu^0_{ijk}, these two terms will yield the first and second terms in Eq. (15), as developed in Appendix A. Eq. (49) becomes

$$\delta W_I^{d,2\text{-alt}} = \frac{1}{V}\sum_{c\in V\cup B} f_i^c l_j^c \delta u^0_{ij} + \frac{1}{2V}\sum_{c\in V\cup B} f_i^c J^c_{jk}\delta u^0_{ijk} - \frac{1}{V}\sum_n\sum_{m\in V}\left(m_i^{nm} + e_{ijk}x_j^{nm}f_k^{nm}\right)\delta\omega_i^0$$
$$-\frac{1}{V}\sum_n\sum_{m\in V}\left(m_i^{nm} + e_{ijk}x_j^{nm}f_k^{nm}\right)x_\ell^n\delta\omega^0_{i\ell} + \frac{1}{V}\sum_{b\in B} m_i^b\left(x_\ell^b - x_\ell^n\right)\delta\omega^0_{i\ell} - \frac{1}{V}\sum_{b\in B} e_{ijk}x_j^{nb}f_k^{nb}\delta\omega_i^0$$
$$-\frac{1}{V}\sum_{b\in B} e_{ijk}x_j^{nb}f_k^{nb}x_\ell^n\delta\omega^0_{i\ell} \tag{B.1}$$

The third term in Eq. (B.1) is zero, since forces and moments at internal contacts are self-equilibrating (as in Eq. (3)). The sixth term in Eq. (B.1) can also be expressed with the notation

$$-\frac{1}{V}\sum_{b\in B} e_{ijk}x_j^b f_k^b\delta\omega_i^0 \tag{B.2}$$

Eq. (19) implies that (B.2) has the alternative form

$$-\frac{1}{V}\sum_{b\in B} e_{ijk}x_j^b f_k^b\delta\omega_i^0 = -\frac{1}{V}\sum_{c\in V\cup B} e_{ijk}f_k^c l_j^c\delta\omega_i^0 \tag{B.3}$$

Because the positions x_j^{nm} are at the contact points, whereas positions x_j^n are at the particle centers, the fourth term in Eq. (B.1) can be rewritten with the internal contact set $c \in V$:

$$-\frac{1}{V}\sum_n\sum_{m\in V}\left(m_i^{nm} + e_{ijk}x_j^{nm}f_k^{nm}\right)x_\ell^n\delta\omega^0_{i\ell} = \frac{1}{V}\sum_{c\in V}\left(m_i^c l_\ell^c + e_{ijk}f_k^c x_j^c l_\ell^c\right)\delta\omega^0_{i\ell} \tag{B.4}$$

where $x_i^c = x_i^{nm} = x_i^{mn}$ for interior contacts, and f_i^c, m_i^c, and l_i^c are defined in Eqs. (16) and (17). This term can be combined with the two remaining $\delta\omega^0_{i\ell}$ terms in Eq. (B.1):

$$\frac{1}{V}\sum_{c\in V\cup B} m_i^c l_\ell^c\delta\omega^0_{i\ell} + \frac{1}{V}\sum_{c\in V} e_{ijk}f_k^c x_j^c l_\ell^c\delta\omega^0_{i\ell} - \frac{1}{V}\sum_{b\in B} e_{ijk}f_k^{nb}x_j^{nb}\left(x_\ell^b - l_\ell^b\right)\delta\omega^0_{i\ell}$$
$$= \frac{1}{V}\sum_{c\in V\cup B}\left(m_i^c l_\ell^c + e_{ijk}f_k^c x_j^c l_\ell^c\right)\delta\omega^0_{i\ell} - \frac{1}{V}\sum_{b\in B} e_{ijk}f_k^b x_j^b x_\ell^b\delta\omega^0_{i\ell} \tag{B.5}$$

We can apply Eq. (20) to the last term in Eq. (B.5), replacing it as follows:

$$-\frac{1}{V}\sum_{b\in B} e_{ijk}f_k^b x_j^b x_\ell^b\delta\omega^0_{i\ell} = -\frac{1}{V}\sum_{c\in V\cup B} e_{ijk}f_k^c J^c_{j\ell}\delta\omega^0_{i\ell} \tag{B.6}$$

Finally, we recombine the parts of $\delta W_I^{d,2\text{-alt}}$ in Eq. (B.1): the first two terms of Eq. (15) and Eqs. (B.3), (B.5) and (B.6). The result is

$$\delta W_I^{d,2\text{-alt}} = \frac{1}{V}\sum_{c\in V\cup B} f_i^c l_j^c\delta u^0_{ij} + \frac{1}{2V}\sum_{c\in V\cup B} f_i^c J^c_{jk}\delta u^0_{ijk} - \frac{1}{V}\sum_{c\in V\cup B} e_{ijk}f_k^c l_j^c\delta\omega_i^0$$
$$+\frac{1}{V}\sum_{c\in V\cup B}\left(m_i^c l_j^c + e_{ijk}f_k^c l_\ell^c x_j^c\right)\delta\omega^0_{i\ell} - \frac{1}{V}\sum_{c\in V\cup B} e_{ijk}f_k^c J^c_{j\ell}\delta\omega^0_{i\ell} \tag{B.7}$$

which is identical to $\delta W_I^{d,2}$ in Eq. (15).

Appendix C. Alternative stress definition

In Sections 3.4 and 3.5, we used the virtual work $\delta W^{d,2}$ of Eq. (5) to derive definitions of average stress quantities. In this section, we instead use the virtual work $\delta W^{d,1}$ of Eq. (4), as in Bardet and Vardoulakis (2001), and show that this approach leads to stress definitions that violate Conditions 1 and 3, as presented in Section 1.

The external and internal virtual works associated with $\delta\ W^{d,1}$ are given in Eqs. (7) and (8), which we repeat:

$$\delta W_E^{d,1} = \frac{1}{V}\sum_n \sum_{b\in B} f_i^{nb}\delta u_i^n + \frac{1}{V}\sum_n \sum_{b\in B}\left(m_i^{nb} + e_{ijk}r_j^{nb}f_k^{nb}\right)\delta\omega_i^n \tag{C.1}$$

$$\delta W_I^{d,1} = -\frac{1}{V}\sum_n \sum_{m\in V} f_i^{nm}\delta u_i^n - \frac{1}{V}\sum_n \sum_{m\in V}\left(m_i^{nm} + e_{ijk}r_j^{nm}f_k^{nm}\right)\delta\omega_i^n \tag{C.2}$$

In this alternative to Eqs. (9) and (10), deformation is not permitted for peripheral particles. Here, an external force f_i^{nb} moves and rotates with its particle about the particle's interior reference point $\mathbf{x}^n$, which implies that the peripheral particles are rigid between their interior reference points and their external contact points. Indeed, the term "external work" many not be appropriate with Eq. (C.1), since $\delta W_E^{d,1}$ involves the products of external forces (f_i^{nb} and m_i^{nb}) and internal displacements (δu_i^n and $\delta\omega_i^n$). Both issues were removed in Eq. (5) by introducing the independent movements δu_i^b and $\delta\omega_i^b$ of the boundary points. The external work done by the forces f_i^{nb} in Eq. (9) differs from that in Eq. (C.1) by the amounts $f_i^{nb}(\delta u_i^b - \delta u_i^n)$, and the differences between the external work done by the moments m_i^{nb} in Eqs. (9) and (C.1) are $m_i^{nb}(\delta\omega_i^b - \delta\omega_i^n) - e_{ijk}r_j^{nb}f_k^{nb}\delta\omega_i^n$. These external work differences are transferred into the internal work of Eq. (10), since this work is produced by deformation within the peripheral particles.

Restricting the virtual displacements and rotations to the continuum fields in Eqs. (12) and (13) gives the following external virtual work:

$$\begin{aligned}\delta W_E^{d,1} = {} & \frac{1}{V}\sum_{b\in B} f_i^b\delta u_i^0 + \frac{1}{V}\sum_{b\in B} f_i^b x_j^n\delta u_{ij}^0 + \frac{1}{2V}\sum_{b\in B} f_i^b x_j^n x_k^n\delta u_{ijk}^0 + \frac{1}{V}\sum_{b\in B}\left(m_i^b + e_{ijk}r_j^{nb}f_k^b\right)\delta\omega_i^0 \\ & + \frac{1}{V}\sum_{b\in B}\left(m_i^b x_j^n + e_{i\ell k}r_\ell^{nb}f_k^b x_j^n\right)\delta\omega_{ij}^0\end{aligned} \tag{C.3}$$

where we now use the superscript notation f_i^b and m_i^b for the boundary forces (replacing f_i^{nb} and m_i^{nb}). The superscript "b" indicates an external contact point, whereas x_i^n is the location of the (interior) reference point $\mathbf{x}^n$ of the peripheral particle that contains the contact b. Vector r_j^{nb} joins the reference point $\mathbf{x}^n$ of particle n to the external contact point b. Because the external forces are in equilibrium, $\sum f_i^b = 0$, and the first sum in Eq. (C.3) will, henceforth, be removed.

We now restrict the virtual displacements in $\delta W_I^{d,1}$ to the fields $\delta\hat{u}_i$ and $\delta\hat{\omega}_i$ of Eqs. (12) and (13), so that Eq. (C.2) becomes

$$\begin{aligned}\delta W_I^{d,1} = {} & -\frac{1}{V}\sum_n \sum_{m\in V} f_i^{nm}\delta u_i^0 - \frac{1}{V}\sum_n \sum_{m\in V} f_i^{nm}x_j^n\delta u_{ij}^0 - \frac{1}{2V}\sum_n \sum_{m\in V} f_i^{nm}x_j^n x_k^n\delta u_{ijk}^0 \\ & - \frac{1}{V}\sum_n \sum_{m\in V}\left(m_i^{nm} + e_{i\ell k}r_\ell^{nm}f_k^{nm}\right)\left(\delta\omega_i^0 + x_j^n\delta\omega_{ij}^0\right)\end{aligned} \tag{C.4}$$

Because the internal contact forces are self-equilibrating (Eq. (3)), the first term in Eq. (C.4) is zero and the second term can be simplified as

$$-\frac{1}{V}\sum_{n}\sum_{m\in V} f_i^{nm} x_j^n \delta u_{ij}^0 = -\frac{1}{V}\sum_{c\in V}\left(f_i^{nm}x_j^n + f_i^{mn}x_j^m\right)\delta u_{ij}^0 = \frac{1}{V}\sum_{c\in V} f_i^c l_j^c \delta u_{ij}^0 \tag{C.5}$$

where the contact force $f_i^c = f_i^{nm} = -f_i^{mn}$ and the branch vector $l_j^c = x_j^m - x_j^n$. In this notation, f_i^c is the contact force exerted by particle m on particle n ; and l_j^c connects x_j^n to x_j^m. The internal contact moments are also self-equilibrating, so the sum of products $m_i^{nm}\delta\omega_i^0$ in Eq. (C.4) is also zero, and the equation can be simplified as

$$\delta W_I^{d,1} = \frac{1}{V}\sum_{c\in V} f_i^c l_j^c \delta u_{ij}^0 + \frac{1}{2V}\sum_{c\in V} f_i^c J_{jk}^c \delta u_{ijk}^0 - \frac{1}{V}\sum_{c\in V} e_{ijk} f_k^c l_j^c \delta\omega_i^0 + \frac{1}{V}\sum_{c\in V}\left(m_i^c l_j^c + e_{i\ell k} f_k^c \left(r_\ell^{mc} x_j^m - r_\ell^{nc} x_j^n\right)\right)\delta\omega_{ij}^0 \tag{C.6}$$

with the symmetric tensor $J_{jk}^c = x_j^m x_k^m - x_j^n x_k^n$. The radial vector r_j^{nc} is measured from the reference point $\mathbf{x}^n$ of particle n to its contact c with neighbor m; radial vector r_j^{mc} is from the reference point $\mathbf{x}^m$ of particle m to the same contact point. The branch vector in Eq. (C.6) can also be expressed as $l_j^c = r_j^{nc} - r_j^{mc}$.

Eqs. (6), (C.3) and (C.6) imply the following equivalences among the force sums:

$$\frac{1}{V}\sum_{b\in B} f_i^b x_j^n = \frac{1}{V}\sum_{c\in V} f_i^c l_j^c \tag{C.7}$$

$$\frac{1}{V}\sum_{b\in B} f_i^b x_j^n x_k^n = \frac{1}{V}\sum_{c\in V} f_i^c J_{jk}^c \tag{C.8}$$

$$\frac{1}{V}\sum_{b\in B}\left(m_i^b + e_{ijk} r_j^{nb} f_k^b\right) = -\frac{1}{V}\sum_{c\in V} e_{ijk} f_k^c l_j^c \tag{C.9}$$

$$\frac{1}{V}\sum_{b\in B}\left(m_i^b + e_{i\ell k} r_\ell^{nb} f_k^b\right)x_j^n = \frac{1}{V}\sum_{c\in V}\left[m_i^c l_j^c + e_{i\ell k} f_k^c\left(r_\ell^{mc} x_j^m - r_\ell^{nc} x_j^n\right)\right] \tag{C.10}$$

Bardet and Vardoulakis (2001) derived these same equations and used them to find expressions for the average stress in a representative volume. For example, Eq. (C.7) leads to the average stress

$$\bar{\sigma}_{ji} = \frac{1}{V}\sum_{b\in B} f_i^b x_j^n = \frac{1}{V}\sum_{c\in V} f_i^c l_j^c \tag{C.11}$$

The difference between this definition and that in Eq. (36) lies in their summation ranges. In Eq. (C.11), the summation on the right is limited to interior contacts, but the summation on the right of Eq. (36) is carried over all contacts, both interior and exterior. Eq. (C.9) implies that the average stress may not be symmetric, even in the absence of contact moments, since

$$e_{ijk}\bar{\sigma}_{ji} = \frac{1}{V}\sum_{b\in B}\left(m_i^b + e_{ijk} r_j^{nb} f_k^b\right) = -\frac{1}{V}\sum_{c\in V} e_{ijk} f_k^c l_j^c \tag{C.12}$$

which can be non-zero even when the moments m_i^b are zero.

Eqs. (C.7)–(C.10) are a valid consequence of equilibrium, but we must also determine whether the sums satisfy the three conditions prescribed in Section 1. In regard to Condition 1, all of the sums in Eqs. (C.7)–(C.10) fail: none is independent of the reference points $\mathbf{x}^n$ that are assigned to the peripheral particles (Fig. 1c). This shortcoming is evident in Eq. (C.9), since shifting a peripheral particle's reference point will alter its location x_j^n and the radial vector r_j^{nb}, which will change the sums on the left of Eqs. (C.7)–(C.10). For example, shifting the reference point $\mathbf{x}^n$ of a single peripheral particle will alter the stress anisotropy in

Eq. (C.9). It might be reasoned that this shortcoming is a consequence of forcing the continuum restriction of Eq. (12) at the discrete points $\mathbf{x}^n$. The shortcoming in the sums is more fundamental, however, particularly in regard to Condition 3, as will be shown below. As for Condition 2, the sums in Eqs. (C.7)–(C.10) are objective for the same reasons given in Section 3.5 for the sums in Eqs. (19)–(22). The third condition is addressed in the following paragraphs.

Moment equilibrium is valid for any choice of a central point. In the first part of this appendix, moment equilibrium has been applied with respect to a different central point for each particle (Eq. (2)), since these central points coincide with the particle reference points $\mathbf{x}^n$. Another possible choice is a single, common central point for all particles in the representative volume, as was done in Section 3.7. With this approach, the moment equilibrium equations $(2)_2$ are replaced with those in Eqs. (46), and the virtual work $\delta W^{d,1-\text{alt}}$ in Eq. (4) becomes

$$\delta W^{d,1\text{-alt}} = \frac{1}{V}\sum_n\left(\sum_{b\in B} f_i^{nb} + \sum_{m\in V} f_i^{nm}\right)\delta u_i^n + \frac{1}{V}\sum_n\left(\sum_{b\in B}\left(m_i^{nb} + e_{ijk}x_j^{nb}f_k^{nb}\right) + \sum_{m\in V}\left(m_i^{nm} + e_{ijk}x_j^{nm}f_k^{nm}\right)\right)\delta\omega_i^n = 0 \tag{C.13}$$

where the superscript "alt" distinguishes the virtual work $\delta W^{d,1-\text{alt}}$ from the work $\delta W^{d,1}$ in Eq. (4). Neglecting the contribution of body forces and moments, f_i^n and m_i^n, the new external and internal works are

$$\delta W_E^{d,1\text{-alt}} = \frac{1}{V}\sum_n\sum_{b\in B} f_i^{nb}\delta u_i^n + \frac{1}{V}\sum_n\sum_{b\in B}\left(m_i^{nb} + e_{ijk}x_j^{nb}f_k^{nb}\right)\delta\omega_i^n \tag{C.14}$$

$$\delta W_I^{d,1\text{-alt}} = -\frac{1}{V}\sum_n\sum_{m\in V} f_i^{nm}\delta u_i^n - \frac{1}{V}\sum_n\sum_{m\in V}\left(m_i^{nm} + e_{ijk}x_j^{nm}f_k^{nm}\right)\delta\omega_i^n \tag{C.15}$$

Although the equilibrium equations (46) are as valid as Eqs. $(2)_2$, the resulting external virtual work expressions (C.1) and (C.14) are different, as are the internal work expressions (C.2) and (C.15). After restricting the displacements and rotations to the continuum fields in Eqs. (12) and (13), the alternative external virtual work is

$$\delta W_E^{d,1\text{-alt}} = \frac{1}{V}\sum_{b\in B} f_i^b\delta u_i^0 + \frac{1}{V}\sum_{b\in B} f_i^b x_j^n\delta u_{ij}^0 + \frac{1}{2V}\sum_{b\in B} f_i^b x_j^n x_k^n\delta u_{ijk}^0 + \frac{1}{V}\sum_{b\in B}\left(m_i^b + e_{ijk}x_j^b f_k^b\right)\delta\omega_i^0 + \frac{1}{V}\sum_{b\in B}\left(m_i^b x_j^n + e_{i\ell k}x_\ell^b f_k^b x_j^n\right)\delta\omega_{ij}^0 \tag{C.16}$$

In this equation, vector x_j^n is measured from the common central point to the reference point $\mathbf{x}^n$ of particle n, since we have constrained the virtual displacements to coincide with the continuum field (12) at these points. The vectors x_j^{nb}, however, are measured to the external contacts, as required for moment equilibrium. The fourth sum in Eq. (C.16) is zero, since the representative volume must be in (external) moment equilibrium.

Because Eqs. (C.3) and (C.16) differ, they will imply different average stresses. To find the alteration of stress, we also write the internal work (C.15) in terms of the continuum variables:

$$\delta W_I^{d,1\text{-alt}} = \frac{1}{V}\sum_{c\in V} f_i^c l_j^c\delta u_{ij}^0 + \frac{1}{2V}\sum_{c\in V} f_i^c J_{jk}^c\delta u_{ijk}^0 + \frac{1}{V}\sum_{c\in V}\left(m_i^c l_j^c + e_{i\ell k}f_k^c x_\ell^c l_j^c\right)\delta\omega_{ij}^0 \tag{C.17}$$

where the x_j^c are measured to the interior contact points, and $f_i^c = f_i^{nm} = -f_i^{mn}$. This internal work expression differs from that in Eq. (C.6). Comparing Eqs. (C.3) and (C.6) with Eqs. (C.16) and (C.17), we see that shifting the central point for moment equilibrium will alter the stress quantities. In particular, the virtual rotation $\delta\omega_i^0$ does no work in $\delta W_I^{d,1-\mathrm{alt}}$, so that each sum in Eq. (C.9) is now zero, and the stress anisotropy in Eq. (C.12) is zero. Moreover, the sums in Eq. (C.10) are now replaced with

$$\frac{1}{V}\sum_{b\in B}\left(m_i^b + e_{i\ell k}x_\ell^b f_k^b\right)x_j^n = \frac{1}{V}\sum_{c\in V}\left(m_i^c l_j^c + e_{i\ell k} f_k^c x_j^c l_\ell^c\right) \tag{C.18}$$

so that the average couple stress and stress moment are altered as well. In summary, stress formulations derived from the work $\delta W^{d,1}$, as with Bardet and Vardoulakis (2001), violate Conditions 1 and 3.

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