Domain heterogeneities in geomaterial modeling: integrating multi-scale FEMxDEM and second-gradient approaches

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Abstract. In the context of finite element modelling, the boundary value problem is often considered to be initially homogeneous. However, such assumption contradicts the observation of real geo-engineering problems and may affect the behaviour of geo-structure. It is thus necessary to consider a heterogeneous domain with a certain degree of variability. In this paper, we tackle this question by using a multi-scale FEM×DEM model with a second gradient enhancement. Pressuremeters are modelled in which, at the macro-scale, FEM model with a second gradient enhancement is used, while at micro-scale, an assembly of grains (called VE – volume elements) is used to numerically derive the constitutive response of geomaterials. Several VEs are simultaneously employed in a single finite element mesh in order to describe the heterogeneity of real engineering issues. The results suggest that when a certain heterogeneity is introduced, the set of possible numerical solutions seems more restrained even though the uniqueness of the solution is not guaranteed.

1 Introduction

The numerical modelling of geomechanical problems presents significant challenges due to material softening behaviour, strain localization and loss of uniqueness in numerical solutions. In the classical Finite Element Method (FEM), these issues often lead to mesh dependency, where the model requires mesh refinement. To address this, a higher-order continuum approach, such as the second-gradient technique [1,2] has been introduced. This technique incorporates an internal length scale to control the strain localization and thus resolve the mesh dependency.

When modelling the geomechanical model by FEM, the boundary value problem (BVP) is conventionally considered to be homogeneous, where a single constitutive law is applied uniformly throughout the domain. However, this contradicts the observation of real geo-engineering problems and may affect the behaviour of geo-structure. Experimental and field observations have demonstrated that geomaterials exhibit intrinsic spatial heterogeneity, which influences the initiation and evolution of failure patterns. These findings highlight the need for a heterogeneous distribution of constitutive material laws across the domain to enhance numerical predictions.

In light of these motivations, this study aims to investigate the role of heterogeneous constitutive laws within a second gradient-enhanced finite element framework. We focus on the pressuremeter problems made of cohesive-frictional granular materials and analysing how spatially varying material properties influence strain localization and multiplicity of numerical solutions. By combining second-gradient theory with heterogeneous constitutive modelling, we evaluate whether this approach can reduce the loss of uniqueness in the resulting numerical solutions.

2 Methodology

The influence of taking into account the heterogeneous BVP is studied based on the concept of the pressuremeter test [3]. A cross-section of the pressuremeter test is considered as shown in Fig. 1(a). The loading conditions are as follows: from an isotropic condition ($\sigma = \sigma_0$), the outer pressure ($p_e = \sigma_0$) is kept constant while we increase the inner pressure five times from the isotropic stress ($p_i = \sigma_0 \rightarrow 5\sigma_0$). To ensure the mechanical stability of the model, two supports are assigned, as shown in the figure.

An enhanced FEM×DEM model is employed in which the cross-section is discretized in 2700 second gradient finite elements [2]. The mesh size is finer in a local zone of about 60cm from the centre of the borehole. Regarding constitutive laws, DEM-based model is used as the first model, while the second gradient model is inspired from [4] with only one parameter D [2,5], which is set to 5E-2 based on recommendations in [6–8]. It should be noted that we use a Volume Element (VE) made of 400 circular grains, simulated by Discrete Element Method (DEM) to define the DEM-based model.

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Grains interact via normal and tangential forces. Rolling resistance is not considered. The normal interaction is determined thanks to normal stiffness (k_n), normal contact overlap (δ) and a cohesion force (f_c) as $f_n = k_n\delta + f_c$, $f_c = -\bar{a}\sigma_0$ where $\bar{a}$ is the mean diameter of granular assembly (VE). The current tangential force (f_t^i) is calculated via the tangential of previous time step (f_t^{i-1}) and an increment of tangential force (Δf_t) as $f_t^i = f_t^{i-1} + \Delta f_t$ with $\Delta f_t = k_t\,\Delta u_t$, where k_t is the tangential stiffness of contact and Δu_t is the relative displacement at the contact point. Tangential force is also limited by Coulomb threshold $|f_t| \leq \mu f_n$, with μ the intergranular coefficient of friction. The detailed description of such a concept is given in [9–11]. DEM parameters are summarized in Table 1.

Table 1. DEM parameters

Parameters	Values
Normal stifness (k_n/σ_0)	1000
Stiffness ratio (k_n/k_t)	1
Friction coefficient (μ)	0.5

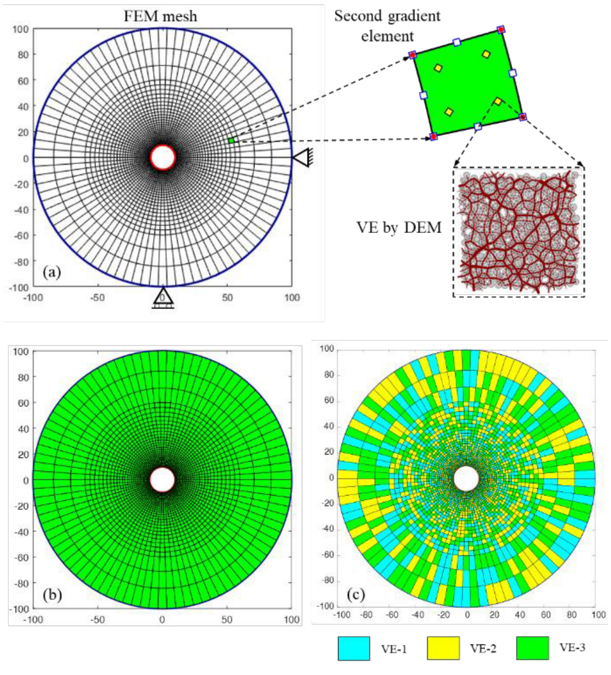

Fig. 1. FEMxDEM model (a) and finite mesh for HO case (b) and HE case (c)

Homogeneous (HO) and heterogeneous (HE) domains are considered as depicted in Fig. 1(b,c). In the HO case, a single DEM-based model (i.e., one VE) is employed throughout the FEM domain. In contrast, the HE case utilizes three distinct DEM-based models (three VEs), which are embedded simultaneously within the finite elements of the BVP. These VEs are generated following the same procedure, ensuring identical minimum and maximum grain radii. However, they differ in terms of grain size distribution and contact orientation. Despite these differences, the VEs exhibit mechanically similar macro- (similar Young modulus, poisson coefficient, dilatancy angle, cohesion and friction angle) and micro-scale (initial void ratio, coordination number) properties, as detail discussed in Ref. [11]:. In the HE case, the VEs are randomly distributed across the FEM mesh.

For each case, we run three simulations, namely s1, s2 and s3. In these three simulations, we vary the maximum time step (Δt_{max}) for each FEM increment while the initial (Δt_0) and minimum (Δt_{min}) time steps are unchanged (Table 2). The time step is automatically adjusted based on the rate of convergence, but it remains within the specified range $[\Delta t_{min}, \Delta t_{max}]$. Since the loadings of computations are rate independent, the maximum and minimum time steps are equivalent to maximum and minimum values of pressure applied for each increment.

Table 2. Time-step parameters for FEM increment

Simulations	$\Delta t_0/\sigma_0$	$\Delta t_{min}/\sigma_0$	$\Delta t_{max}/\sigma_0$
s1	4.10^{-3}	3.10^{-3}	1.10^{-1}
s2	4.10^{-3}	3.10^{-3}	4.10^{-2}
s3	4.10^{-3}	3.10^{-3}	2.10^{-2}

3 Numerical results

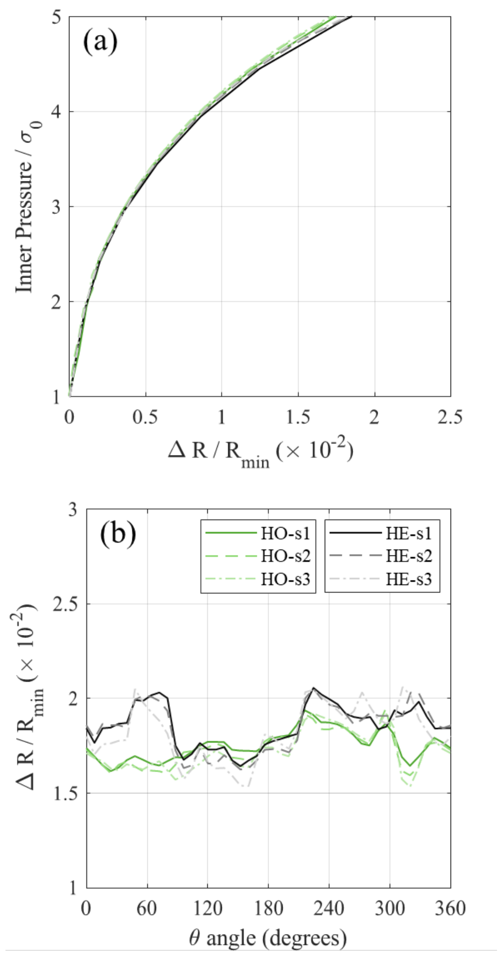

Fig. 2. Macroscopic curves.

Pressuremeter curves for six simulations (three for each HO and HE cases) are shown in Fig. 2(a). These curves display the relationship between normalized inner pressure and the strain in the cavity. The strain in the cavity is defined as the variation of radial displacement to the initial value of the internal radius of the borehole. The six curves are almost the same up to $p_i = 4.0\sigma_0$ then slightly diverge. The inner displacement at the end of the simulation shown in Fig. 2(b) confirms an anisotropic deformation of the inner boundary. This is a remarkable feature of the proposed FEM×DEM approach that naturally accounts for anisotropic in a very straightforward way. In the sub-figures, in each HO or HE case, the inner deformation shows similarities between simulations. However, considerable differences are observed between HO and HE cases.

Fig. 3, composed of six sub-figures, compares the shear band occurrence at the end of the simulation (i.e. $p_i = 5.0\sigma_0$). In both HO and HE cases, one can observe that when loading parameters change (s1, s2 to s3), the shear band patterns are different. This is proof of the loss of uniqueness of the numerical solutions. This problem is encountered even with a domain enriched by heterogeneities. However, comparing two rows of figures in Fig. 3 (HO and HE cases) reveals that in HE case, stronger similarities between s1, s2 and s3 are found.

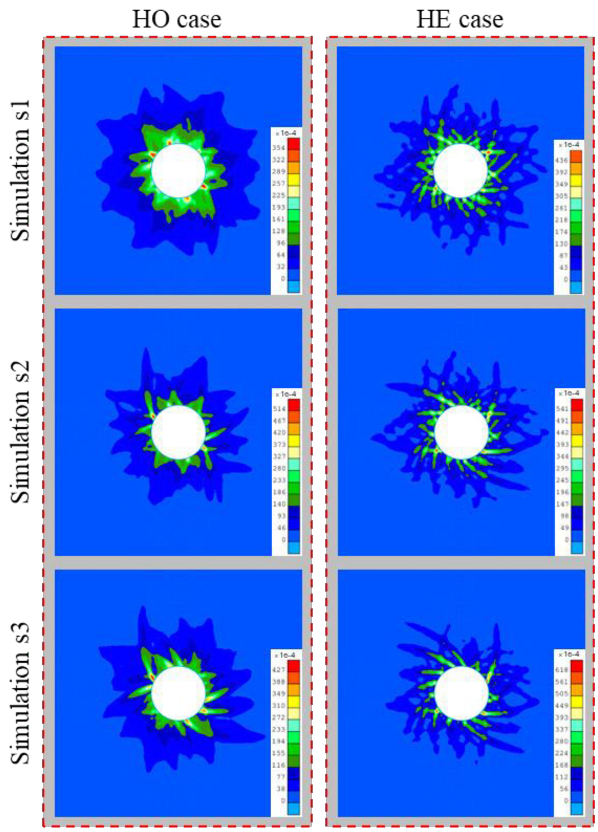

Fig. 3. Strain localization patterns.

As also shown in ref. [11], the loss of uniqueness in boundary value problems (BVPs) originates from microscale behavior characterized by internal variables. These internal variables could be divided into two groups: type A - internal variables which do not evolve during loading (grain shape and sizes, grain contact properties) and type B - internal variables which evolve during the calculation (void ratio, fabric tensor, etc.). These internal features predominantly control the development of shear deformation modes. As also demonstrated in ref. [11], type B internal variable predominate the strain localization mode if single-VE is used in the simulation, which is also in agreement with [12]. When multiple volume elements (VEs) are considered simultaneously, the resulting strain localization pattern seemed to manifest as a superposition of the distinct modes observed in single-VE simulations. The present results therefore indicate that enhancing domain heterogeneity may offer a viable means of constraining the solution space, even though it does not guarantee uniqueness.

4 Conclusions

In this paper, we employ a multi-scale FEM×DEM model enhanced with a second-gradient technique to introduce and evaluate the impact of heterogeneous domains on macroscopic behaviour and shear band patterns. Both homogeneous and heterogeneous cases were examined, demonstrating that the loss of uniqueness in the numerical solutions occurs when the loading parameters are modified. Even with a constitutive model with many ingredients, like the DEM-based model, the loss of uniqueness cannot be avoided. However, thanks to introducing a heterogeneous domain, a promising strategy to reduce the set of results has been proposed. Indeed, with a HE case mixed of three different DEM-based models, the results show that if a certain heterogeneity is introduced, the set of possible numerical solutions seems more restrained even though the uniqueness of the solution is not guaranteed.

References

[1] Chambon, R., Caillerie, D., Matsushima, T. (2001). Plastic continuum with microstructure, local second gradient theories for geomaterials: localization studies, Int. J. Solids Struct., 38(46), pp. 8503–27.
[2] Matsushima, T., Chambon, R., Caillerie, D. (2002). Large strain finite element analysis of a local second gradient model: application to localization, Int. J. Numer. Methods Eng., 28, pp. 499–521.
[3] Clarke, B.G. (2022). Pressuremeters in geotechnical design, CRC Press.
[4] Mindlin, R.D. (1965). Second gradient of strain and surface-tension in linear elasticity, Int. J. Solids Struct., 1(4), pp. 417–38.
[5] Bésuelle, P., Chambon, R., Collin, F. (2006). Switching deformation modes in post-localization solutions with a quasibrittle material, J. Mech. Mater. Struct., 1(7), pp. 1115–34.
[6] Marinelli, F., Sieffert, Y., Chambon, R. (2015). Hydromechanical modeling of an initial boundary value problem: Studies of non-uniqueness with a second gradient continuum, Int. J. Solids Struct., 54, pp. 238–57, Doi: 10.1016/j.ijsolstr.2014.10.012.

[7] Nguyen, T.K., Claramunt, A.A., Caillerie, D., Combe, G., Dal Pont, S., Desrues, J., Richefeu, V. (2017).FEM × DEM: A new efficient multi-scale approach for geotechnical problems with strain localization. EPJ Web of Conferences, vol. 140,.

[8] Desrues, J., Argilaga, A., Caillerie, D., Combe, G., Nguyen, T.K., Richefeu, V., Dal Pont, S. (2019). From discrete to continuum modelling of boundary value problems in geomechanics: An integrated FEM-DEM approach, Int. J. Numer. Anal. Methods Geomech., 43(5), Doi: 10.1002/nag.2914.

[9] Nguyen, T.K., Desrues, J., Vo, T.T., Combe, G. (2022). FEM×DEM multi-scale model for cemented granular materials: Inter- and intra-granular cracking induced strain localisation, Int. J. Numer. Anal. Methods Geomech., 46(5), pp. 1001–25, Doi: 10.1002/nag.3332.

[10] Nguyen, T.K., Desrues, J., Vo, T.T., Combe, G. (2024). Macro-micro analysis of ground response to circular tunnel excavation in granular media, Eur. J. Environ. Civ. Eng., 28(12), pp. 2862–80, Doi: 10.1080/19648189.2024.2327849.

[11] Nguyen, T.K., Vo, T.T., Nguyen, N.H.T., Combe, G. (2024). Variability and loss of uniqueness of numerical solutions in FEM×DEM modeling with second gradient enhancement, Int. J. Numer. Anal. Methods Geomech., 48(9), pp. 2381–407, Doi: 10.1002/nag.3737.

[12] Zhao, J., Guo, N. (2015). The interplay between anisotropy and strain localisation in granular soils: A multiscale insight, Geotechnique, 65(8), pp. 642–56, Doi: 10.1680/geot.14.P.184.