Journal of Science and Technology in Civil Engineering, HUCE (NUCE), 2021, 15 (4): 111–122

COUPLED FINITE-DISCRETE ELEMENT MODELING AND POTENTIAL APPLICATIONS IN CIVIL ENGINEERING

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Article history:
Received 06/8/2021, Revised 20/9/2021, Accepted 24/9/2021

Abstract

Since its appearance at the last of seventy decades, the Discrete Element Modeling (DEM) has been widely used in the modeling of geomaterials but regrettably limited to small scales problems by considering grains interactions. Recently, a new trend has emerged in combining DEM with other methods. The coupled approach allows extending the methods toward a wide range of civil engineering applications. Among them, FEM×DEM coupling has been the topic of research over the past decade. The FEM×DEM coupling has been mainly developed in two categories: direct interaction and multi-scale coupled models. In the first regard, this paper summarizes the basic principle of FEM and DEM, then reviews a number of possible direct coupling strategies between FEM and DEM together with potential applications in civil engineering. The second objective is to develop a model that combines these two above mentioned methods in a multi-scale approach. The results obtained by the developed model have been proved to efficiently tackle the complicated problem in engineering applications by assessing both macro and micro features and establishing the linking information between them.

Keywords: DEM; FEM; numerical methods; coupling methods; civil engineering applications.

https://doi.org/10.31814/stce.huce(nuce)2021-15(4)-10

1. Introduction

Besides theoretical and experimental approaches, numerical method plays an important role, in many cases, this is the only way to solve the civil engineering boundary value problems (BVP). Several popular numerical methods, such as Finite Element Method (FEM), Discrete Element Method (DEM), Material Point Method (MPM), Smoothed-particle hydrodynamics (SPH) or other Meshfree Methods... have been frequently used in the field of civil engineering applications [1–4]. The nature of the problem and the research's objective determine which method is most appropriate. The Finite Element Method (FEM) and the Discrete Element Method (DEM) are two of the most widely used approaches for modeling civil engineering issues. Each method is based on different set of assumptions and is also suitable for different specific purposes. In terms of problem scales, most of the current research works have employed FEM for large scale problems, while the DEM is used to describe the micro-scale, the scale of which the interaction between the particles constituting the material is

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considered. The DEM has been recognized to be a perfect solution for problems in which the overall response is characterized by micro-scale phenomenon. In fact, the number of particles in real structure or experiment is much more than in numerical modeling by DEM. With the availability of computing resources, it seems not feasible to consider the full-scale modeling of structures accounting for the realistic number of grains in a DEM model. In such cases, other numerical approaches like FEM, MPM, SPH, etc. are required.

In order to take advantage of both above-mentioned method (i.e. FEM and DEM), many studies combining the two methods in a unified simulation have been proposed recently. They can be distinguished in two main families: direct interaction between FEM×DEM which includes surface or volume coupling [5–9]; and multi-scale coupling in which FEM is employed at macro scale while DEM is used at smaller scale [10–14]. Unlike the former which couples the two methods directly, the latter combines FEM and DEM by bridging the scales between them. This allows modeling the real problems at the macroscopic scale, by taking into consideration the inherent properties of geomaterials via micro-scale interactions. As a result, a fullfield measurement can be achieved, and the behavior of materials/structure can be studied at pertinent scales.

Motivated by the emerging trends in bridging the gap between macroscopic observation and its microscopic origins; by the necessity of taking advantage of common methods, this paper reviews several concurrent FEM×DEM coupling approaches. And then focusing on the development of a coupled FEM×DEM model in a multi-scale approach (named FEM×DEM integrated coupling). The developed multi-scale model enables the possibility to fill the gap between macroscopic observation and its microscopic origins. After presenting the methodology, validation tests, the paper investigates the behavior of granular materials in a complex case, the pressurized hollow cylinder test. By analyzing the microscopic features and macro failure, several microscopic aspects related to the strain localization, that cannot simply be described by phenomenological constitutive law, have been successfully revealed.

2. Scales separation in civil engineering

As shown in Fig. 1, the scales in the civil engineering field can be separated from the interaction between the particles of the material (micro scale) to the real problem with specified boundary conditions (macro scale). From a numerical point of view, to study the structure/material at pertinent scales, the DEM is suitable for small-scale problems, while problems in the real-engineering scale should be analyzed by FEM. However, FEM is based on many assumptions, and describing the behavior of materials by taking into account the interactions between their constituent elements is a real challenge, even for advanced constitutive law. To meet that requirement, many studies have proposed to combine FEM and DEM in a single unified description, in order to take the advantage of the two

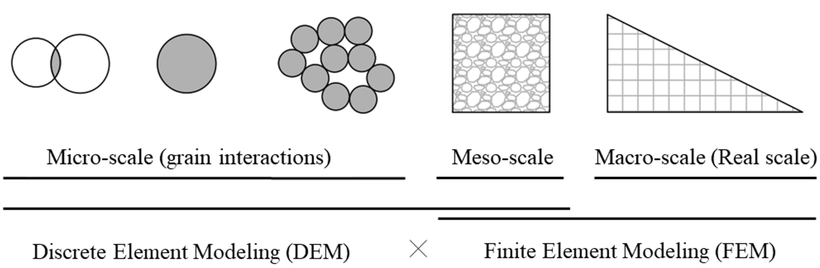


Figure 1. Separation of scales in civil engineering

methods and to describe as correctly as possible the behavior of materials/structure by considering its microscopic features.

3. Brief of Finite Element Method (FEM)

The FEM (Finite Element Method) is a numerical method that may be used to solve a wide range of engineering issues that interest both engineers and scientists. Originally, this method was used to solve boundary value problems for partial or linear differential equations. The problem is presented in the weak form, which serves as the basis for FEM implementation.

The FEM is a method of Galerkin type, which consists in seeking an approximation of the unknown field (e.g. displacement in mechanics) in a discretized form which is a linear combination of predetermined basic functions. In the FEM, the field is divided into sub-domain, of triangular or quadrangular form in general for a 2D problem. These sub-domains are the finite elements of the geometric discretization, the vertices of the elements are the nodes. Each node is associated with a shape function that is equal to one in this node and zero in the other nodes.

This method was initially developed to solve linear problems and has been applied to a great variety of applications, in which non-linear and coupled phenomena can be encountered. The non-linearity can come from the constitutive law or the presence of large deformations. In general, one brings back the resolution of the non-linear problem to that of a series of problems linearized by the iterative method of Newton, the linear problem of each iteration being solved by the FEM. For more details on this FEM method, the reader can refer to the text-book [1].

4. Discrete Element Method (DEM)

The classical Discrete Element Method (DEM) was first proposed by Cundall and Strack [15] to model the cohesionless granular assembly made of 2D disks. This method has been increasingly developed over four decades and has been applied for almost all kinds of geomaterials such as sand, concrete, and rock [16–19]. The DEM allows modeling the geomaterial at a small scale by considering the interaction between its particles. The DEM considers the elements (particles) independently, from which the motion of particles is based on the equation of Newton's second law. This method handles the interaction of a set of 2D circular disks, 3D spheres, polygons, ... Interactions between the elements (particles) are modeled through the interaction contact model by involving the interaction forces. The computation cycle of the DEM is presented in Fig. 2. Over the past four decades, the DEM has been widely used to study the behavior of geomaterials with emphasis on micro-scale phenomenon-induced macroscopic response with heterogeneity and anisotropy.

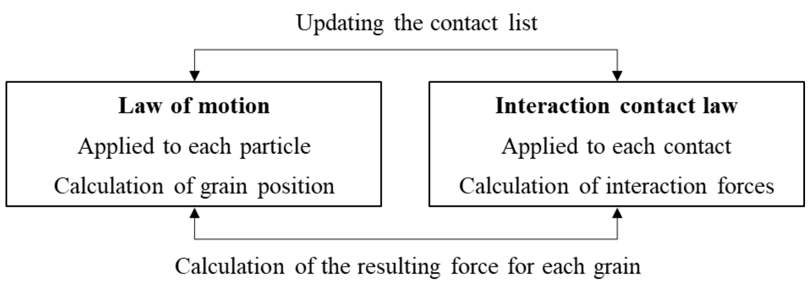


Figure 2. Discrete Element Method cycle

4.1. DEM Governing equations

The equations that govern motion particles (velocity and rotation) are given by:

$$M \cdot \ddot{\vec{x}}_i = \sum_j \vec{F}_{ji} + \vec{r} \tag{1}$$

$$\underline{\underline{I}} \cdot \ddot{\vec{\theta}}_i = \sum_j \vec{\Gamma}_{ji} + \vec{m}_r \tag{2}$$

where M and $\underline{\underline{I}}$ is the mass and inertial matrix of grain i; $\ddot{\vec{x}}_i$ and $\ddot{\vec{\theta}}$ is the acceleration and angular acceleration of grain i; $\vec{F}_{ji}$ is the force exerted from j to i; $\vec{\Gamma}_{ji}$ is the moment of $\vec{F}_{ji}$ with respect to the gravity center of grain i; $\vec{r}$ is the external force and $\vec{m}_r$ is its moment with respect to the gravity center of grain i. Eqs. (1)–(2) are used to numerically discretize the second law of Newton.

4.2. Interaction contact model

The contact model describes the interaction between grains in contacts. The interaction forces are normal forces, tangential forces, rolling resistance, and eventually cohesive forces. Several contact models are possible to model different rheology or different kind of materials. For example, the interaction forces components in the case of cohesionless granular materials (e.g. dry sand) are different from cohesive-frictional granular materials (e.g. sandstone), even the assumption of circular or spherical grains are used. In this case, the grains are assumed to be rigid, and the contact deformation is described by the possible interpenetration between grains in contact. The interpenetration is very small compared to grains' size.

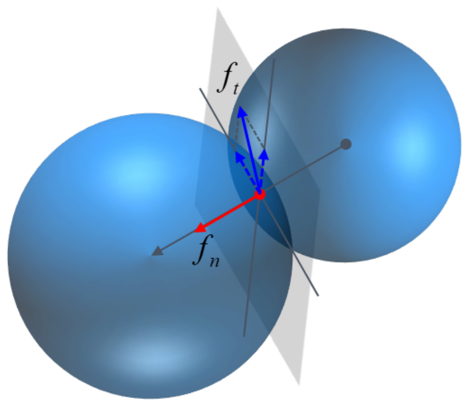


Figure 3. Illustrative image of two grains in contacts

The normal and tangential contact forces are noted f_n and f_t, respectively. They are calculated as follows:

$$f_n = -k_n \cdot \delta + f_c \tag{3}$$

$$f_t = -k_t \cdot u_t \tag{4}$$

where δ is the overlap between two contacted particles; u_t is the relative tangential displacement. To reproduce cohesive-frictional granular materials, a local cohesion f_c is introduced and tangential force is limited by Coulomb threshold as:

$$f_t \leq \mu \cdot |f_n| = \tan\varphi \cdot |f_n| \tag{5}$$

where μ and φ are intergranular coefficient and friction angle.

The stress tensor σ is determined by the homogenized formula:

$$\sigma = \frac{1}{V} \sum_c \vec{f}_c \otimes \vec{l} \tag{6}$$

where $\vec{f_c}$ is contact force and $\vec{l}$ is the branch vector joining the centers of two particles in contact. V is the volume of granular assembly and c is the contact list. The interaction contact model could be varied from case to case and depend on the materials. We recommend the reader to [4] for other interaction contact models.

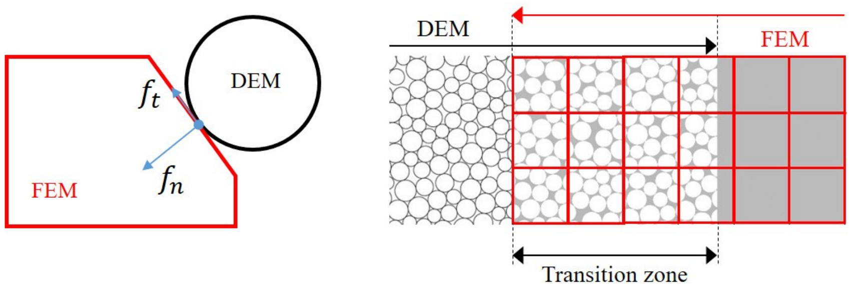
5. FEM×DEM coupling models with direct interaction

5.1. Principle

FEM and DEM have their own advantages, but some gaps need to be filled and supported by other methods. Therefore, the combination of two methods to benefit their advantages has been interested in research since the 80s decade of the twentieth century [5, 6, 20, 21]. In this section, the paper reviews some important contributions and suggesting the possible application in the field of civil engineering.

a. Surface coupling

In this approach, the problem is divided into separate domains that do not overlap. Each of these separate domains is calculated by FEM or DEM. The calculations of the two methods are handled independently. The interaction between the two methods is reflected in the fact that when there is a collision/contact between the FEM and DEM, the interaction force is considered as an external force for the other element, or alternatively, they are considered as boundary conditions for the other elements. Each domain is separately solved by FEM or DEM (Fig. 4(a)).



(a) Surface coupling (b) Volume coupling

Figure 4. FEM×DEM coupling with direct interaction

b. Volume coupling with a transition zone

The idea of volume coupling is similar to surface coupling presented in the previous sub-section. The difference lies in the fact that between the two methods (FEM and DEM), there is an overlapping domain. At this transition region, it can be considered that the behavior of the DEM depends on the FEM or that the behavior in this region is the sum of the responses from FEM and DEM (Fig. 4(b)).

5.2. Applications

The combined FEM×DEM method can be used to simulate and study the behavior of structural elements, for example, concrete beams [22]. The entire concrete beam is simulated by the FEM. The region with large predicted tensile stress is simulated by DEM method. This combination allows describing the flexural behavior of beams while taking into account the occurrence and propagation of cracks in the concrete in the tensile zone. In the cracking area, instead of meshing by the FEM, DEM was used to simulate the occurrence, growth, and propagation of cracks in concrete beams. In addition, the application can also be extended to the study of steel-concrete composite structures in which structural steel is modeled by FEM and concrete is modeled by DEM. In the geotechnical field, [5] investigate the shallow landslide problem by FEM×DEM coupling. The studied area was simulated separately by FEM in the area far from the slope and DEM at the potential slope failure. This simulation used a direct interaction region between the FEM and DEM. The failure occurred at the slope which is expressed by the transition from the steady-state to the unstable state.

In addition to simulating the working and behavior of load-bearing members, soil mechanics problems, ground-structure interaction, the direct combination of FEM×DEM is shown to efficiently model several problems in the field of transport. [23, 24] used the coupled approach to model two typical applications: (i) simulation of the behavior of soil and rock masses under repetitive loads caused by trains and (ii) interaction between tire and roadbed. In both cases, the soils are modeled by DEM whether the rest of the structure used FEM.

6. Multi-scale coupling: FEM×DEM integrated model

6.1. Method development

The principle of multi-scale coupling between FEM and DEM is schematized in Fig. 4. The macro-structure is discretized into finite elements. At each finite element, a representative volume element (RVE) by DEM, is assigned to the integration points (Gauss points). The deformation gradient is then applied to each Gauss point, thanks to the DEM computation, we obtain the corresponding Cauchy stress. Next, we determine the elementary stiffness matrix and then assemblage these matrices to obtain the global one. The non-linear equation system is generally solved by Newton-Raphson method. The above process is repeated for each calculation step until the convergence condition is satisfied. The computation cycle and algorithm of the FEM×DEM integrated approach are described in Fig. 5 and Table 1. In this development, in-house code is used.

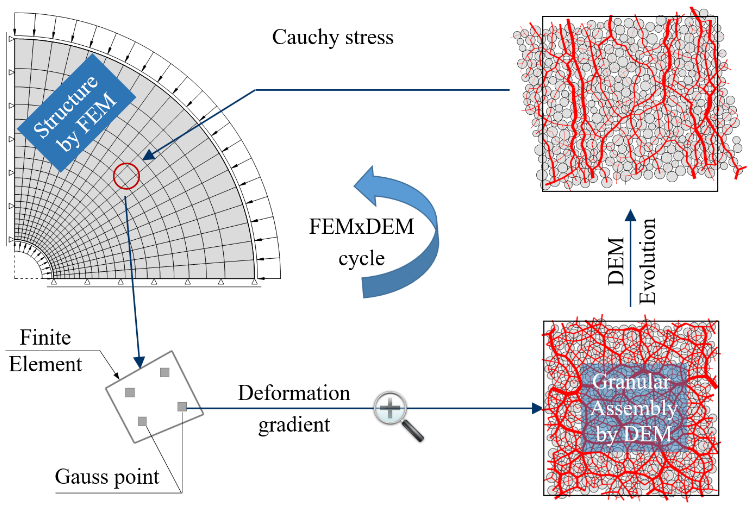


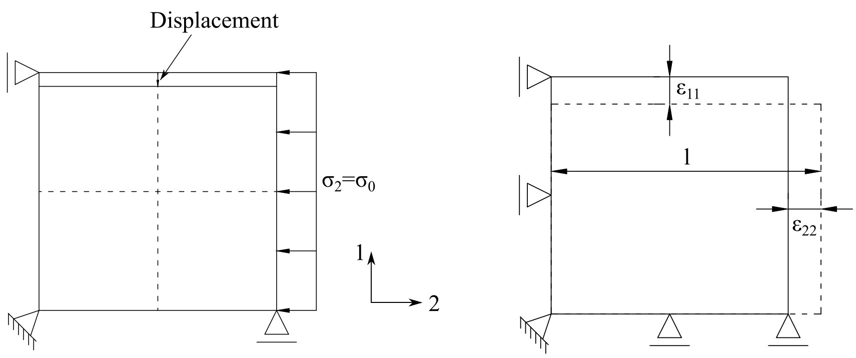
Figure 5. FEM×DEM integrated coupling: computation cycle

Table 1. FEM×DEM integrated algorithm

1. FEM discretization into finite element mesh
2. Each Gauss point in a finite element is assigned a DEM assembly
3. Impose boundary conditions to FEM mesh
4. For each global loading step
For each iteration in the Newton-Raphson resolution
4.1. Compute the current stress and internal variables by DEM computation
4.2. Compute the tangent operator
4.3. Assemblage of the global stiffness matrix
4.4. Solve system equation $F = K \cdot u$
4.5. Update the stress, nodal values, and internal variables
4.6. Verify convergence criterion
5. Perform the next loading step and repeat step 4

6.2. Model verification

We first consider the elementary test under biaxial loading conditions. The top surface is compressed vertically while the constant confining pressure is applied on the left boundary. The elementary test is composed of one Q8 finite element with four integration points (Gauss points). Other boundary conditions are given in Fig. 6. Regarding DEM part, we assign a similar dense granular assembly of 400 grains at each integration Gauss point. The number of grains used in DEM calculation is taken as suggested by [25–27].



(a) Initial configuration (b) Deformed configuration

Figure 6. Biaxial elementary test

The multi-scale response by FEM×DEM simulation is compared to that by DEM computation. As shown in Fig. 7, a good agreement is found in terms of macroscopic stress and volumetric strain versus axial strain. The behavior is typical of a dense granular assembly showing a hardening regime followed by softening regime after reaching the peak in stress-strain response. Regarding strain evolution, the evolution of the volumetric strain first shows a contracting phase followed by a dilating phase after a minimum of axial strain.

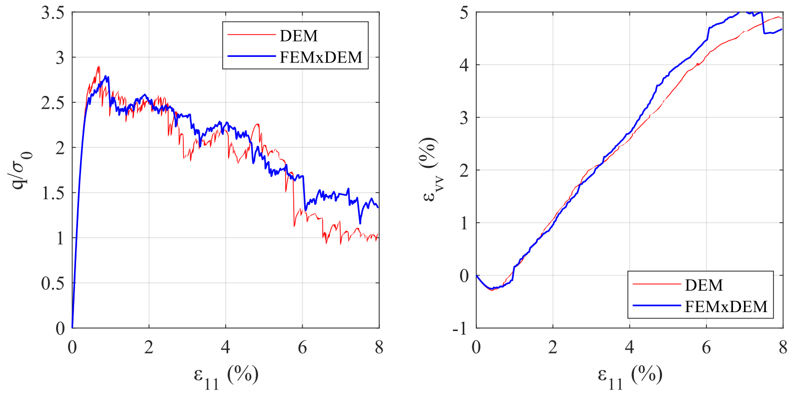


Figure 7. Elementary tests: comparison between FEM×DEM and DEM

6.3. Hollow cylinder model

The objective of this simulation is to reproduce the behavior of the material in the mid-plane section of the hollow cylinder (Fig. 8), assuming plane strain conditions in the axial direction. Because of the symmetric problem, only one-fourth of a plane section is modeled. It is discretized by using 400 eight-nodes quadrilateral order-2 elements with 4 integration points, with the geometry and the loading conditions shown in Fig. 8. According to the experimental test performed by [28, 29], internal and external radii are r_{int} = 7 mm and r_{ext} = 43 mm, respectively. The computation has been performed in two steps: starting from a homogeneous state of isotropic compression σ_0, first the internal pressure (σ_{int}) is decreased to zero then the external pressure (σ_{ext}) is increased up to 4 times the initial isotropic stress (σ_0). At microscopic level, 400 circular disks are used to define granular assembly which is inserted at integration point of finite element. The key parameter of the micromechanical model is summarized in Section 4.

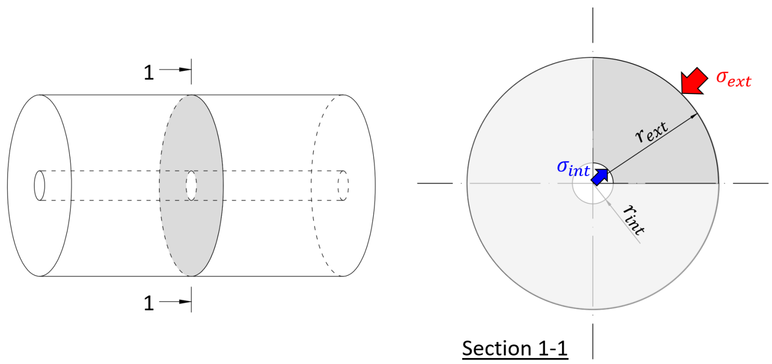


Figure 8. Hollow cylinder problem

From an isotropic stress state, decreasing internal stress σ_{int} produces a redistribution of stress, especially on the internal side. In this zone, ortho-radial stress increases and becomes major principal stress. On the internal side, deviatory stress increase reaches a peak corresponding to the maximum strength of the material and then decreases. Simultaneously, mean stress strongly diminishes in the area near the hole (internal side) leading to the breaking of the micro cohesion link between particles.

Fig. 9 shows the deformation mode in the model at different stages of the loading in terms of the second invariant of strain tensor: (a, b) 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, consistent with experimental work reported by [30, 31]. This is the result of the inherent strain-softening exhibited by the material. 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 [12]. In order to restore a mesh independent behavior in such computations, higher-order constitutive models in which a second gradient model is used with success can be introduced, as according to [32, 33].

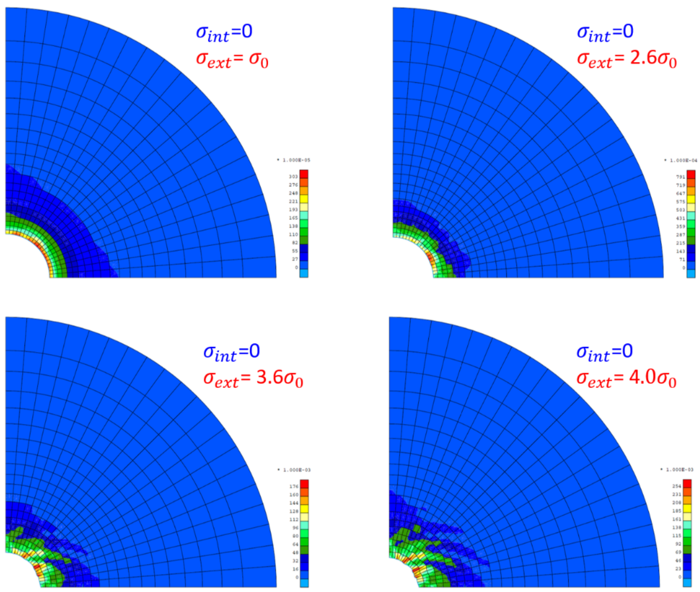


Figure 9. Hollow cylinder: illustration of strain localization by 2nd invariant of strain tensor

It is interesting to put this result in the general context of the loss of uniqueness of the solution. When such a loss of uniqueness is encountered, numerical modeling is moved towards one or more possible solutions. However, different solutions have common characteristics such as shear band orientation (e.g. Sieffert et al. [34]). Thus the result shown here is one of the possible solutions. Obviously, due to the development of shear bands, radial displacements of the internal side are irregular. By approaching the external side, this far zone is not affected by strain localization, radial displacements are almost constant.

Multi-scale modeling by FEM×DEM approach gives a unique way to get further insight on the material behavior at the microscale, within the shear band. Some selected Gauss points are chosen to highlight this feature. Fig. 10 shows the shapes of RVE at the end of the simulation. The width of the force chain is proportional to the normal contact force. RVE No. 16 in the shear band is subjected to complex loading. Its deformation is combined by traction and shear. This RVE shape is monitoring by shear band development. Chains forces tend to move forward the major stress principal direction (orthoradial). Especially, located in the shear band, micro fissure by breakage of cohesion is clearly showed in this RVE. In the homogeneous area, RVE No. 362 does not change much in the distribution of force chains. However, increasing external pressure induce increasing in contact force, as illustrated by more intense force chains.

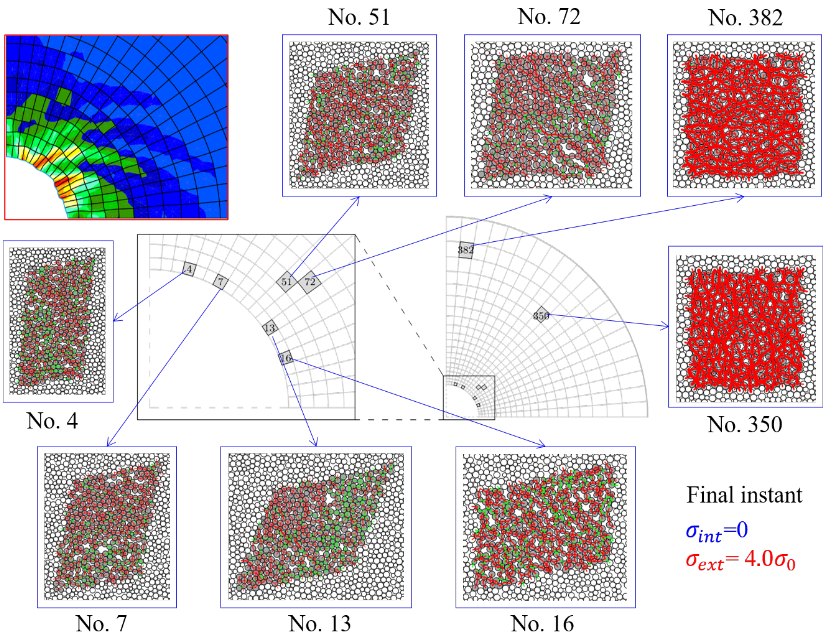


Figure 10. Microscopic insights hollow cylinder problems

7. Conclusions

Based on the separation scales in engineering applications, the paper reviews some FEM×DEM coupling strategies together with potential applications in civil engineering fields.

After a general introduction of the two methods as well as the scope of their application, the study has pointed out the gap between the two methods, as a basis for proposing the combined method FEM×DEM. The principle of coupling between the two methods has been presented in three forms, including surface/volume coupling and multi-scale integrated coupling. These couplings have been illustrated by examples in the civil engineering field. The coupling methods have a wide range of applications, from analyzing the behavior of structural elements to studying the interaction between the ground and structure or other problems in more particular transportation issues.

Finally, we developed a multi-scale integrated approach in which FEM is used at the macroscopic level and DEM at the microscopic level. After describing the methodology, model verification is then presented via biaxial elementary test. Application of the method to a hollow cylinder problem showing the strain localization occurred at macro-scale. This macroscopic behavior has its origin from microscopic evolutions. This unique result demonstrates the capability of the developed model to deal with complicated civil engineering problems.

Besides its advantages, the multi-scale model developed in this study still has some limitations. On the one hand, the result in section 6 shows mesh dependency. To regularize the issue, a local or non-local second gradient model has to be implemented [35, 36]. The microscopic model by DEM in this study, on the other hand, was applied for spheres or disks. Irregular grain shapes or clusters of grains should be utilized to describe geomaterials like soil, rock, or concrete in a more realistic way.

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