ABSTRACT: The objective of the paper is to demonstrate the calculation of micromorphic continuum stress measures based directly on three-dimensional (3D) ellipsoidal discrete element (DE) simulations over representative volume elements (RVE) within the DE domain representing granular media. We will demonstrate these calculations for two simulations: (1) pile penetration, and (2) cavity expansion. All calculations are assumed to be performed in the current configuration with respect to a large deformation micromorphic continuum mechanics analysis. The micromorphic continuum stresses include the unsymmetric third order couple stress tensor $m_{ijk}$, symmetric second order micro-stress tensor $s_{ij}$, and unsymmetric second order Cauchy stress tensor $\sigma_{ij}$. The DE continuum stress measure due to Christoffersen et al. (1981) and Rothenburg & Selvadurai (1981), is used as the symmetric “micro-element” stress tensor $\sigma'_{ij}$ for micromorphic continuum mechanics (Eringen & Suhubi 1964). The balance equations solved are the balance of linear and angular momenta for the DE simulations, whereas the micromorphic continuum stress measures are only used to interpret the DE simulation results, at the moment.

1 INTRODUCTION

To date, homogenized continuum modeling of granular materials has considered primarily traditional continuum mechanics as the overlaying framework (Christoffersen et al. 1981, Rothenburg and Selvadurai 1981, Chang et al. 1992, Borja and Wren 1995, Muhlhau et al. 2000, Peters 2005, Andrade and Tu 2009) or higher order methods like micropolar continuum mechanics or enhanced continua with strain gradients (Chang and Gao 1995, Walsh and Tordesillas 2004, Pasternak and Muhlhaus 2005, Gardiner and Tordesillas 2006). These methods involve attempts to either replace the underlying discrete particle mechanics with an equivalent continuum constitutive model, or provide a continuum framework to which to up-scale the discrete particle mechanics through underlying Discrete Element Method (DEM) simulations (Cundall & Strack 1979) via hierarchical up-scaling procedures. We are interested in both approaches, but follow here the spirit of the latter class of methods (hierarchical up-scaling), and we use micromorphic continuum mechanics as the overlaying continuum mechanics framework. In the paper, we focus only on the micromorphic continuum stress measures, and consider micromorphic deformation and strain measures for future work. We focus on the micromorphic theory because of the additional kinematics it provides, through not only the micro-rotation of a micro-element volume (e.g., the Representative Volume Element (RVE) of a granular material), but also micro-stretch and micro-shear. The micropolar theories were primarily motivated for granular materials because of the additional rotational degrees of freedom of the individual particles, but these theories miss the ability to model clusters of particles that also shear and compact/dilate.

1.1 Brief background on the kinematics of a micromorphic continuum at finite strain

Figure 1 presents the mapping from the reference configuration $B_0$ to the current configuration $B$ through the deformation gradient $F_{kK}$ $(dx_k = F_{kK}dX_K)$ and micro-deformation tensor $\chi_{kK}$ $(\xi_k = \chi_{kK}\Xi_K)$. $\Xi_K$ is the relative position vector between the centroid $C$ of the macro-element differential volume $dV$ and the centroid $C'$ of the micro-element differential volume $dV'$ in the reference configuration $B_0$. Similarly, $\xi_k$ is the relative position vector between the centroid $c$ of the macro-element differential volume $dv$ and the centroid $c'$ of the micro-element differential volume...
\[ \sigma_{kl} = \frac{1}{2v_{RVE}} \sum_{\epsilon=1}^{M} (f_k^\epsilon b_l^\epsilon + b_l^\epsilon f_k^\epsilon) \]
Regueiro 2010).

To continue in this direction, we define, based on the previous discussion, a volume average for the symmetric micro-stress $s_{kl}$ and unsymmetric couple stress $m_{klm}$ as

$$s_{kl} \defeq \frac{1}{\Omega_{\alpha}^{\text{avg}}} \int_{\Omega_{\alpha}^{\text{avg}}} \sigma'_{kl} dv'$$

$$m_{klm} \defeq \frac{1}{\Omega_{\alpha}^{\text{avg}}} \int_{\Omega_{\alpha}^{\text{avg}}} \sigma'_{kl} \xi_m dv'$$

Before moving on, recall that balance equations are derived by localizing an integral over the body $B$ in the current configuration. We consider discrete approximations to these integrals (e.g., an eventual Gaussian quadrature rule), such that

$$\int_B (\bullet) dv = \sum_{\alpha=1}^{n_{\text{avg}}} \int_{\Omega_{\alpha}^{\text{avg}}} (\bullet)' dv' \approx \sum_{\alpha=1}^{n_{\text{avg}}} (\bullet)_\alpha W_{\text{avg}}^{\text{avg}} \Omega_{\alpha}^{\text{avg}}$$

$$\int_{\Omega_{\alpha}^{\text{avg}}} (\bullet)' dv' \approx \sum_{RVE} (\bullet)' W^{RVE} v^{RVE}$$

where $W_{\text{avg}}$ and $W^{RVE}$ are the weights of integration, which for now we assume $W_{\text{avg}} = W^{RVE} = 1$ (later, these will take appropriate values in the context of a FE, FD, or meshfree numerical implementation).

For example, the micromorphic continuum symmetric micro-stress $s_\alpha$ at point $c_\alpha$ within averaging domain $\Omega_{\alpha}^{\text{avg}}$ can be calculated as,

$$\langle s_{kl} \rangle_\alpha = \frac{1}{\Omega_{\alpha}^{\text{avg}}} \sum_{RVE} \sigma'_{kl} v^{RVE}$$

and likewise for the micromorphic continuum unsymmetric couple stress $m_\alpha$ as

$$\langle m_{klm} \rangle_\alpha = \frac{1}{\Omega_{\alpha}^{\text{avg}}} \sum_{RVE} \sigma'_{kl} \xi_m v^{RVE}$$

The question then becomes how to calculate the micromorphic continuum unsymmetric Cauchy stress $\sigma_\alpha$ at point $c_\alpha$. Recall from the micromorphic continuum theory (Eringen & Suhubi 1964) that the stresses are defined as follows,

$$s_{mk} dv \defeq \int_{dv} \sigma'_{mk} dv'$$

$$\sigma_{kl} n_\alpha da \defeq \int_{da} \sigma'_{kl} n'_\alpha da'$$

$$m_{klm} n_\alpha da \defeq \int_{da} \sigma'_{kl} \xi_m n'_\alpha da'$$

Thus, the volume average definition for $s$ in (2) and (5) is in line with micromorphic continuum theory in (7), whereas the volume average definition for $m$ in (3) and (6) is an assumption when compared to (9). The unsymmetric Cauchy stress $\sigma$, however, cannot be uniquely determined from (8), nor can it be estimated by a volume average of $\sigma'$ because this is the definition for $s$. Thus, we resort to the balance of first moment of momentum to calculate $\sigma$.

The balance of first moment of momentum of the micromorphic theory, integrated over the body $B$ in the current configuration, is written as (Eringen & Suhubi 1964, Eringen 1999),

$$\int_B \left[ \sigma_{mk} - s_{mk} + m_{km} \ell + \rho (\ell_{km} - \omega_{km}) \right] dv = 0$$

where $\rho$ is the mass density, $\ell_{km}$ the body force couple per unit mass, and $\omega_{km}$ the micro-spin inertia. We can analyze each term separately, with in mind that we want to solve for $\sigma_\alpha$ at point $c_\alpha$:

$$\int_B \sigma_{mk} dv = \sum_{\alpha=1}^{n_{\text{avg}}} (\sigma_{mk})_\alpha \Omega_{\alpha}^{\text{avg}}$$

$$\int_B s_{mk} dv = \sum_{\alpha=1}^{n_{\text{avg}}} (s_{mk})_\alpha \Omega_{\alpha}^{\text{avg}} = \sum_{\alpha=1}^{n_{\text{avg}}} \sum_{RVE} \sigma'_{kl} v^{RVE}$$

$$\int_B m_{km} dv = \int_{\partial B} m_{km} n_\alpha da$$

$$\approx \sum_{\alpha=1}^{n_{\text{avg}}} \sum_{RVE} \sigma'_{kl} \xi_m n'_\alpha v^{RVE}$$

$$\int_B \rho \ell_{km} dv \approx \sum_{\alpha=1}^{n_{\text{avg}}} \sum_{RVE} \rho' g_{km} \xi_m v^{RVE}$$

$$\int_B \rho \omega_{km} dv \approx \sum_{\alpha=1}^{n_{\text{avg}}} \sum_{RVE} \rho' g_{km} \xi_m v^{RVE}$$
where \( g_k \) is the gravity acceleration vector, \( \rho' \) is the mass density of particles in \( v^{RVE} \), and \( a_k^\xi = \xi_k \) is the acceleration of the relative position vector which is important for dynamics problems, as will be seen for the cavity expansion problem in the Numerical Examples. We calculate \( a_k^\xi \) based on the motion of the relative position vector \( \xi_k \), which tracks the centroids of the RVEs \( c^* \) with respect to the centroid of the averaging domain \( c_\alpha \). In this case, the RVEs are assumed to move with the particles, as for the cavity expansion example in Section 3.2. Then, substituting (11)-(12) into (10), we can solve for the micro-morphic continuum unsymmetric Cauchy stress \( \sigma_\alpha \) at point \( c_\alpha \). Note that as \( \xi \to 0 \), \( \sigma_\alpha = s_\alpha \), and the Cauchy stress is symmetric (i.e., it is the same as the symmetric micro-stress, and vice versa). Thus, for certain continuum mechanics problems of interest to geotechnical and geological engineers, the granular material can be treated as a classical continuum such that the assumption \( \xi \to 0 \) is valid. For specific problems of interest, however, the discrete nature of the granular material from the perspective of a penetrometer in sand, or tire rolling through gravel, \( \xi \) is finite, and thus a generalized continuum theory like micromorphic continuum mechanics may provide additional insight into the mechanics of granular media. At the very least, it will be relevant for overlap coupling procedures, as shown in Fig.2, where the degree of freedom (dof) mismatch between DEM and classical FEM in the overlap region is apparent, and the additional dof in the micromorphic continuum should improve such procedures.

3 NUMERICAL EXAMPLES

We demonstrate the hierarchical up-scaling procedure in Section 2 for calculating the three micromorphic continuum stresses \( (\sigma_{ij}, s_{ij}, m_{ijk}) \) by conducting three-dimensional (3D) ellipsoidal DE simulations for two examples: (1) pile penetration, and (2) cavity expansion. Particle properties are indicated in Table 1.

For comparison purposes in the results, we also represent the various stress measures. For both mean and octahedral shear stress in Fig.5, the shear stress increases as the particles in \( \Omega^\alpha \) shear with respect to each other during pile penetration. Now let us compare the various stress measures. For both mean and

![Figure 4: Side view of pile penetration simulation, showing averaging domain \( \Omega^\alpha \) drawn by box in the initial penetration zone.](image)

### 3.1 Pile penetration

This example is run quasi-statically, with the ‘pilé’ represented as a large ellipsoidal particle for now (see Fig.4). Further details are found in Yan et al. (2010). The averaging domain \( \Omega^\alpha_{\text{avg}} \) is drawn by a box in the initial penetration zone, and is divided into \( 2 \times 2 \times 2 = 8 \) RVEs. These RVEs are fixed. For comparison purposes, the mean couple stress and deviatoric couple stress are defined as follows,

\[
(p_{\text{m}})_{m}^\alpha \; \text{def} \; \frac{1}{3} (m_{\text{aam}})_{\alpha}
\]

\[
\implies p_{\alpha}^\text{couple} = \sqrt{\p_{\alpha}^\text{couple} \cdot \p_{\alpha}^\text{couple}}
\]

\[
\text{dev}(m_{lkm})_{\alpha} \; \text{def} \; (m_{lkm})_{\alpha} - (p_{\text{m}}^\alpha)_{\alpha} \delta_{lkm}
\]

\[
\implies \sigma_{\text{oct,couple}} = \sqrt{\frac{1}{3} \sqrt{\text{dev}(m_{\alpha}) \cdot \text{dev}(m_{\alpha})}}
\]

The plots of mean stress and octahedral shear stress are shown in Fig.5, calculated over the averaging domain \( \Omega^\alpha_{\text{avg}} \) as discussed in Section 2. They compare the following six stress results: (i) symmetric micro-stress \( s_\alpha \), (ii) unsymmetric Cauchy stress \( \sigma_\alpha \), (iii) unsymmetric Cauchy stress \( \sigma_\alpha \) without micro-spin inertia \( \rho \omega \) term in (10), (iv) unsymmetric Cauchy stress \( \sigma_\alpha \) without micro-spin inertia \( \rho \omega \) and body force couple \( \rho \ell \) terms, (v) unsymmetric couple stress \( m_\alpha \), and (vi) unsymmetric granular stress \( \Omega^\alpha \). It is observed that for each mean stress history in Fig.5, as the pile penetrates through the averaging domain \( \Omega^\alpha_{\text{avg}} \) (see box in Fig.4), the mean stress increases in compression (negative), and then begins to decrease as the pile passes through \( \Omega^\alpha_{\text{avg}} \) (the depth of \( \Omega^\alpha_{\text{avg}} \) is 0.03m). Similarly, for octahedral shear stress in Fig.5, the shear stress increases as the particles in \( \Omega^\alpha_{\text{avg}} \) shear with respect to each other during pile penetration. Now let us compare the various stress measures. For both mean and

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus ( E ) (Pa)</td>
<td>( 2.9 \times 10^{10} )</td>
</tr>
<tr>
<td>Poisson’s ratio ( \nu )</td>
<td>0.25</td>
</tr>
<tr>
<td>specific gravity ( G_s )</td>
<td>2.65</td>
</tr>
<tr>
<td>inter-particle coeff. of friction ( \mu )</td>
<td>0.5</td>
</tr>
<tr>
<td>inter-particle contact damping ratio</td>
<td>5%, 30%</td>
</tr>
<tr>
<td>particle radii (m)</td>
<td>0.001 ( \sim ) 0.0025</td>
</tr>
<tr>
<td>viscous damping ratio</td>
<td>2.0/( \Delta t ), 0</td>
</tr>
<tr>
<td>time step ( \Delta t ) (sec)</td>
<td>( 5.0 \times 10^{-6}, 5.0 \times 10^{-7} )</td>
</tr>
</tbody>
</table>

Table 1: Parameters for quartz sand/gravel. If there is a second number, it is associated with the cavity expansion simulation.
octahedral shear stress, the symmetric micro-stress $s_\alpha$ and unsymmetric granular stress $\sigma_{\Omega}$ are not equal, indicating that the granular stress is unsymmetric. The unsymmetric Cauchy stress $\sigma_\alpha$, as a result of accounting for the couple terms in the balance of first moment of momentum in (10), (11)-(12), shows a reduced value when compared to $s_\alpha$ and $\sigma_{\Omega}$ in Fig.5, and the effect of acceleration and gravity force couple terms $\rho\omega$ and $\rho\ell$ are negligible. Recall the units of the couple stress, which are Pa.m. Thus, to compare the couple stress values on the same plot, the mean and octahedral shear couple stresses are normalized by the relative position vector $\xi$, which has unit of length; also, $-p_\text{couple}$ is plotted. Note, the main comparison is between $s_\alpha$ and $\sigma_\alpha$ to see the effect of the length scale (i.e., the relative position vector $\xi$) through the couple stress divergence term in the balance of first moment of momentum. Further work will consider various-sized averaging domains and RVEs to better understand this assumption of length scale (i.e., $\xi$), and its influence on the stresses (and in turn, constitutive equations).

3.2 Cavity expansion

This example is run dynamically, where the cavity expansion is started by a high initial outward velocity of an interior cluster of particles, that then pushes the remaining particles (initially at rest under gravity) upward in a box, that then settle down again by gravity (see Fig.7). The changing averaging domain $\Omega_{\text{avg}}$ is indicated by the box drawn at various times in Fig.7. This domain is in turn further divided into $4 \times 4 \times 3 = 48$ RVEs. Figure 6 displays the comparison of the stress values over the simulation time for mean and octahedral shear stresses. It is observed that as the cavity expands and pushes the particles up (Fig.7(b)), all mean stress values approach 0 (Fig.6) because there are few particle contacts. As the particles settle by gravity, the mean stress increases in compression (negative), until they come to rest. Similarly for the octahedral shear stress, as the particles reach their maximum height (and least number of contacts) at 0.025s, the octahedral shear stress approaches 0 (Fig.6). Upon settling, the octahedral shear stress increases again, and then decreases to a steady state value when the particles come to rest. Here, the symmetric micro-stress $s_\alpha$ and unsymmetric granular stress $\sigma_{\Omega}$ are equal, as there is little shearing of particles as compared to the pile penetration problem. For this dynamic example, the significance of the micro-spin inertia $\rho\omega$ and gravity force couple $\rho\ell$ are evident on the calculation of unsymmetric Cauchy stress $\sigma_\alpha$. 

Figure 5: Mean and octahedral shear stress versus time for the various stress measures of the pile penetration example.

Figure 6: Mean stress and octahedral shear stress versus time for the various stress measures of the cavity expansion example.
Figure 7: Side view of cavity expansion simulation, showing averaging domain $\Omega_{\text{avg}}^\alpha$ drawn by box, moving with particles at different simulation times: (a) 0.000s, (b) 0.075s, and (c) 0.375s.

4 CONCLUSIONS

The paper focussed on deriving the equations to calculate the three stresses within a micromorphic continuum theory, for an averaging domain $\Omega_{\text{avg}}^\alpha$ using 3D ellipsoidal DEM simulations: (1) symmetric micro-stress $s_\alpha$, (2) unsymmetric Cauchy stress $\sigma_\alpha$, and (3) unsymmetric couple stress $m_\alpha$. The stresses $s_\alpha$ and $m_\alpha$ could be calculated directly from volume average definitions, whereas $\sigma_\alpha$ required evaluating the balance of first moment of momentum. Stress results for pile penetration and cavity expansion DEM simulations were compared. It was observed that depending on the example, significant shearing can generate an unsymmetric granular stress $\sigma_\alpha^{(1)}$ as well as Cauchy stress $\sigma_\alpha$ (for pile penetration), and that for dynamics (cavity expansion), the role of micro-spin inertia and gravity couple force can significantly affect the calculation of Cauchy stress $\sigma_\alpha$.

Such a hierarchical multiscale framework for estimating micromorphic stresses, when extended to include the calculation of micromorphic strains, can be used to estimate material parameters of micromorphic constitutive models, as well as which parameters may be set to zero, and also how to estimate the length scale (directly related to the relative position vector $\xi$ in the micromorphic theory). This relies on the DEM model (or other underlying discrete physics-based model) to be physically relevant itself, and there are open questions on that issue that are beyond the scope of the paper (e.g., interparticle constitutive relations, particle shape/fracture, particle mineralogy and crystallographic orientation effects, pore water and air effects, ...).

Future work includes further investigation of the size of the averaging domain $\Omega_{\text{avg}}^\alpha$ and corresponding RVE sizes $r_{\text{RVE}}$ within $\Omega_{\text{avg}}^\alpha$, their relative position vectors $\xi$, and resulting stress calculations.

5 ACKNOWLEDGEMENTS

We would like to acknowledge funding for the research from ONR MURI grant N00014-11-1-0691.

REFERENCES


RAR also acknowledges support from a UPS Foundation visiting professorship in the Department of Civil and Environmental Engineering at Stanford University during the writing of the paper.