Hierarchical Multiscale Modeling of Strain Localization in Granular Materials: A Condensed Overview and Perspectives

Jidong Zhao

Abstract This paper presents a brief overview on hierarchical multiscale modeling (HMM) of granular media and its application in simulating and understanding the phenomenon of strain localization. The general principles, solution procedures and advantages of existing HMM approaches are reviewed and compared. Focuses are devoted to the new cross-scale findings and insights offered by recent HMM studies on identification of key micro-structural origins and micro-mechanisms underpinning different deformations bands in granular materials. Limitations, challenges and opportunities pertaining to multiscale modeling of granular media are discussed.

1 Introduction

Multiscale modeling tops the trending words across many disciplines of engineering and science for over two decades, and has become a focal topic of interest in the study of granular materials recently. Granular media represent a wide range of materials that are of tremendous importance for many branches of engineering and industry, including cohesion-less sand, unconsolidated rocks, crushed coal, agricultural grains and chemical powders. Our fundamental understanding on the behavior of granular media, especially their mechanical behavior such as strength, stiffness and localized deformation patterns, has been largely built upon phenomenological characterizations, empirical descriptions and continuum-based modeling. While these traditional approaches have gained certain success in helping us meet the primary needs on design and operation of engineering problems, there are numerous occasions where the multiscale nature of granular media

J. Zhao (✉)
Hong Kong University of Science and Technology, Kowloon, Hong Kong
e-mail: jzhao@ust.hk

J. Zhao
Hong Kong University of Science and Technology Shenzhen
Research Institute, Kowloon, Hong Kong

E. Papamichos et al. (eds.), *Bifurcation and Degradation of Geomaterials with Engineering Applications*, Springer Series in Geomechanics and Geoengineering, DOI 10.1007/978-3-319-56397-8_44

has to be rigorously taken into account in order to attain accurate, comprehensive understanding, *strain localization* being a representative one of them.

There has been compelling recent experimental evidence, especially from test data based on advanced modern facilities such as X-ray micro computerized tomography (X-ray micro CT) and Digital Imaging Correlation (DVC), indicting that the initiation, formation, (sometimes) transition and finalization of strain localization bear intimate correlations with intricate microstructural mechanisms and controlling factors originated from the grain scale of a granular material [1–5, 14]. The corresponding theoretical and computational developments on this subject have apparently lagged behind their experimental counterpart. There has been a strong urge for the development of next-generation modeling and analysis tools, which, if ideally available, may not only retain the robustness and rigor of conventional continuum-based approaches in dealing with practical boundary value problems while voiding being phenomenological, but also incorporate fully the grain-scale granular mechanics showcased by prevailing micromechanics approaches and experimental observations. A special class of multiscale modeling methods, namely, the Hierarchical Multiscale Modeling (HMM) approaches, has been developed recently to take a step forward towards this direction. This paper serves as a condensed review of the latest advance of the HMM methods, with an emphasis placed on their unique roles in helping us gain new cross-scale understanding of strain localization in granular media.

2 Hierarchical Multiscale Modeling (HMM) of Granular Media

2.1 Principle and Methodology

Principle: The concept of HMM typically exploit a hierarchical discrete-continuum coupling scheme to solve a boundary value problem for granular media (see e.g., [8]). In the HMM framework, a continuum approach (e.g., FEM) is employed to discretize the concerned domain and find its solution subjected to the prescribed boundary conditions according to similar ways as conventional continuum approaches. It departs from conventional ways in that a HMM approach does not require a constitutive model to be assumed at the material point of the continuum domain. Rather, the constitutive relations are derived from the solution of a discrete-particle assembly of Representative Volume Element (RVE) attached to each material point of the continuum domain whereby the RVE receives deformations and other state variables as boundary condition from the macro scale and is solved by a discrete-based method (e.g., DEM). In essence, the HMM retains the robustness and flexibility of FEM in handling BVPs (which is a pitfall for DEM), while avoid assuming phenomenological constitutive models as required by conventional continuum approaches. Meanwhile, it fully capitalises the strength of discrete-based methods in reproducing the highly nonlinear, path-dependent mechanical behavior of a granular material. Moreover, the hierarchical structure offers a direct pathway to link the macro observations with their underpinning microstructural mechanisms, a feature highly desirable for multiscale understanding of strain localization in granular media.

Methodology: A dominant majority of existing HMM approaches for granular media have employed FEM to solve the continuum boundary value problem, and DEM for the solution of the boundary value problem of the particle assembly [3, 6, 8, 9, 17, 18, 21–25], Nitka et al. [23] and Liu et al. [20]. Figure 1a demonstrates a typical flowchart for the sequential iterative macro-micro solution procedure of HMM of dry granular media based on a hierarchical FEM-DEM coupling [8]. Since the DEM computation for each RVE is independent, the HMM approach can fully adopt parallel computing techniques for each RVE in the macro domain to enhance the computational efficiency. In existing HMM studies, the DEM commonly uses deformable particles of either spherical or elliptical shapes with linear or nonlinear contact and friction laws governing their contacts. Only exception is the study by Kaneko et al. [16] where the called Granular Element Method (GEM) based on rigid, frictional circular disks was adopted for the RVE solution. Notably, while most of the studies have been formulated under 2D conditions for the sake of simplicity, [9] and Liu et al. [20] have presented 3D HMM formulations and demonstrative examples.

Global-local solution schemes: In deriving the global-local solutions of the HMM approach, the implicit Newton-Raphson (NR) solution scheme with sequential macro-micro iterations has been commonly adopted to solve the non-linear problems for granular media [8, 21]. In particular, Meier et al. [21] used the elastic modulus as the tangent operator for frictionless particles based on Taylor's assumption. Note that the Taylor's assumption may potentially render the material response unrealistically stiffer and less dissipative. Guo and Zhao [8] found that the use of a secant elastic modulus for general granular particles (with friction) could work efficiently and robustly, noting that the perturbation method as advised in Nitka et al. [23] could cause issues of potential non-convergence and relatively low computational efficiency. Shahin et al. [25] suggested that a modified Newton-Raphson approach could be more robust when the quadratic convergence of a NR scheme was lost. Liu et al. [20] have recently proposed an explicit solution procedure for HMM which was claimed to be more efficient than the implicit iterative procedures aforementioned.

2.2 Selection and Benchmark of RVE for HMM

The selection of proper Representative Volume Element (RVE) is critical to the HMM approaches in two-fold. *First*, a proper RVE should faithfully represent the typical material behavior of the simulated granular material observed in the lab. Indeed, a RVE can be considered a virtual specimen equivalent to that used in a

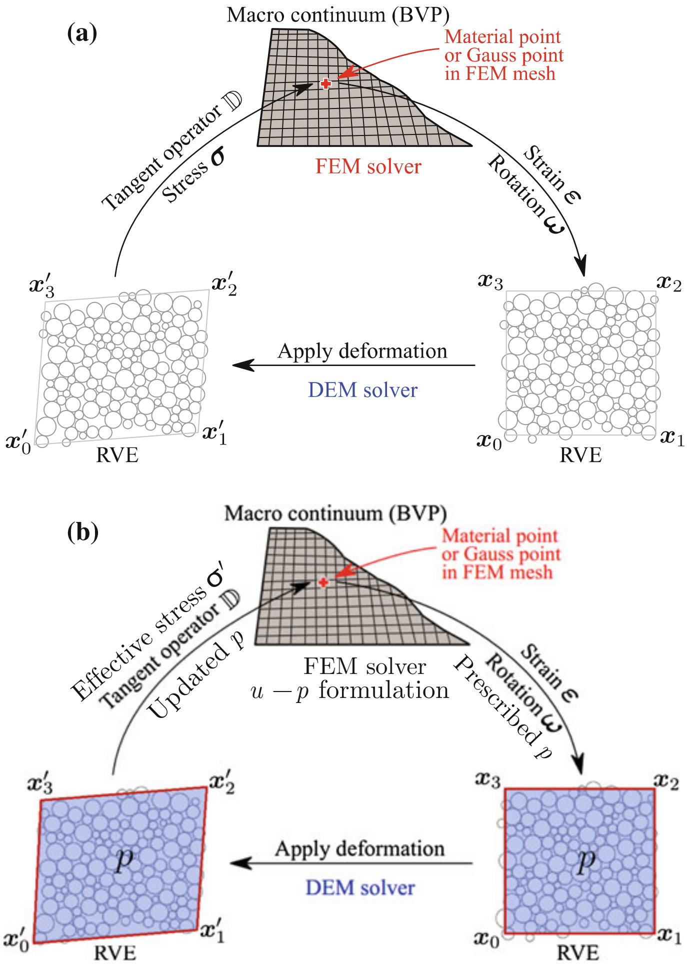

Fig. 1 Illustration of Hierarchical Multiscale Modeling of granular media with *FEM* × *DEM* coupling. **a** *HMM of Dry granular media*: FEM discretizes the macroscale BVP and passes the deformation gradients as boundary conditions for the meso-scale RVE modeled by DEM. The deformed RVE returns tangent operators and stresses for FEM to advance its global solution [8]. **b** *HMM of saturated granular media*: The FEM solves the BVP based on *u-p* formulation. It passes the deformation gradients and prescribes pore water pressure on the RVE. The DEN solution of the RVE returns the effective stress based on Terzaghi's principle of effective stress, the tangent operator and an updated value for the pore water pressure to FEM for iterative global solution [9]

typical laboratory element tests. *Second*, the selection of a RVE should make it computationally affordable as its DEM solution constitutes a typical HMM may involve hundreds of thousand RVE to be computed at each loading step. While constitutive features governing the DEM including contact models and geometry of particles have been extensively discussed in the DEM community, the most critical issue regarding HMM computation boils down to the number of particles to be included in a typical RVE. For 2D case, a size of RVE with a few hundred particles appears to be widely agreed by most study to offer good predictions of material behavior with reasonable computational efficiency. For example, Kaneko et al. [16] examined 16 different RVE size (2D) and aspect ratio in terms of their fabric isotropy and concluded that 200 particles would make an acceptable RVE for their multiscale approach. Meier et al. [21] examined the contact normal density function and average Cauchy stress of RVEs containing particle numbers from 70350 to 700 and concluded that the 700-particle RVE could offer reasonable results for 2D simulations. Guo and Zhao [8] and Nguyen et al. [24] both recommended 400 particles would serve a balanced choice for HMM of 2D problems. For 3D case, Guo and Zhao [11] suggested that a RVE with 1000 particles would be a reasonable unit cell for HMM simulations, while the number suggested Liu et al. [20] was 4000. Note that Shahin et al. [25] have more recently examined the effects of inhomogeneity and imperfection in a RVE on the prediction of strain localization in biaxial compression test simulations. In the future, if faster, more advanced parallel computing facilities can be inexpensively accessible, the number of particles considered in a RVE may be reasonably increased to yield more representative material responses.

Equally important is the benchmarking of the chosen RVE to ensure its prediction is valid and representative of typical granular responses. Guo and Zhao [8] and Liu et al. [20] compared the single-scale RVE response with the Gauss point response of HMM single element tests under either biaxial compression or simple shear to benchmark their methods. Note that Guo and Zhao [10] and Guo et al. [12] further employed their HMM approach and investigated some classic geomechanics problems, including retaining wall, footing and cavity expansion in thick-walled hollow cylinder.

2.3 Hydro-Mechanical Coupling for Saturated Granular Media

The presence of pore fluids in a porous, saturated granular medium may lead to strong hydro-mechanical coupling effects underpinning many aspects of its engineering performance. Micromechanics-based approaches for direct modeling of particle-fluid interactions, such as those based on DEM-CFD (Computational Fluid Dynamics) or DEM-LBM (Lattice Boltzmann Method) coupling, are too expensive to be affordably paired with HMM approaches to solve a practical problem. Moreover, these approaches commonly require complicated considerations and treatments of moving boundaries at the interface of fluid and particles. Guo and Zhao [9, 13] recently proposed adapting the fixed-stress split method with the seminal $\boldsymbol{u}$-p formulation to solve the global governing equations in the HMM, and exploiting the classic Terzaghi's effective stress principle to derive effective stress from the RVE. Wang and Sun [26] presented a similar method. The stress tensor homogenized from a typical DEM assembly according to Love's formula is based on the interparticle contact forces of the soil particles. It is hence a clear measure of the effective stress as defined by Carl Terzaghi. This micro-scale based effective stress added by the macro pore water pressure (as an unknown) makes up the total stress in the global equilibrium equation. Therefore, the entire hydro-mechanical coupling problem can be solved in the HMM framework efficiently and robustly, without resorting to expensive micromechanically based coupling. The entire solution procedure can be readily adapted from the one proposed for dry granular media by Guo and Zhao [8]. As illustrated in Fig. 1b, the pore water pressure is passed down to the RVE as an additional prescribed boundary condition on its calculation, before being updated and passed up to the macro material point again together with the homogenized effective stress and tangent stiffness matrix, and an updated permeability based on new void ratio and fabric structure of the RVE. All the rest of the solution procedure remains the same as in the dry case. Guo and Zhao [9, 13] benchmarked their coupled hydro-mechanical HMM approach with classic Terzaghi's 1D consolidation problem and the 2D consolidation under a strip footing, while Wang and Sun [26] verified their formulation on 1D consolidation problem.

2.4 Non-conventional Continuum Enrichment and Finite Strain

To resolve mesh-dependency issue and to capture size effects, Li et al. [18] presented a micro-macro homogenization method for Cosserat continuum, and Li et al. [17] further developed a mixed FEM of gradient Cosserat continuum with second-order computational homogenization for granular media based on Hu-Washizu variational principle. Liu et al. [20] developed a coupled FEM and DEM nonlocal multiscale method wherein the macro finite element solution was based on a nonlocal strain formulation. Finite strains were considered by Miehe et al. [22] and Liu et al. [20]. A side note on finite strain is made here. When the stress is homogenized from a RVE from interparticle contact forces, both translation and rotation of all particles of the entire RVE are totally considered. Consequently, the attained stress tensor may have already included contributions of co-rotational terms for the assembly (e.g., according to the manner of Jaumann stress rate). Therefore, it appears that the general HMM formulation (e.g., [8]) may well consider finite strain case already.

3 Multiscale Modeling of Strain Localization in Granular Media

The various HMM approaches have been applied to simulating strain localization in granular media. Biaxial compression tests have been a popular example in most of these HMM studies (see, e.g., [3, 8, 9, 13, 16, 22, 23]). Strain localization in 3D problems such as triaxial compression and extension on cubic and cylindrical samples have also been investigated by HMM approaches [11, 26]. The following provides a brief summary of major new cross-scale findings pertaining to strain localization revealed by the various HMM studies.

3.1 Alternative Localization Indicators

Cumulative deviatoric and void ratio have long been considered good indicators for localized shear bands in granular media. In addition, Zhao and Guo [28] found that cumulative particle rotation extracted from their HMM simulations can be an equally good localization too (see Fig. 2a, b, d. Meanwhile, both Guo and Zhao [8] and Zhao and Guo [28] demonstrated that the localized pattern for the intensity of fabric anisotropy defined by interparticle contact-normals was not consistent with the accumulated deviatoric strain, and suggested that the contact-normal-based fabric anisotropy was as good as an indicator for strain localization in granular media (c.f. Figure 2e with the rest figures). However, Zhao and Guo [28] employed clumped particles in RVE and showed that the intensity distribution of particle-orientation-based fabric anisotropy was highly consistent with that of deviator strain, and hence can be used as a localization indicator (see, Fig. 2c).

3.2 2D Versus 3D Loading Conditions

Guo and Zhao [11] employed 3D HMM approach to predict the occurrence of granular media subjected to 3D loading conditions. The multiscale modeling concluded that localized shear failure could be easier to occur under plane-strain conditions, and triaxial extension conditions could prohibit deformation localization and lead to diffuse failure mode instead. Indeed, as summarized in Fig. 3, their multiscale modeling indicates a cylindrical sample may tend to undergo bulging

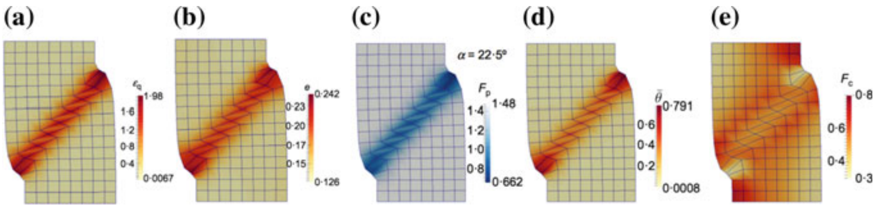

Fig. 2 Localization patterns predicted by HMM simulations of biaxial shear tests (Zhao and Guo [28]), in terms of **a** cumulative deviatoric strain, **b** void ratio, **c** intensity of particle-orientation-based fabric anisotropy, **d** cumulative particle rotation and **e** intensity of contact-normal-based fabric anisotropy

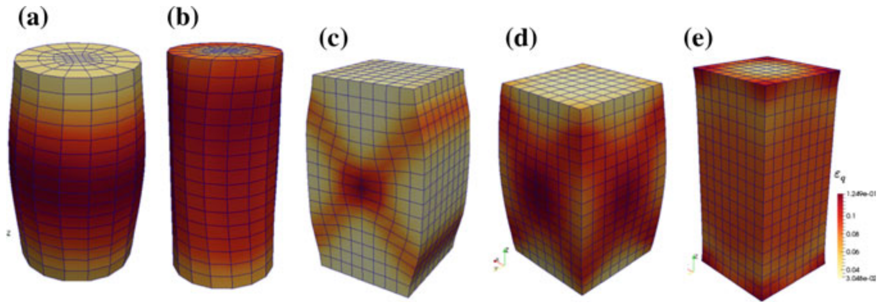

Fig. 3 Shear strain contours predicted by HMM tests simulations of uniform **a** cylindrical sample under triaxial compression condition (CTC), **b** cylindrical sample under triaxial extension condition (CTE), **c** cubic sample under plane-strain biaxial compression condition (PBC), **d** cubic sample under triaxial compression condition (CTC) and **e** cubic sample under triaxial extension condition (CTE) [11]

failure under triaxial compression (Fig. 3a) but fail diffusively under triaxial extension condition (Fig. 3b), whilst a cubic specimen is prone to develop octopus-shaped localizations under triaxial compression condition Fig. 3d and cross planar shear bands under plane-strain biaxial compression Fig. 3c, while it fails in diffuse mode under triaxial extension Fig. 3e. The 3D HMM simulations also showed that, if shear banding occurs, the shear band angle (relative to the minor principal stress direction) decreases from CTC, to PBC and further to CTE loading conditions (or equivalently with the increase of intermediate principal stress ratio). These findings are indeed consistent with experimental observations (e.g., [15]).

3.3 Pore Water Pressure Dissipation and Shear Banding

Guo and Zhao [9] employed a hydro-mechanical coupling HMM formulation to simulate a globally undrained biaxial compression test on saturated dense sand. A striking finding is as follows: (a) An obvious flux flow pattern was found proceeding to a clear strain localization incepts when the porosity of the entire sample remains relatively uniform (Fig. 4a). (b) The formation of strain localization is intimately related to a surge of pore water flux flowing from the rest of the sample into the dilative shear band (e.g., Fig. 4b). (c) When the shear band is fully developed, the flux flow across the entire sample becomes vanishingly small (Fig. 4c, d). Nevertheless, the overall distribution of pore water pressure field in the sample is relatively uniform over the shearing process. The HMM simulation seems to suggest that in saturated granular media, the flow plays a driver role in causing localized dilation and inducing strain localization, not the opposite process that the pore dilation acts a local sucking sink for local flux flow.

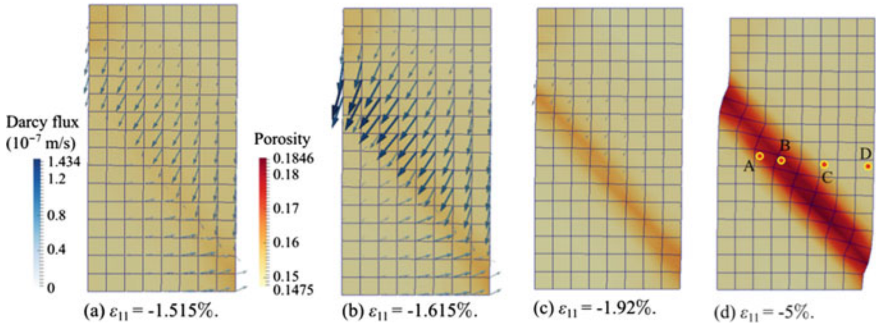

Fig. 4 Augmented illustration of strain localization and Darcy flux patterns of a saturated dense sand sample during globally undrained biaxial shear [9]. Note in the figures the thicker and longer arrows indicate stronger flux of pore fluid flow

3.4 Critical State Reached Within Shear Bands

Guo and Zhao [8] found the material response extracted from the RVE at Gauss point within the shear band formed under drained biaxial shear reached critical state, with constant stress, fabric anisotropy and volumetric strain. The finding confirms early pure DEM simulations by Fu and Dafalias [7] and the anisotropic critical state theory [19, 27]. Indeed, only material points located within the shear band(s) can possibly undergo excessively large shear deformation (e.g., in [7], the shear strain amounts to over 400%) to reach the critical state. While in conventional laboratory tests, such high shear strain levels are difficult to attain under proportional loading conditions.

4 Conclusions and Outlook

A condensed overview was made on hierarchical multiscale modeling of granular media, in particular relation to the simulation of strain localization in these materials. The principle, methodology and solution schemes on HMM were summarized. Recent new advances of HMM in simulating saturated granular media and further gradient or nonlinear enrichments were discussed. Some interesting new findings attained by various HMM studies on strain localization were highlighted. As shown, hierarchical multiscale modeling provides a new, effective toolbox for us to model and understand the multiscale nature of granular media, and opens up new grounds for exciting research. Exploratory future directions on hierarchical multiscale modeling of granular media include: (1) experimental microstructural characterization, verification and validation of the RVE; (2) characterization of realistic particle shapes for RVEs; (3) fully micromechanically-based modeling of fluid-particle interactions for the RVE to receive and pass information to the macro-scale domain; (4) consideration of particle crushing in hierarchical multi-scale modeling; (5) integrated multiscale modeling of continuous-discontinuous domains/stage transitions; (6) Hierarchical multiscale modeling of cohesive granular media; (7) Hierarchical multiscale modeling of dynamic problems in granular media.

Acknowledgements The study was partially supported by Research Grants Council of Hong Kong via a Collaborative Research Fund Project (No. C6012-15G) and by National Science Foundation of China through Project No. 51679207.

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