Computational multiscale methods for granular materials

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Abstract The fine-scale heterogeneity of granular material is characterized by its polydisperse microstructure with randomness and no periodicity. To predict the mechanical response of the material as the microstructure evolves, it is demonstrated to develop computational multiscale methods using discrete particle assembly-Cosserat continuum modeling in micro- and macro- scales, respectively. The computational homogenization method and the bridge scale method along the concurrent scale linking approach are briefly introduced. Based on the weak form of the Hu–Washizu variational principle, the mixed finite element procedure of gradient Cosserat continuum in the frame of the second-order homogenization scheme is developed. The meso-mechanically informed anisotropic damage of effective Cosserat continuum is characterized and identified and the microscopic mechanisms of macroscopic damage phenomenon are revealed. [doi:10.1063/2.1301101]

Keywords granular material, discrete particle assembly, gradient Cosserat continuum, computational homogenization, bridge scale method, damage characterization

I. INTRODUCTION

Most of granular materials are highly heterogeneous, composed of voids and particles with different sizes and shapes. Geological matter, soil and clay in nature, geo-structure, concrete, etc. are practical examples among them. From the microscopic view, a local region in the medium is occupied by particles with small but finite sizes and granular material is naturally modeled as an assembly of discrete particles in contacts within the frame of micromechanics. On the other hand, the local region is identified with a material point in the overall structure and this discontinuous medium can then be represented by an effective continuum on the macroscopic level.

As a continuum model is concerned, it should be noted that conventional Cauchy continuum theories are based on the local assumption, i.e., the length scale of the microstructure characterizing material constitutive behaviors is much less than the wavelength of deformation field occurring in the continuum, which may no longer hold for granular materials. A non-classical continuum model, taking into account the discrete nature of the microstructure of granular materials, should be adopted.

For granular material modeled as a discrete particle assembly, each discrete particle possesses finite size and independent rotational degrees of freedom (DOF) in addition to translational DOF in the kinematics and is capable of bearing and transmitting couples from one particle to the other in contact in the kinetics. Then it is natural and reasonable to adopt the Cosserat continuum model for macroscopic description of a material point at which a discrete particle assembly within the representative microstructure is assigned.[1] Indeed, D'Addetta et al.[2] and Ehlers et al.[3] pointed out that granular material should be homogenized as Cosserat continuum with non-symmetric macroscopic stress tensor and couple stresses. The structure of the derived meso-mechanically informed degraded isotropic constitutive relations of granular materials also demonstrated the rationality of adopting Cosserat continuum models for granular materials.[4] The micro-rotations defined as independent DOF at each mathematical point in Cosserat continuum play an important role in properly transiting the effect of rotations of particles within the representative microstructure via its boundary to the macroscopic continuum and vice versa. It is remarked that as the micro-rotations introduced as independent DOF into Cosserat continuum are constrained to equal the macro-rotations defined with the derivatives of the translational displacements, the Cosserat continuum theory reduces to couple stress theory. On the other hand, the gradient Cosserat continuum model also includes the strain gradients and the energy-conjugated stress moments introduced in the Toupin–Mindlin gradient theory of Cauchy continuum.[1,5]

The two distinct scale nature and the discrete particle assembly-continuum modeling of granular material leads to the construction of a continuum-based constitutive model characterizing macroscopic mechanical behavior at a material point in terms of the information about the properties and responses of the microstructure attributed to the macroscopic point of granular material. To establish micromechanically informed macroscopic constitutive relation and to predict macroscopic response at a material point as its microstructure evolves are the two main tasks presented to multi-scale mechanics of granular materials.

The discreteness and discontinuity of granular material in its micro-scale are its important characters distinct from other media. The fine-scale heterogeneity of

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granular material characterized by different microstructures with no periodicity at different material points possesses randomness in spatial distribution. In view of random heterogeneity, polydispersity, non-periodicity of micro-structural topology, morphology and high nonlinearity due to multi-body contacts among a great number of particles as the microstructure of granular material evolves, it is almost impossible to obtain equivalent constitutive relations and material properties of granular materials modeled as continua as a result of analytical or semi-analytical homogenization techniques. Instead, one has to resort to computational multiscale methods.[6–13] In addition, to solve for initial and boundary value problems of granular structures with multiscale numerical methods, it is also required to develop computational multiscale methods for discrete particle assembly-Cosserat continuum modeling.

Computational multiscale methods attempt to reproduce real responses of heterogeneous granular materials at the macroscopic continuum level on the basis of the information provided by the microscopic modeling of discrete particle assembly and to further reveal the micromechanical mechanisms of the macroscopic behaviors. Several computational multiscale approaches have been proposed to achieve these goals.[6–8] Among them is the asymptotic homogenization approach.[7] Many contributions have been devoted to the development of multiscale asymptotic expansion method for periodic structures along this approach. The method provides effective overall properties as well as local stress and strain values. The recent studies have proved multiscale asymptotic expansion methods to be more predictive. They have been used to replace heterogeneous Cosserat media by an effective one.[7] Several schemes are possible depending on the ratio between the Cosserat length scale and the size of heterogeneities.[14–16] However, it was also reported that the methods are usually restricted to very simple microscopic geometries (or medium with periodic micro structure) and simple material models, mostly at small strains.[8]

Taking into account the microscopic characteristics of granular materials described above and the complexity and nonlinearity of microstructural behaviors, the concurrent scale linking approach, instead of the hierarchical approach, should be adopted. The two promising computational multiscale methods along the category of concurrent methods are introduced in the present paper. They are the computational homogenization method (i.e., the global-local nested analysis scheme)[11–13,17,18] and the bridge scale method.[9,10] Both of them possess their respective advantages.

The computational homogenization method has received increasing attentions due to its suitability for modeling the mechanical response of heterogeneous materials characterized by complex micro-structures varying with loading history and with no periodicity, for which to formulate a closed-form macroscopic constitutive relation derived from detailed description of the microstructures and micromechanical behaviors is usually unfeasible. The approach is based on the average-field theory and the concept of a representative volume element (RVE) assigned at each integration point of the computational grid of macroscopic continuum.[19] The average-field theory for classical Cauchy continuum has been well developed and widely applied to multi-scale analysis and computation of composites. An abundant literature deals with this subject.[19–24]

Nevertheless, fewer contributions[1,7,13–16,25] have been devoted to the development of the homogenization scheme for Cosserat continuum. Among them a micro-macro computational homogenization scheme for discrete particle assembly-Cosserat continuum modeling of granular materials is proposed.[13] The consistent macroscopic modulus tensor and the macroscopic constitutive relation defined at the sampling point are formulated in terms of the averaged behavior of associated microstructures. With the proposed scheme, one enables the incorporation of large deformations and arbitrary material behaviors including history dependence while does not need to specify the phenomenological constitutive relation or to determine macroscopic constitutive parameters a priori at selected macroscopic points.

However, the main disadvantage of most (the first-order) existing homogenization methods developed in the computational homogenization approach lies in their intrinsic assumption of the uniformity of the macroscopic stress–strain fields attributed to the boundaries of each RVE, so that microstructural size effects and the gradients of macroscopic fields along the boundaries of the RVE can not be taken into account. As the absolute sizes of the RVE and the high strain gradients within the RVE have to be considered, the macroscopic energy product will be wrongly predicted and even the Hill–Mandel energy condition will no longer hold in the homogenization procedure using classical (the first-order) continuum model in the macroscopic level.[26]

Among the different schemes[8,14,16–18,27–29] proposed to overcome this disadvantage is the gradient-enhanced computational homogenization procedure[17,18] presented for heterogeneous Cauchy continua, in which not only the macroscopic deformation tensor but also its gradient are used to prescribe the essential boundary conditions on a microstructural RVE. The deficiency of the homogenization procedure using the classical continuum model in the macroscopic level can be remedied in the homogenization procedure using the gradient-enhanced macroscopic continuum model, in which the additional macroscopic energy product attributed to the strain gradients is taken into account.

The adoption of gradient Cosserat continuum model for the macro-scale modeling in computational multiscale methods requires the development of the finite element procedure of gradient Cosserat continuum. The key issues arising in the development are the appearance of strain gradients and how to attain the C^1 continuity of the displacement interpolation for a displacement-based finite element, i.e., both translational displacements and their first-order derivatives are required to be continuous across inter-element boundaries.[30] The direct strategy to achieve the C^1 continuity requirement is to use the Hermitian interpolation. Indeed Hermitian finite elements are truly C^1 continuous, in which the displacement field is the only field needed to be discretized using a C^1 continuity element.[31]

To circumvent C^1 continuity requirement in the development of displacement-based finite elements with high-order displacement interpolations, certain authors devoted to develop mixed finite elements fulfilling the C^1 continuity requirement only in a weak form for different strain gradient continua using couple stress theory[32,33] and Toupin–Mindlin theory,[18,34–36] respectively. An overview of finite element formulations and implementations for gradient elasticity in statics and dynamics was given by Askes and Aifantis.[37] To authors' knowledge, so far there has been no work published in the literature for finite element methods of gradient-enhanced Cosserat continuum and related finite element procedure, particularly in the frame of second order computational homogenization. Indeed a mixed finite element procedure based on the Hu–Washizu variational principle for gradient Cosserat continuum in the second-order computational homogenization for granular materials is presented and briefly described in this paper.

A fundamental problem presented in computational multiscale methods for discrete particle assembly-Cosserat continuum modeling of granular materials is how to identify local damage and elasto-plastic failures in macroscopic continuum and to reveal micromechanical mechanisms of failure process occurring in the granular structure. To achieve this objective, it is required to detect the micro-slip, the loss, the generation and the re-orientation of contacts[38] within a typical meso-structure consisting of a reference particle and its intermediate neighboring particles as the deformation proceeds, and then to quantitatively describe their effects on the mechanical behavior of the meso-structure and to trace the evolution of force chains leading to the force chain collapse.

The micromechanically informed macroscopic damage characterization of granular materials is briefly introduced. The micromechanically informed macroscopic damage factor tensor to characterize anisotropic material damage of effective Cosserat continuum is formulated with no need of specifying macroscopic phenomenological damage criterion and damage evolution role. In addition, the microscopic mechanisms of macroscopic damage phenomenon are revealed.[4]

The purpose of this paper is to introduce our research work achieved in the past years on developing computational multiscale methods for granular materials. The computational homogenization methods using Cosserat and gradient Cosserat continuum models in the macro-scale are first reviewed in Section II. The mixed finite element procedure based on the weak form of Hu–Washizu variational principle for the gradient Cosserat continuum in the second-order homogenization is presented in Section III. Section IV briefly describes the bridge scale method for discrete particle assembly-Cosserat continuum modeling. Meso-mechanically informed anisotropic damage characterization of Cosserat continuum for granular materials is reviewed in Section V followed by discussions in Section VI.

II. COMPUTATIONAL HOMOGENIZATION METHODS

The computational homogenization methods for heterogeneous granular medium described in the paper are based on the average-field theory and the concept of RVE. The medium is modeled as classical Cosserat continuum or gradient Cosserat continuum in the macroscale for the 1st or 2nd order computational homogenization procedure, respectively. On the other hand, a material point in the medium is modeled as a discrete particle assembly within the RVE representing the microstructure of the medium in the micro-scale. As soon as the boundary conditions are imposed to the peripheral particles of the discrete particle assembly of the RVE, the micromechanical behaviors can be evaluated by means of the existing discrete element model[39] based on the distinct element method.[40]

To transit mechanical properties and variables between the macroscopic Cosserat continuum and the microscopic discrete particle assembly within the RVE in a manner consistent with the continuum theory, it is also required to model the RVE as an effective Cosserat continuum. The link between the discrete particle assembly within the RVE and its effective Cosserat continuum is achieved via the discrete contacting points of peripheral particles of the particle assembly with the boundary of the effective classical Cosserat continuum. Through those discrete contacting points the boundary conditions prescribed to the RVE of effective classical Cosserat continuum are imposed to the discrete particle assembly. On the other hand, with the help of the effective Cosserat continuum of the RVE, the discrete element method (DEM) solutions resulting from the microscopic boundary value problem for the discrete particle assembly of the RVE can be upscaled to macroscopic mechanical measures and micromechanically informed macroscopic constitutive relations can also be formulated.

To downscale and determine the microscopic boundary value problem for the RVE subjected to macroscopic strain-stress measures as external loads of the RVE, the generalized Hill's lemma derived for heterogeneous Cosserat continuum in the first-order computational homogenization is given below[13,25]

$$\begin{aligned}&\overline{\sigma_{ji}\varepsilon_{ji}}+\overline{\mu_{ji}\kappa_{ji}}-\bar{\sigma}_{ji}\bar{\varepsilon}_{ji}-\bar{\mu}_{ji}\bar{\kappa}_{ji}=\\&\quad\frac{1}{V}\int_S(n_k\sigma_{ki}-n_k\bar{\sigma}_{ki})(u_i-\bar{u}_{i,j}x_j)\,\mathrm{d}\,S+\\&\quad\frac{1}{V}\int_S(n_k\mu_{ki}-n_k\bar{\mu}_{ki})(\omega_i-\bar{\omega}_i)\,\mathrm{d}\,S,\end{aligned}\tag{1}$$

where $\bar{\sigma}_{ji}$, $\bar{\mu}_{ji}$ and $\bar{\varepsilon}_{ji}$, $\bar{\kappa}_{ji}$ are denoted as the volume average Cauchy stresses and couple stresses and the volume average strains and curvatures over the domain of the RVE, prescribed to equal the corresponding macroscopic stress and strain measures at the given sample point. $\overline{\sigma_{ji}\varepsilon_{ji}}$, $\overline{\mu_{ji}\kappa_{ji}}$ are denoted as the volume averages of the microscopic products $\sigma_{ji}\varepsilon_{ji}$, $\mu_{ji}\kappa_{ji}$ over the domain of the RVE. σ_{ki}, μ_{ki}, u_i, ω_i at the right hand side of Eq. (1) are the stress measures, the translational displacements and the micro-rotations at the point with the coordinates x_j and outward normal n_k on the boundary S of the RVE of effective Cosserat continuum. $\bar{u}_{i,j}, \bar{\omega}_i$ are regarded as the derivatives of translational displacements and micro-rotations at the given macroscopic sample point. To ensure the satisfaction of the Hill–Mandel energy condition for the homogenization procedure, it is required as the downscaling rule to enforce that the two boundary integrals at the right hand side of Eq. (1) vanish in a pointwise (strong) or a integral (weak) manner.

It is found that the periodic boundary conditions commonly adopted for Cauchy continuum are only admissible to be prescribed on the RVE in the weak form for the pair of variables u_i and σ_{ki} but not for the pair of variables ω_i and μ_{ki} for Cosserat continuum.[25] In addition, the microstructure of the RVE for heterogeneous granular material does not possess periodicity. It is interesting to notice that Hill–Mandel energy condition for Cosserat continuum holds in the strong manner if and only if kinematically admissible translational displacements and statically admissible couple stresses given below are prescribed, i.e.

$$u_i|_S = \bar{u}_{i,j}x_j, \quad m_i|_S = (n_k\mu_{ki})|_S = n_k\bar{\mu}_{ki}. \tag{2}$$

With the discrete counterpart of the boundary conditions (2) prescribed on the discrete N_c points of the peripheral particles contacting with the boundary, the rate constitutive equations for micromechanically informed macroscopic Cauchy stresses and curvatures were derived and given in the forms[13]

$$\begin{aligned}\dot{\bar{\boldsymbol{\sigma}}} &= \boldsymbol{D}_{\sigma E} : \dot{\bar{\boldsymbol{\Gamma}}} + \boldsymbol{D}_{\sigma\mu} : \dot{\bar{\boldsymbol{\mu}}},\\ \dot{\bar{\boldsymbol{\kappa}}} &= \boldsymbol{D}_{\kappa E} : \dot{\bar{\boldsymbol{\Gamma}}} + \boldsymbol{D}_{\kappa\mu} : \dot{\bar{\boldsymbol{\mu}}},\end{aligned} \tag{3}$$

where $\dot{\bar{\boldsymbol{\Gamma}}} = \dot{\bar{\Gamma}}_{ji} = \dot{\bar{u}}_{i,j}$, $\boldsymbol{D}_{\sigma E}$, $\boldsymbol{D}_{\sigma\mu}$, $\boldsymbol{D}_{\kappa E}$, $\boldsymbol{D}_{\kappa\mu}$ are the fourth-order constitutive modular tensors, depending on the microstructure of the discrete particle assembly within the deformed RVE.

To overcome the deficiency of the first-order homogenization procedure using classical continuum model in the macro-scale described above, the gradient-enhanced computational homogenization procedure for discrete particle assembly-gradient Cosserat continuum modeling of granular material was proposed.[26,41] The generalized Hill's lemma for heterogeneous gradient Cosserat continuum in the second-order computational homogenization is given below

$$\begin{aligned}&\overline{\sigma_{ji}\varepsilon_{ji}} + \overline{\mu_{ji}\kappa_{ji}} - \bar{\sigma}_{ji}\bar{\varepsilon}_{ji} - \bar{\mu}_{ji}\bar{\kappa}_{ji} - \bar{\Sigma}_{lji}\bar{E}_{lji} = \\ &\frac{1}{V}\int_S (n_k\sigma_{ki} - n_k\bar{\sigma}_{ki})(u_i - \bar{u}_{i,j}x_j - \\ &\frac{1}{2}\bar{u}_{i,jl}x_jx_l)\,\mathrm{d}\,S + \frac{1}{V}\int_S (n_k\mu_{ki} - n_k\bar{\mu}_{ki}) \cdot \\ &(\omega_i - \bar{\omega}_i - \bar{\omega}_{i,l}x_l)\,\mathrm{d}\,S,\end{aligned} \tag{4}$$

where $\bar{\Sigma}_{lji}$, $\bar{E}_{lji}$ are denoted as the stress moment and strain gradient, $\bar{u}_{i,jl}$, $\bar{\omega}_{i,l}$ are the second-order derivative of translational displacements and the curvature defined at the sample point in the macroscopic gradient Cosserat continuum. Satisfaction of Hill–Mandel energy condition for gradient Cosserat continuum can be achieved by enforcing the following boundary conditions on the boundary of the RVE, i.e.

$$u_i|_S = \bar{u}_{i,j}x_j + \frac{1}{2}\bar{u}_{i,jl}x_jx_l, \quad \omega_i|_S = \bar{\omega}_i + \bar{\omega}_{i,l}x_l. \tag{5}$$

The macroscopic stress measures can be expressed in the forms of boundary integrals along the boundary of the RVE and further discretized into the discrete quantities assigned at the N_c contacting points of the peripheral particles of the particle assembly with the boundary of the RVE. With the discrete counterpart of the boundary conditions (5) prescribed on the discrete N_c contacting points and the formulae for macroscopic stress measures $\bar{\sigma}_{ji}$, $\bar{T}_k$, $\hat{\bar{\Sigma}}_{jlk}$, $\bar{\mu}^0_{ji}$ expressed in terms of boundary integrals along the boundary of the effective Cosserat continuum of the RVE, and then discretized into the microscopic discrete quantities assigned at the N_c contacting points of the peripheral particles with the boundary of the RVE, the micromechanically informed macroscopic constitutive relations linking rate macro-stress and strain measures for macroscopic gradient Cosserat continuum of heterogeneous granular materials are given by[41]

$$\dot{\bar{\boldsymbol{\sigma}}} = \boldsymbol{D}_{\sigma\Gamma} : \dot{\bar{\boldsymbol{\Gamma}}} + \boldsymbol{D}_{\sigma\hat{E}} \vdots \dot{\hat{\bar{\boldsymbol{E}}}} + \boldsymbol{D}_{\sigma\omega} \cdot \dot{\bar{\boldsymbol{\omega}}} + \boldsymbol{D}_{\sigma\kappa} : \dot{\bar{\boldsymbol{\kappa}}}. \tag{6}$$

$$\dot{\bar{\boldsymbol{T}}} = \boldsymbol{D}_{T\Gamma} : \dot{\bar{\boldsymbol{\Gamma}}} + \boldsymbol{D}_{T\hat{E}} \vdots \dot{\hat{\bar{\boldsymbol{E}}}} + \boldsymbol{D}_{T\omega} \cdot \dot{\bar{\boldsymbol{\omega}}} + \boldsymbol{D}_{T\kappa} : \dot{\bar{\boldsymbol{\kappa}}}. \tag{7}$$

$$\dot{\hat{\bar{\boldsymbol{\Sigma}}}} = \boldsymbol{D}_{\hat{\Sigma}\Gamma} : \dot{\bar{\boldsymbol{\Gamma}}} + \boldsymbol{D}_{\hat{\Sigma}\hat{E}} \vdots \dot{\hat{\bar{\boldsymbol{E}}}} + \boldsymbol{D}_{\hat{\Sigma}\omega} \cdot \dot{\bar{\boldsymbol{\omega}}} + \boldsymbol{D}_{\hat{\Sigma}\kappa} : \dot{\bar{\boldsymbol{\kappa}}}. \tag{8}$$

$$\dot{\bar{\boldsymbol{\mu}}}^0 = \boldsymbol{D}_{\mu\Gamma} : \dot{\bar{\boldsymbol{\Gamma}}} + \boldsymbol{D}_{\mu\hat{E}} \vdots \dot{\hat{\bar{\boldsymbol{E}}}} + \boldsymbol{D}_{\mu\omega} \cdot \dot{\bar{\boldsymbol{\omega}}} + \boldsymbol{D}_{\mu\kappa} : \dot{\bar{\boldsymbol{\kappa}}}. \tag{9}$$

where $\dot{\bar{\boldsymbol{\sigma}}}$, $\dot{\bar{\boldsymbol{T}}}$, $\dot{\hat{\bar{\boldsymbol{\Sigma}}}}$, $\dot{\bar{\boldsymbol{\mu}}}^0$ are the boldfaced forms of macroscopic rate stress measures, i.e., rate Cauchy stress, symmetric part of rate stress moment, rate internal torque, generalized rate couple stress $\dot{\bar{\mu}}^0_{ji}$ defined as $\dot{\bar{\mu}}^0_{ji} = \dot{\bar{\mu}}_{ji} - e_{ikl}\dot{\check{\bar{\Sigma}}}_{jkl}$ with $\dot{\check{\bar{\Sigma}}}_{jkl}$ being the skew-symmetric part of rate stress moment, e_{ikl} being the permutation tensor. $\dot{\hat{\bar{\boldsymbol{E}}}}$ is the boldfaced form of macroscopic strain gradient $\dot{\hat{\bar{E}}}_{ljk} = \dot{\bar{u}}_{k,jl}$. All of the sixteen constitutive modular tensors shown in Eqs. (6)–(9) depend on the microstructure and its evolution of the discrete particle assembly within the deformed RVE.

The capability of the second-order computational homogenization approach proposed for granular materials in accounting for the size effect is demonstrated by an example with a set of six RVEs. The six RVEs

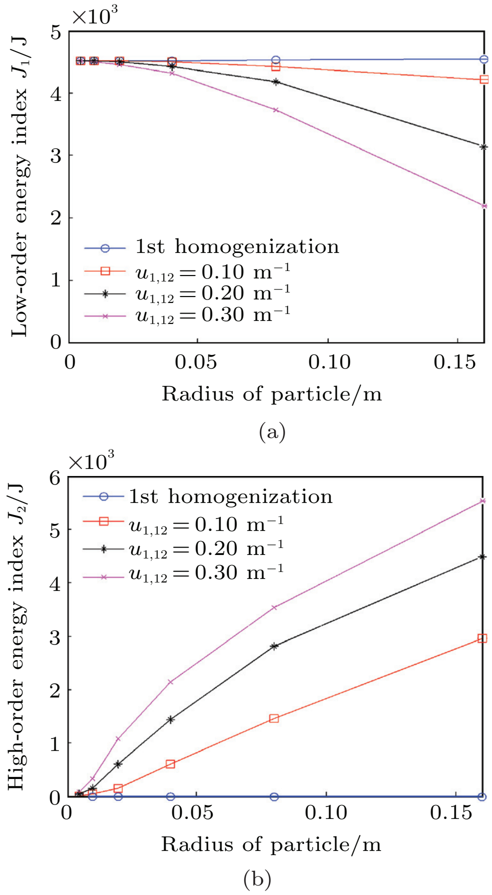


Fig. 1. Curves for RVE averaged low- (a) and high- (b) order energy indexes versus the characteristic microstructural size

possess the same micro-structural topology and morphology composed of 40 uniform round particles but with different particle radii increasing form 0.005 m to 0.160 m. Figure 1 plots low and high order energy density products J_1, J_2 versus the radius of particle in the macroscopic Cosserat and gradient Cosserat continua obtained by the first-order and the proposed second-order homogenization schemes respectively as the RVEs are subjected to varying macroscopic strain gradient $u_{1,12} = 0.1\,\mathrm{m}^{-1}$, $0.2\,\mathrm{m}^{-1}$, $0.3\,\mathrm{m}^{-1}$ in addition to $u_{1,1} = -0.015\,\mathrm{m}^{-1}$ and $u_{2,2} = -0.005\,\mathrm{m}^{-1}$. Both the size effect and the effect of the high-order deformation mode $u_{1,12}$ imposed to the RVE boundary are illustrated.

III. MIXED FINITE ELEMENT PROCEDURE FOR GRADIENT COSSERAT CONTINUUM IN SECOND-ORDER COMPUTATIONAL HOMOGENIZATION

The weak form of the Hu–Washizu variational principle for gradient Cosserat continuum in the frame of micro-macro computational homogenization of heterogeneous granular materials can be written as

$$\int_\Omega \delta u_i[(\sigma_{ji} - \Sigma_{kji,k})_{,j} - b_i^{\mathrm{f}}]\,\mathrm{d}\,\Omega + \int_\Omega \delta\omega_i[\mu_{ji,j} + e_{ijk}(\sigma_{jk} - \Sigma_{ljk,l}) - b_i^{\mathrm{m}}]\,\mathrm{d}\,\Omega - \int_\Omega \delta\rho_{ji}(\Psi_{ji} - u_{i,j})\,\mathrm{d}\,\Omega = 0, \tag{10}$$

with the weak form of rate stress–strain constitutive relations, in addition to the micromechanically informed constitutive relations (6)–(9), given by

$$\begin{aligned}
&\textstyle\int_\Omega \delta\Gamma_{ji} D^{\sigma\hat{E}}_{jinml}(\dot{\hat{E}}_{nml} - \dot{\eta}_{nml})\,\mathrm{d}\,\Omega = 0,\\
&\textstyle\int_\Omega \delta\eta_{kji} D^{\hat{\Sigma}\hat{E}}_{kjinml}(\dot{\hat{E}}_{nml} - \dot{\eta}_{nml})\,\mathrm{d}\,\Omega = 0,\\
&\textstyle\int_\Omega \delta\omega_i D^{T\hat{E}}_{inml}(\dot{\hat{E}}_{nml} - \dot{\eta}_{nml})\,\mathrm{d}\,\Omega = 0,\\
&\textstyle\int_\Omega \delta\kappa_{ji} D^{\mu\hat{E}}_{jinml}(\dot{\hat{E}}_{nml} - \dot{\eta}_{nml})\,\mathrm{d}\,\Omega = 0,
\end{aligned} \tag{11}$$

where and hereafter the over-bars applied to denote macroscopic variables in the frame of computational homogenization in Section II are dropped for clarity. Ω is the domain of macroscopic gradient Cosserat continuum, b_i^{f} and b_i^{m} are the body force and body moment per unit volume of the medium. A second-order tensor $\boldsymbol{\Psi}$ as a field function is introduced to express the strain gradient defined as a third-order tensor $\boldsymbol{\eta}$ such that at any point in the domain Ω one may have

$$\eta_{kji} = \frac{1}{2}(\psi_{ki,j} + \psi_{ji,k}). \tag{12}$$

The strain gradient will no longer be defined as the second derivative of assumed displacement field in the frame of proposed mixed finite element (FE) procedure. Instead with the Hu–Washizu variational principle, the relation between the strain gradients and the 2nd order derivatives of the displacements in gradient Cosserat continuum is enforced in the weak form given by $\int_\Omega \delta\hat{\Sigma}_{kji}(\eta_{kji} - \hat{E}_{kji})\,\mathrm{d}\,\Omega = 0$, which can be transformed into the constraint imposed to the equality $\psi_{ji} = u_{i,j}$ in the weak form given by

$$\int_\Omega \delta\rho_{ji}(\Psi_{ji} - u_{i,j})\,\mathrm{d}\,\Omega = 0, \tag{13}$$

in which ρ_{ji} is defined and termed as Lagrange multipliers to be determined in the proposed mixed FE procedure. Equation (10) can be re-expressed as

$$\int_\Omega \delta\varepsilon_{ji}\sigma_{ji}\,\mathrm{d}\,\Omega + \int_\Omega \delta\kappa_{ji}\mu_{ji}\,\mathrm{d}\,\Omega + \int_\Omega \delta E_{kji}\Sigma_{kji}\,\mathrm{d}\,\Omega + \int_\Omega \delta\rho_{ji}(\Psi_{ji} - \Gamma_{ji})\,\mathrm{d}\,\Omega = \int_S (\delta u_i t_i + \delta\omega_i m_i + \delta u_{i,j} g_{ji})\,\mathrm{d}\,S + \int_\Omega (\delta u_i b_i^{\mathrm{f}} + \delta\omega_i b_i^{\mathrm{m}})\,\mathrm{d}\,\Omega, \tag{14}$$

in which t_i, m_i, g_{ji} are the surface traction, the surface couple and the surface high-order generalized traction.

The introduction of incompatible strain gradient η_{kji} into Eq. (14) leads to

$$\begin{aligned}&\int_{\Omega}\delta\Gamma_{ji}\sigma_{ji}\,\mathrm{d}\,\Omega+\int_{\Omega}\delta\omega_k T_k\,\mathrm{d}\,\Omega+\\&\quad\int_{\Omega}\delta\kappa_{ji}(\mu_{ji}^{0}-e_{ikl}\hat{\Sigma}_{jkl})\,\mathrm{d}\,\Omega+\\&\quad\int_{\Omega}\delta\eta_{kji}\hat{\Sigma}_{kji}\,\mathrm{d}\,\Omega+\\&\quad\int_{\Omega}(\delta\Psi_{ji}-\delta\Gamma_{ji})\rho_{ji}\,\mathrm{d}\,\Omega+\\&\quad\int_{\Omega}\delta\rho_{ji}(\Psi_{ji}-\Gamma_{ji})\,\mathrm{d}\,\Omega=\\&\quad\int_{S}(\delta u_i t_i+\delta\omega_i m_i+\delta\Psi_{ji}g_{ji})\,\mathrm{d}\,S+\\&\quad\int_{\Omega}(\delta u_i b_i^{\mathrm{f}}+\delta\omega_i b_i^{\mathrm{m}})\,\mathrm{d}\,\Omega.\end{aligned}\tag{15}$$

As an incremental procedure is concerned, with omission of rate virtual kinematic quantities such as $\delta\Gamma_{ji},\delta\omega_k,\delta\kappa_{ji},\delta\eta_{kji},\delta\Psi_{ji},\delta\rho_{ji},\delta u_i$ in the derivation of tangent stiffness matrices, the rate form of Eq. (15) can be written in the boldfaced vector-matrix form below for convenience of its implementation in the FE procedure

$$\begin{aligned}&\int_{\Omega}\delta\boldsymbol{\Gamma}^{\mathrm{T}}\dot{\boldsymbol{\sigma}}\,\mathrm{d}\,\Omega+\int_{\Omega}\delta\boldsymbol{\omega}^{\mathrm{T}}\dot{\boldsymbol{T}}\,\mathrm{d}\,\Omega+\\&\quad\int_{\Omega}\delta\boldsymbol{\eta}^{\mathrm{T}}\dot{\hat{\boldsymbol{\Sigma}}}\,\mathrm{d}\,\Omega+\int_{\Omega}\delta\boldsymbol{\kappa}^{\mathrm{T}}(\dot{\boldsymbol{\mu}}^{0}-\boldsymbol{H}\dot{\hat{\boldsymbol{\Sigma}}})\,\mathrm{d}\,\Omega+\\&\quad\int_{\Omega}(\delta\boldsymbol{\Psi}^{\mathrm{T}}-\delta\boldsymbol{\Gamma}^{\mathrm{T}})\dot{\boldsymbol{\rho}}\,\mathrm{d}\,\Omega+\int_{\Omega}\delta\boldsymbol{\rho}^{\mathrm{T}}(\dot{\boldsymbol{\Psi}}-\dot{\boldsymbol{\Gamma}})\,\mathrm{d}\,\Omega=\\&\quad\int_{S}(\delta\boldsymbol{u}^{\mathrm{T}}\dot{\boldsymbol{t}}+\delta\boldsymbol{\omega}^{\mathrm{T}}\dot{\boldsymbol{m}}+\delta\boldsymbol{\Psi}^{\mathrm{T}}\dot{\boldsymbol{g}})\,\mathrm{d}\,S+\\&\quad\int_{\Omega}(\delta\boldsymbol{u}^{\mathrm{T}}\dot{\boldsymbol{b}}^{\mathrm{f}}+\delta\boldsymbol{\omega}^{\mathrm{T}}\dot{\boldsymbol{b}}^{\mathrm{m}})\,\mathrm{d}\,\Omega.\end{aligned}\tag{16}$$

The translational displacements $\boldsymbol{u}$, the microrotations $\boldsymbol{\omega}$, the displacement gradients $\boldsymbol{\Psi}$ and the Lagrange multipliers $\boldsymbol{\rho}$ are taken as the primary variables in interpolation approximations of proposed mixed FE procedure. Denoting their nodal values with $\bar{\boldsymbol{U}}^{\mathrm{T}}=\begin{bmatrix}\bar{\boldsymbol{u}}^{\mathrm{T}} & \bar{\boldsymbol{\omega}}^{\mathrm{T}} & \bar{\boldsymbol{\Psi}}^{\mathrm{T}} & \bar{\boldsymbol{\rho}}^{\mathrm{T}}\end{bmatrix}$, one may interpolate $\boldsymbol{u},\boldsymbol{\omega},\boldsymbol{\Psi},\boldsymbol{\rho}$ at any point within the FE mesh with their nodal values in the forms

$$\boldsymbol{u}=\boldsymbol{N}_u\bar{\boldsymbol{u}},\ \ \boldsymbol{\omega}=\boldsymbol{N}_\omega\bar{\boldsymbol{\omega}},\ \ \boldsymbol{\Psi}=\boldsymbol{N}_\Psi\bar{\boldsymbol{\Psi}},\ \ \boldsymbol{\rho}=\boldsymbol{N}_\rho\bar{\boldsymbol{\rho}},\tag{17}$$

where $\boldsymbol{N}_u,\boldsymbol{N}_\omega,\boldsymbol{N}_\Psi,\boldsymbol{N}_\rho$ are interpolation functions for $\boldsymbol{u},\boldsymbol{\omega},\boldsymbol{\Psi},\boldsymbol{\rho}$, respectively. The spatial derivatives of primary variables $\boldsymbol{u},\boldsymbol{\omega},\boldsymbol{\Psi}$ at any point within the FE mesh can be expressed in terms of $\bar{\boldsymbol{u}},\bar{\boldsymbol{\omega}},\bar{\boldsymbol{\Psi}}$ respectively by

$$\boldsymbol{\Gamma}=\boldsymbol{B}_u\bar{\boldsymbol{u}},\quad \boldsymbol{\eta}=\boldsymbol{B}_\Psi\bar{\boldsymbol{\Psi}},\quad \boldsymbol{\kappa}=\boldsymbol{B}_\omega\bar{\boldsymbol{\omega}},\tag{18}$$

where $\boldsymbol{B}_u,\boldsymbol{B}_\Psi,\boldsymbol{B}_\omega$ are the spatial derivatives of shape functions $\boldsymbol{N}_u,\boldsymbol{N}_\Psi,\boldsymbol{N}_\omega$, respectively.

The particular forms of interpolation functions $\boldsymbol{N}_u,\boldsymbol{N}_\omega,\boldsymbol{N}_\Psi,\boldsymbol{N}_\rho$ depend on construction of the multivariable mixed FE in consideration. A particular multivariable mixed FE is designed. It is termed as the quadrilateral element QU38L4 with 36 nodal DOFs and 4 Lagrange multipliers, i.e., 18 DOFs for translational displacements defined at 9 nodes, 4 DOFs for microrotations and 16 DOFs for displacement gradients defined at 4 corner nodes, 4 Lagrange multipliers defined at the element center. With Eqs. (16)–(18) the tangent stiffness matrices of the mixed FE QU38L4 can be derived and numerically integrated with the 2×2 Gauss quadrature scheme. The presented mixed FE passes the four typical patch tests, i.e., constant biaxial tension- compression strain, constant shear strain, constant strain gradient, constant microcurvature and shear strain tests.

IV. THE BRIDGE SCALE METHOD

Base on the bridging scale method (BSM) initially presented for molecular dynamics-Cauchy continuum modeling in nano mechanics,[9] a new version of the BSM that couples the discrete particle assembly modeling using DEM and the Cosserat continuum modeling using FEM at both micro-macro scale levels was proposed for multiscale analysis of granular materials. The whole computational domain is decomposed into two nested regions. The coarse scale region denoted by macroscopic (MS), which is modeled with Cosserat continuum and numerically simulated by the FEM, covers the whole medium for the simulation. While the fine scale region modeled with the discrete particle assembly and numerically simulated by the DEM is limited to a localized region denoted by DEM region for accurately simulating plasticity, crushing and discontinuous failure phenomena in microscopic scale.

With the bridging scale projection operator, the total displacement (including translations and microrotations) field is decomposed into coarse and fine scales. Based on the virtual work principle applied to the FEM nodes of the Cosserat continuum and the particle centers of the discrete particle assembly respectively, two decoupling sets of equations of motion of the combined coarse-fine scale system, resulting a multiscale DEM–FEM solution scheme, are formulated. As a consequence, different time step sizes for the time integration schemes in coarse and fine scales are permitted to be adopted, and both computational accuracy and efficiency of the proposed BSM are greatly enhanced.

One crucial issue of the BSM is how to properly present a multiscale interfacial condition between MS and DEM regions, which can appropriately embody the interaction and transition of kinematic and kinetic quantities at the interface. To impose the interfacial condition applied to the DEM region by the MS region, a layer of virtual interfacial particles in the MS region are fictitiously collocated and appended to the peripheral particles of the DEM region along the interface between the MS and DEM regions.

In the case of quasi-static loading, there exists no propagation of high frequent waves and the wave propagation effect in the DEM region can be neglected. Then it is desired to provide a simplified but efficient interface condition between the MS and DEM regions. It is assumed that the fine scale displacements defined at the virtual interfacial particles in the MS region are assigned to be zero, i.e., the displacements of peripheral particles of the DEM region along the interface are entirely determined in terms of the FE nodal displacements in the MS region.

As dynamic response problems with high and/or medium frequencies are concerned, it is necessary to taken into account the effect of wave propagation in granular media. To properly simulate the propagation of the waves with high frequencies originated from the DEM region, which should be allowed to pass through the interface and traveling into the medium outside the DEM region in the numerical simulation. Then the effects of those fine scale DOFs defined at the virtual discrete particles on the proximate peripheral particles of the DEM region have to be kept. It is achieved by taking into account the external force acting upon the proximate peripheral particles of the DEM region due to the fine scale DOFs of the virtual discrete particles. Indeed an effective and efficient scheme for non-reflecting boundary condition prescribed on the interface between the MS and DEM regions is developed for the proposed BSM using discrete particle assembly-Cosserat continuum concurrent modeling with the coupled DEM–FEM method.[10]

The good performance of the developed non-reflecting boundary condition in eliminating spurious reflected waves at the interfaces between the MS and DEM regions is demonstrated by a soil-foundation problem (Fig. 2) subjected to a uniformly distributed periodic pressure load normal to the surface of the cylindrical pit with the loading history $q_n = q_{n,0}\cos(\omega t)$ ($q_{n,0} = 1.0$ MPa, $\omega = 2\pi f$, $f = 200$ Hz) in Fig. 3.

V. MESO-MECHANICALLY INFORMED ANISOTROPIC DAMAGE CHARACTERIZATION

The study of micromechanical behaviors for granular material modeled as a discrete particle assembly is carried out from three distinct scales. In the micro-scale study one is concentrated on a typical contacting point and inter-particle contact behavior of two typical particles in contact. While in the macro-scale study, one focuses on the overall mechanical behavior of a granular structure consisting of a huge number of discrete particles as a boundary value problem performed by DEM solvers and its numerical solution.

It is remarked that the micro-scale and the macro-scale studies termed above do not relate to the microstructure and its evolution and their effects on the micro-structural constitutive behaviors leading to the local material failure. To reveal micromechanical mech-

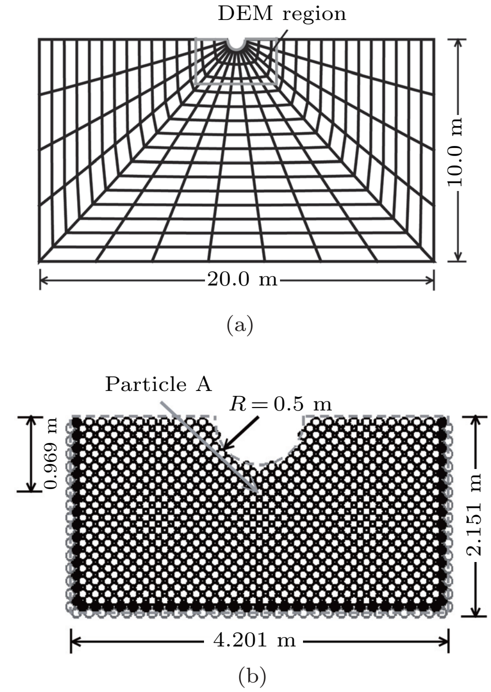


Fig. 2. A soil foundation with a half-circular pit of 0.5 m radius centered on its surface and FEM meshes (a) and schematic of the DEM region (b).

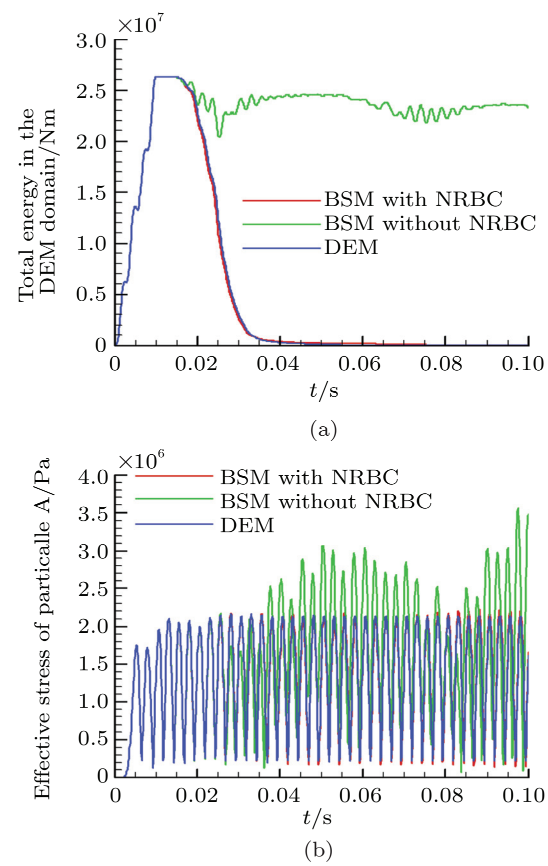


Fig. 3. The evolution of total energy (a) and effective stress (b) evolution in the DEM region of the foundation.

anisms of failure process occurring in the granular structure, it is required to detect the micro-slip, the loss, the generation and the re-orientation of contacts[42] among a small group of particles consisting of a reference particle and its neighboring particles within the microstructure as the deformation proceeds, and then to quantitatively describe their effects on the mechanical behavior of the microstructure and to further trace the evolution of force chains leading to the force chain collapse. One has to perceive the local character of material failure and avoid smearing out intrinsic heterogeneity and anisotropy of granular material, in order to accurately capture the real weakened location where failure process is triggered and then to correctly trace and characterize the real failure process.

The study of meso-mechanical behavior of the small group of particles, with the help of homogenization procedure, is the foundation to establish the meso-mechanically informed macroscopic constitutive model of the effective Cosserat continuum and to identify the macroscopic plastic and damage variables in the continuum in terms of microscopic material parameters characterizing the microstructure and its evolution and microscopic response variables characterizing microscopic local failure process.

To perform the meso-scale study for granular material, based on the concept of Voronoi cell,[43,44] a Voronoi cell model which is capable of representing typical microstructure of granular material and is generated with a Voronoi tessellation of discrete particle assembly was presented.[4] The Voronoi cell termed in this paper represents an effective porous Cosserat continuum element, in which voids and discontinuities exist, with the volume of the Voronoi cell assigned to the reference particle. Nevertheless, it is remarked that a Voronoi cell model includes not only the reference particle laid inside the Voronoi cell but also its intermediate neighboring particles. The contacting forces and moments acting on the reference particle via the contacting points depend on not only the movements of the reference particle itself but also its neighboring particles in contacts. As the mechanical behaviors for the effective continuum element, i.e., the reference Voronoi cell, are concerned, the motions of the intermediate neighboring particles of the reference particle have to be taken into account in the modeling of the constitutive behaviors of the reference Voronoi cell.

With the proposed Voronoi cell model the meso-mechanically informed macroscopic non-linear constitutive relations and constitutive modular tensors of effective Cosserat continuum are formulated. The averaged Cauchy stresses and coupled stresses exerted on the Voronoi cell in the two dimensional case can be expressed in the forms

$$\bar{\sigma}_{ji}^{\mathrm{A}} = \bar{\sigma}_{ji}^{\mathrm{Ae}} - \bar{\sigma}_{ji}^{\mathrm{Ae}},\ \bar{\mu}_{j3}^{\mathrm{A}} = \bar{\mu}_{j3}^{\mathrm{Ae}} - \bar{\mu}_{j3}^{\mathrm{Ae}}\quad (i,j=1,2) \tag{19}$$

where $\bar{\sigma}_{ji}^{\mathrm{Ae}}$ and $\bar{\mu}_{j3}^{\mathrm{Ae}}$ stand for reductions of average Cauchy stresses and couple stresses due to relative plastic displacements between the reference particle A and its neighboring particles in contact. The elastic parts $\bar{\sigma}_{ji}^{\mathrm{Ae}}$ and $\bar{\mu}_{ji}^{\mathrm{Ae}}$ are given in terms of the average strains and curvatures $\bar{\varepsilon}_{lk}^{\mathrm{A}}, \bar{\kappa}_{l}^{\mathrm{A}}$ of the Voronoi cell A of anisotropic Cosserat continuum, i.e.

$$\begin{aligned}
&\bar{\sigma}_{ji}^{\mathrm{Ae}} = D_{jilk}^{\mathrm{e}\sigma\varepsilon}\bar{\varepsilon}_{lk}^{\mathrm{A}} + D_{jil}^{\mathrm{e}\sigma\kappa}\bar{\kappa}_{l}^{\mathrm{A}},\\
&\bar{\mu}_{j3}^{\mathrm{Ae}} = D_{j3mi}^{\mathrm{e}\mu\varepsilon}\bar{\varepsilon}_{mi}^{\mathrm{A}} + D_{j3i}^{\mathrm{e}\mu\kappa}\bar{\kappa}_{i}^{\mathrm{A}},
\end{aligned} \tag{20}$$

with the definition of strain tensor $\bar{\varepsilon}_{lk}^{\mathrm{A}} = \bar{u}_{k,l}^{\mathrm{A}} + e_{3kl}\bar{\omega}^{\mathrm{A}}$. Then the meso-mechanically informed elastic secant modular tensors depending on the current status of the microstructure are given by

$$\begin{aligned}
D_{jilk}^{\mathrm{e}\sigma\varepsilon} = \frac{r_{\mathrm{A}}}{V_{\mathrm{A}}}\sum_{c=1}^{\mathrm{m}} h(u_n^{C\mathrm{At}})[-(k_{\mathrm{A}}^{\mathrm{c}} + k_{\mathrm{B}}^{\mathrm{c}})t_i^{\mathrm{c}}n_j^{\mathrm{c}}t_k^{\mathrm{c}}n_l^{\mathrm{c}} +{}\\
k_n^{\mathrm{c}}(r_{\mathrm{A}} + r_{\mathrm{B}})n_i^{\mathrm{c}}n_j^{\mathrm{c}}n_k^{\mathrm{c}}n_l^{\mathrm{c}}],
\end{aligned} \tag{21}$$

$$D_{jil}^{\mathrm{e}\sigma\kappa} = \frac{-r_{\mathrm{A}}}{V_{\mathrm{A}}}\sum_{c=1}^{\mathrm{m}} h(u_n^{C\mathrm{At}})k_{\mathrm{B}}^{\mathrm{c}}(r_{\mathrm{A}} + r_{\mathrm{B}})t_i^{\mathrm{c}}n_j^{\mathrm{c}}n_l^{\mathrm{c}},$$

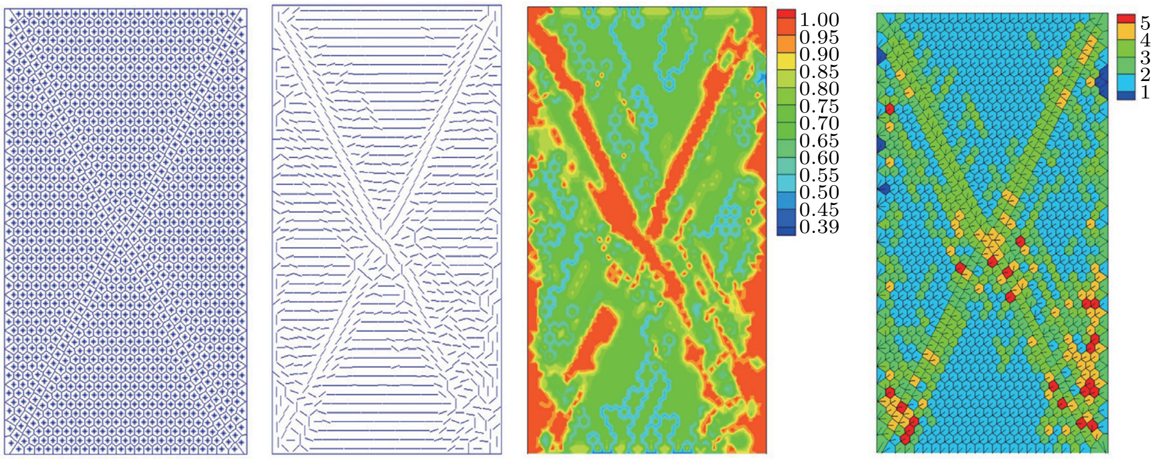
$$D_{j3mi}^{\mathrm{e}\mu\varepsilon} = \frac{-r_{\mathrm{A}}^2}{V_{\mathrm{A}}}\sum_{c=1}^{\mathrm{m}} h(u_n^{C\mathrm{At}})(k_{\mathrm{A}}^{\mathrm{c}} + k_{\mathrm{B}}^{\mathrm{c}})t_i^{\mathrm{c}}n_m^{\mathrm{c}}n_j^{\mathrm{c}}, \tag{22}$$

$$\begin{aligned}
D_{j3i}^{\mathrm{e}\mu\kappa} = \frac{r_{\mathrm{A}}}{V_{\mathrm{A}}}\sum_{c=1}^{\mathrm{m}} h(u_n^{C\mathrm{At}})[r_{\mathrm{A}}r_{\mathrm{B}}(r_{\mathrm{A}} + r_{\mathrm{B}})(k_s^{\mathrm{c}} - k_r^{\mathrm{c}}) +{}\\
k_\theta^{\mathrm{c}}(r_{\mathrm{A}} + r_{\mathrm{B}})]n_j^{\mathrm{c}}n_i^{\mathrm{c}},
\end{aligned} \tag{23}$$

where $h(u_n^{C\mathrm{At}})$ is the Heaviside unit function depending on the value of current overlap u_n^{CAt} between the reference particle A with its intermediate neighboring particle B, $r_{\mathrm{A}}, r_{\mathrm{B}}$ are the radii of the two particles, V_{A} is the volume of the Voronoi cell A, $t_i^{\mathrm{c}}, n_j^{\mathrm{c}} (i,j=1,2)$ are components of the local Cartesian coordinate axes $\boldsymbol{t}_{\mathrm{A}}^{\mathrm{c}}$ and $\boldsymbol{n}_{\mathrm{A}}^{\mathrm{c}}$ assigned to the particle A, and $k_{\mathrm{A}}^{\mathrm{c}} = -k_s^{\mathrm{c}}r_{\mathrm{A}} - k_r^{\mathrm{c}}r_{\mathrm{A}}$, $k_{\mathrm{B}}^{\mathrm{c}} = -k_s^{\mathrm{c}}r_{\mathrm{B}} + k_r^{\mathrm{c}}r_{\mathrm{B}}$, $k_n^{\mathrm{c}}, k_s^{\mathrm{c}}, k_r^{\mathrm{c}}, k_\theta^{\mathrm{c}}$ are stiffness coefficients for repulsive normal compression, sliding and rolling frictions, rolling friction moment between two particles in contact.

The derived meso-mechanically informed macroscopic constitutive relation (20) of effective Cosserat continuum reveals that the Cauchy stresses are not only constitutively related to the strains but also to the curvatures defined in Cosserat continuum, likewise, the couple stresses are not only constitutively related to the curvatures but also to the strains. As the derived meso-mechanically informed anisotropic constitutive relations (20)–(23) are degraded to the isotropic ones, it is found that the structure of the degraded isotropic constitutive relations agrees with that of the macroscopic constitutive relations directly given in the classical theory of Cosserat continuum. It also demonstrates the rationality of adopting Cosserat continuum models for granular materials. In addition, the isotropic elastic modular tensors degraded from Eqs. (21)–(23) are verified by comparisons of them with those given by classical Cosserat continuum theory and are used to identify the elastic constitutive parameters of isotropic Cosserat continuum.

According to the concept of continuum damage mechanics[45] and the elastic damage models,[45,46] the



(a) Deformed cell grid (b) Maximum principal damage directions (c) Maximum principal damage values (d) Number of loss of contacts

Fig. 4. Damage characterizations at the end of loading history.

material damage can be defined as a reduction in the elastic stiffness of material identified with the elastic modular tensor. It is appropriate to note that macroscopic effective Cosserat continuum for granular material with its microstructure represented by the present Voronoi cell model is anisotropic generally in its intrinsic nature. It implies that not only undamaged (initial) elastic modular tensor, but also the material damage of the effective Cosserat continuum for granular material are anisotropic.

In the frame of macroscopic phenomenological theory of continuum damage mechanics, with given undamaged elastic modular tensor $\boldsymbol{D}_0$ and the damage factor tensor $\boldsymbol{d}$ determined by the assumed damage criterion and damage evolution law at damaged (current) material state for a material point, the damaged elastic modular tensor $\boldsymbol{D}_t = \boldsymbol{D}_t(\boldsymbol{D}_0, \boldsymbol{d})$ is then determined.

Whereas in the frame of micromechanically based macroscopic damage mechanics, the damaged elastic modular tensor is directly determined and evaluated according to the current meso-structure associated to the reference Voronoi cell. One does need specifying neither macroscopic (phenomenological) damage criterion nor damage evolution law to determine the damage factor tensor. Contrarily the damaged elastic modular tensor $\boldsymbol{D}_t$ is first determined according to the current contact state of the reference particle with its intermediate neighboring particles in the frame of micromechanics of granular materials. The meso-mechanically informed macroscopic damage factor tensor $\boldsymbol{d} = \boldsymbol{d}(\boldsymbol{D}_t, \boldsymbol{D}_0)$ to characterize anisotropic material damage of effective Cosserat continuum is formulated and determined with given undamaged and damaged elastic modular tensors for the reference Voronoi cell assigned at a material point. The symmetry of the damaged elastic modular matrix $\boldsymbol{D}_t$ is fully determined by Eqs. (21)–(23) and is independent of whether the hypothesis of elastic strain equivalence or the hypothesis of elastic energy equivalence being employed.

A rectangular panel example subjected to a uniaxial compression between two rigid plates applied by a vertical displacement control is performed to demonstrate the proposed micromechanically informed damage characterization. Figure 4 illustrates deformed Voronoi cell grid, the distribution of maximum principal damage directions, the distribution of maximum principal damage value, and the distribution of "number of loss of contacts" revealing the main meso-mechanical mechanism of macroscopic damage, at the end of loading history when the panel fully collapses. It is interesting to notice that the shear bands in the panel only fully develop at the end of loading history (i.e., the panel collapses), when the damage simultaneously fully develops along the shear bands. The principal directions and values of the derived damage factor tensor along with numerical results reveal the microscopic mechanisms of macroscopic damage phenomenon, i.e., loss of contacts, re-orientation of contacts of the reference particle with its intermediate neighboring particles and concomitant volumetirc dilatation of the Voronoi cell.

VI. DISCUSSIONS

The micromechanically informed macroscopic damage factor tensor $\boldsymbol{d}$ at the current configuration of the Voronoi cell is defined on the bases of its initial microstructure characterized by $\boldsymbol{D}_0$. However, $\boldsymbol{D}_0$ is not certainly most stiff among all of possible particle collocation patterns describing the meso-structure for the reference particle.

Therefore, it is possible to result in a negative definite damage matrix $\boldsymbol{d}$ for a Voronoi cell with a deformed particle collocation pattern as it is subjected to certain external conditions and interactions with its neighboring particles. Physically, a negative definite damage matrix $\boldsymbol{d}$ implies a re-collocation of the particles for the

Voronoi cell resulting in a reinforced current microstructure as compared with its initial microstructure assigned at the local material point in the macroscopic continuum. This can be regarded as a microscopic mechanism of self-healing process of granular materials.

It is cognized from the developed micromechanically informed constitutive model for granular materials that the microscopic mechanisms of progressive macroscopic elastic damage-healing and elastoplastic processes are interrelated, i.e., the loss and generation of contact between each two intermediate neighboring particles, the change in the volume of the RVE (Voronoi cell), the change in the orientation of contact will be simultaneously accompanied with the slips between each two particles in contact governed by Coulomb law of friction. A further study for micromechanically informed coupled elastoplastic and damage-healing characterization of Cosserat continuum for granular materials is required.

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