# FEM × DEM Multi-scale Analysis of Boundary Value Problems Involving Strain Localization

**J. Desrues, T.K. Nguyen, G. Combe and D. Caillerie**

**Abstract** The paper presents a FEM × DEM multiscale modeling analysis of boundary value problems involving strain localization in cohesive granular materials. At the microscopic level, a discrete element method (DEM) is used to model the granular structure. At the macroscopic level, the numerical solution of the boundary value problem (BVP) is obtained via a finite element method (FEM) formulation. In order to bridge the gap between micro- and macro-scale, the concept of representative volume element (REV) is applied: the average REV stress and the consistent tangent operators are obtained in each macroscopic integration point as the results of DEM simulation. The numerical constitutive law is determined through the DEM modeling of the microstructure to take into account the discrete nature of granular materials. The computational homogenization method is described and illustrated in the case of a hollow cylinder made of cohesive-frictional granular material, submitted to different internal and external pressures. Strain localization is observed to occur at the macro scale in this simulation.

## 1 Introduction

When modeling boundary value problems encountered in geotechnical engineering, the designer has often to consider the risk of localized failure. Besides long-standing works on experimental characterization of shear banding in laboratory tests and physical models, trying to catch as realistically as possible the localized failure in computational geomechanics has been the subject of theoretical and numerical works for a long while in the IWBDG community.

Recently, multi-scale analysis using a numerical approach of the homogenization of the microstructural behavior of materials to derive the constitutive response at

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the macro scale has become a new trend in numerical modeling. In recent years, different authors have proposed multi-scale approaches (Kouznetsova et al. 2001; Miehe and Dettmar 2004; Meier et al. 2008) to investigate the behavior of materials by using informations from the micro level. As for granular media, a two-scale fully coupled approach can be defined by using FEM at the macroscale, together with DEM at the microscale (Nitka et al. 2009, 2011; Guo and Zhao 2013). Despite an evident computational cost penalty with respect to mono-scale approaches like FEM and DEM, two-scale FEM $\times$ DEM approach allows one to perform real-size grain micro-structure modeling on real-size macroscopic problems, without facing the intractable problem of dealing with trillions of grains in a fully DEM mapped full field problem. Using this approach, microscale related features such as the inherent and induced anisotropy of the material, or material softening/hardening with strain, flow naturally from the microscale DEM model to the macroscale FEM model. An implementation of the FEM $\times$ DEM method in the FEM code Lagamine (ULg) (University of Liège, Belgium) is presented, and representative results are discussed, including aspects related to strain localization.

## 2 Multi-scale Coupling Method

A two-scale numerical homogenization approach by FEM $\times$ DEM is considered, Fig. 1. At the microscopic scale level (for each FEM Gauss point), the constitutive equation $\sigma = \Theta(\varepsilon)$ is numerically obtained by a DEM simulation on a

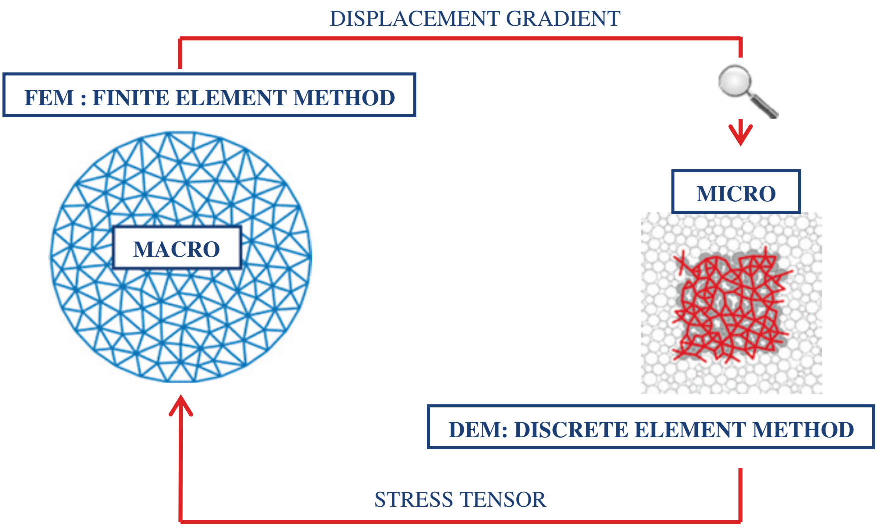



**Fig. 1** Computational homogenization scheme

representative elementary volume (REV). The stress response of the REV is computed using the classical homogenization formula defined in Weber (1966):

$$\sigma_{ij} = \frac{1}{S}\sum_{c=1}^{N_c} f_i^c \cdot l_j^c \tag{1}$$

where S is the volume of the REV (area in 2D). $f_i^c$ and $l_j^c$ are respectively the component $i$ of the contact forces acting in contact c and the component $j$ of the branch vector $l$ joining the mass centers of two grains in contact.

At the macroscopic level, a numerical solution for the BVP is obtained using FEM. In every Gauss point of all the elements of the mesh, a specific REV is attached and followed all along the computation, and the stress in this Gauss point at the time $t$ results from the whole deformation history of the REV. A consistent tangent stiffness matrix $C_{ijkl}$ is computed by numerical perturbation, giving the stress increment as a function of the displacement gradient:

$$d\sigma_{ij} = C_{ijkl} \cdot \frac{\partial du_k}{\partial x_l} \tag{2}$$

## 3 Micro-scale (DEM) Model

The numerical model of the granular material behavior is herein obtained by a DEM approach (soft-contact dynamics type) using periodic boundary conditions (PBC), following (Radjaï and Dubois 2011). The specific REV associated to each Gauss point is made of a dense packing of 400 polydisperse disks, as shown in Fig. 2. Comparing the response of different REVs involving an increasing number of disks, this choice leads to a response reasonably close to the asymptotic one. All grains interact via linear elastic laws and Coulomb friction when they are in contact (Cundall and Strack 1979). Accordingly, the normal repulsive contact force $f_{el}$ is related to the normal apparent interpenetration $\delta$ of the contact as $f_{el} = k_n \cdot \delta$, where $k_n$ is a normal stiffness coefficient ($\delta > 0$ if a contact is present, $\delta = 0$ if there is no contact). The tangential component $f_t$ of the contact force is proportional to the tangential elastic relative displacement, with a tangential stiffness coefficient $k_t$. In order to model cohesive-frictional granular materials, a local cohesion is introduced at the level of each pair of particles by adding an attractive force $f_c$ to $f_{el}$; $f_c$ is constant for each contact. The overall normal force for two grains in contact is $f_n = f_{el} + f_c$. The Coulomb condition $\|f_t\| \leq \mu \cdot f_{el}$ requires an incremental evaluation of $f_t$ in each time step, which leads to some amount of slip each time one of the equalities $f_t = \pm\mu \cdot f_{el}$ is imposed. In that study, $k_n$ is such that $\kappa = k_n / \sigma_2 = 1{,}000$ (Combe and Roux 2003), where $\sigma_2$ is the 2D isotropic pressure. The stiffness ratio is $k_n / k_t = 1$. The adhesion force $f_c$ is defined by reference to the mean level of pressure as suggested by Gilabert et al. (2007): $p^* = f_c / (a \cdot \sigma_2)$ where $a$ is the typical diameter of grains. So $p^*$ is a ratio scaling the attractive part of the mean stress in the sample with the repulsive part due to particle overlap. Hereafter, $p^* = 1$. The intergranular friction angle is $\mu = 0.5$.

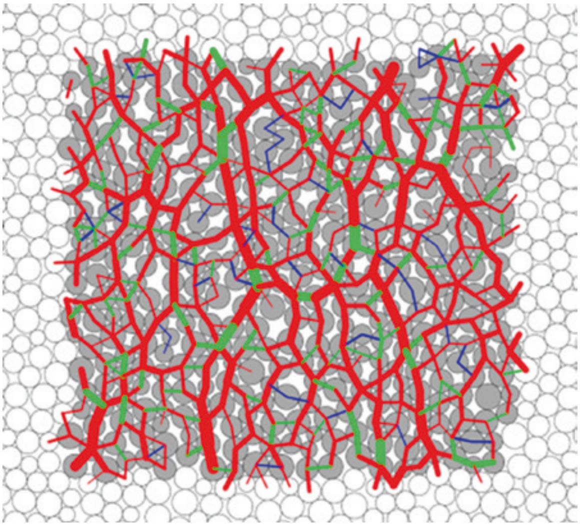


**Fig. 2** A REV of 400 particles with PBC. The contact forces are displayed with the following conventions: the width of the lines joining the centers of two particles in contact is proportional to the amplitude of the normal force. *Red*, *green*, *blue lines* distinguish respectively compressive forces with cohesion ($f_n > 0, f_c < 0$), cohesionless contacts ($f_n > 0, f_c = 0$) and attractive contacts ($f_n < 0, f_c < 0$)

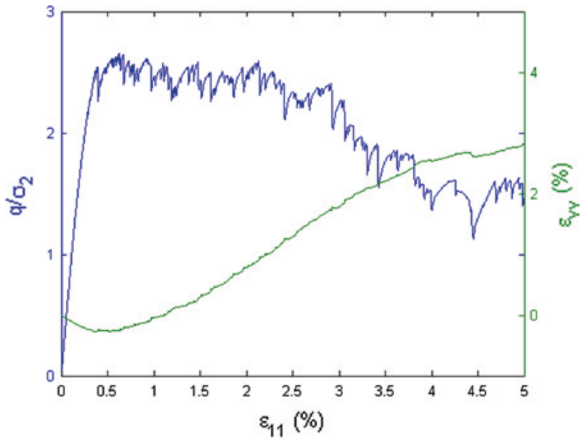



**Fig. 3** Mechanical response of the REV of 400 cohesive-frictional discs submitted to a biaxial loading. The *blue curve* corresponds to the evolution of the normalized vertical deviatoric stress $\left(q/\sigma_2\right), q = \sigma_1 - \sigma_2$ versus the vertical strain $\varepsilon_{11}$. The *green curve* displays the evolution of the volumetric strain $\varepsilon_{vv} = tr(\varepsilon)$ along the biaxial compression. Strain softening is obtained as the result of the degradation of the contact strength and distribution

A degradation of the cohesion is taken into account by considering a vanishing of $f_c$ at a contact when sliding or separation occurs. This corresponds to a simple model of granular materials with brittle cemented contacts. The mechanical response of the REV exhibits strain softening (Fig. 3).

## 4 FEM × DEM Simulation of BVPs

The FEM × DEM approach was implemented in the FEM code Lagamine that is able to perform finite strain analysis. The implementation consisted in inserting the DEM modeling code as a new constitutive law, and solving some specific difficulties linked to the determination of the consistent tangent operator. Different BVPs were studied, showing strain localization due to the inherently strain-softening behavior of the micro-scale model. The case of a biaxial test has been presented in Nguyen et al. (2013). Due to lack of space, the present paper concentrates on the results of the simulation of a pressurized hollow cylinder, using 400 eight-nodes quadrilateral order-2 elements with 4 integration points, with the geometry shown in Fig. 4 and the loading conditions in Fig. 5: starting from an homogeneous state of isotropic compression, first the internal pressure is decreased to zero then the external pressure is increased up to 4 times the initial isotropic stress.

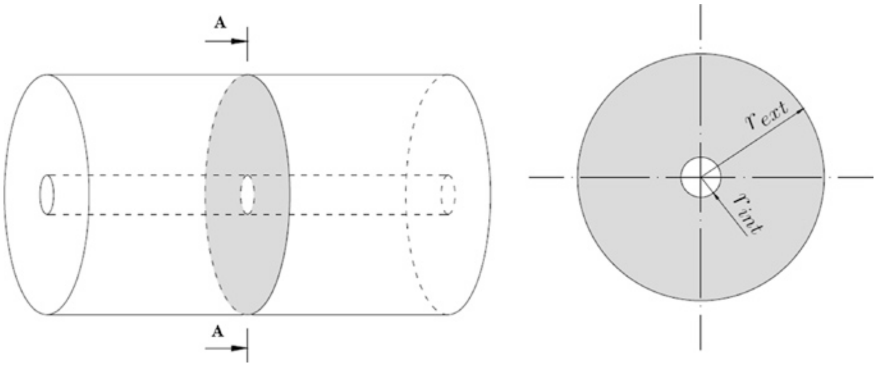



**Fig. 4** 2D model of a hollow cylinder

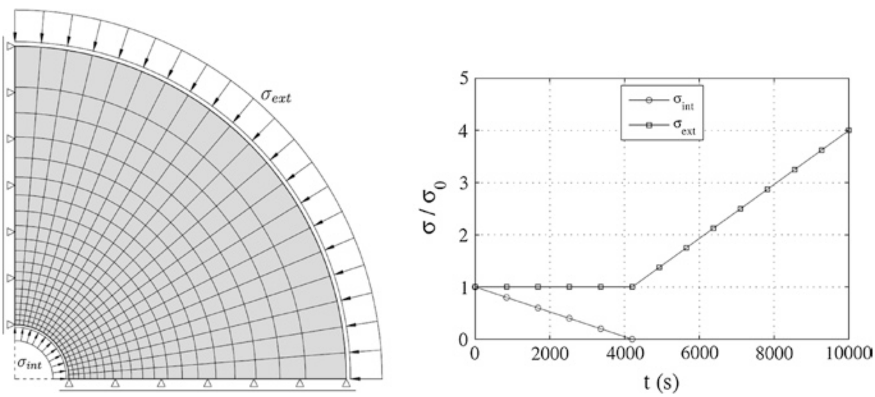



**Fig. 5** Modeling of 2D hollow cylinder: discretization in finite elements and loading conditions

Figure 6 shows the deformation mode in the model at different stages of the loading: (a) after internal pressure drop, (b) and (c) after large external pressure increase. In (a), the deformation is more or less axisymmetric with a strong gradient in the radial direction in the immediate vicinity of the internal wall; but in (b) and (c) strain localization has taken place, organized in spiral shear bands originated at the internal wall and progressing significantly inside the cylinder, as illustrated in more details in the zoom at t = 10,000 s in Fig. 7. This is the result of the inherent strain softening exhibited by the material as shown in Fig. 3. This result shows the ability of the FEM × DEM scheme to produce complex and realistic computations in BVPs. On the other hand, it is well known that implementing strain softening constitutive laws in FEM produces mesh dependency: the deformation concentrates in zones as narrow as the mesh permits, independently of any material parameter. Such pathologic response is observed here, as in the biaxial test simulation in Nguyen et al. (2013). In order to restore a mesh independent behavior in such computations, higher order constitutive models can be introduced, as in Chambon et al. (2001); Matsushima et al. (2002) in which a second gradient model is used with success.

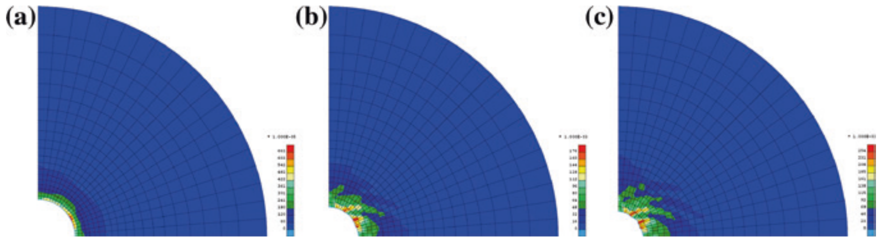
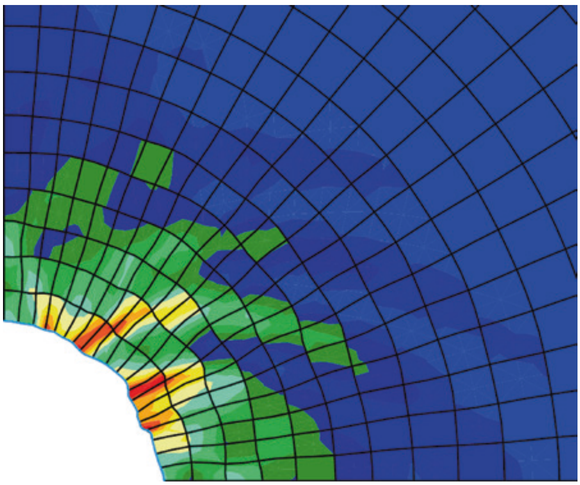



**Fig. 6** Strain localization: 2nd invariant of strain tensor. **a** t = 4,400 s. **b** t = 9,000 s. **c** t = 10,000 s

**Fig. 7** Strain localization at t = 10,000 s



## 5 Conclusion

A two-scale approach to investigate the behavior of cohesive granular materials has been presented, combining DEM at the micro-scale with FEM modeling at macroscopic level. The FEM × DEM mechanical response of a cohesive-frictional granular material submitted to a hollow cylinder pressurization test was analyzed and strain localization was detected. The results obtained allow to validate the approach and open new perspectives. Further developments will concern the use of a second gradient extension of the model in the FEM formulation, to overcome mesh dependency and restore objectivity of the post-localization simulations.

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