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On the efficiency of coupled discrete-continuum modelling analyses of cemented materials

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Abstract

Computational load of discrete element modelling (DEM) simulations is known to increase with the number of particles. To improve the computational efficiency hybrid methods using continuous elements in the far-field, have been developed to decrease the number of discrete particles required for the model. In the present work, the performance of using such coupling methods is investigated. In particular, the coupled wall method, known as the “wall-zone” method when coupling DEM and the continuum Finite Differences Method (FDM) using the Itasca commercial codes PFC and FLAC respectively, is here analysed. To determine the accuracy and the efficiency of such a coupling approach, 3-point bending tests of cemented materials are simulated numerically. To validate the coupling accuracy first the elastic response of the beam is considered. The advantage of employing such a coupling method is then investigated by loading the beam until failure. Finally, comparing the results between DEM, DEM-FDM coupled and FDM models, the advantages and disadvantages of each method are outlined.

1. Introduction

Large-deformation problems in geotechnical engineering, such as pile penetration, are notoriously difficult to simulate using continuum approaches due to both material and geometrical non-linearities (Monforte et al., 2019) and because of mesh distortion related issues (Yang et al., 2020). To overcome these difficulties advanced numerical methods have been developed. Oliynyk et al., (2021) for example used large deformation PFEM (Particle Finite Element Method) analyses to simulate CPTu tests in structured soils, Ko et al., (2016) simulated pile penetration using the Finite Differences Method (FDM) based on Coupled Eulerian-Lagrangian (CEL) method whilst Yang et al., (2020) adopted the Arbitrary Lagrangian–Eulerian (ALE) method to tackle the same problem. Continuum approaches hence have made progress to tackle the numerical complexities stated above. Nonetheless, the quality of the results will always depend on the ability of the constitutive relationship to capture the soil behaviour. Since the discrete element method (DEM) was proposed, it has become a viable alternative to continuum approaches for studying large deformation soil/rock – structure interaction problems and, unlike continuum methods, it does not require a constitutive relationship at the elementary scale because the material behaviour is a direct result of microscale interactions. Nonetheless DEM models require large numbers of particles to produce reliable predictions, making computational cost the main drawback of this approach (Cai et al., 2007). When studying large-scale or even laboratory scale boundary value problems (BVPs), millions of particles are usually needed making the DEM unsuitable. At present, there are two main ways to reduce particle numbers and improve the computational efficiency of large-size BVPs: 1) upscaling the size of particles (Ciantia et al., 2015, 2019; Coetzee, 2019); 2) employing discrete-continuum coupling methods. The former method shifts the natural particle size distribution of the material and for this reason it doesn't guarantee the reproduction of the actual mechanical response at the particle scale and hence requires a time-consuming verification phase. The latter method can be applied to problems where portions of the model are expected to fall within a small strain regime based on a priori knowledge and can hence be directly stimulated with continuum methods. The coupled discontinue-continuum method hence has characteristics that make it a good candidate to simulate

BVPs where large deformations and failure are expected in small portions of the domain. One of the more representative of these coupling methods is the DEM-FDM coupling approach proposed by Zhou et al., (2012) implemented in the Itasca software PFC3D. In this approach, also called “wall-zone”, the forces of discrete particles acting on the vertices of the coupling-wall are transmitted to the continuum element nodes, then the velocities of continuum elements are calculated in the continuum zone and transmitted to the discrete particles through the vertices of the coupling-wall.

In this contribution the accuracy and the efficiency of such a coupling approach, is investigated by simulating 3-point bending tests of a beam-shaped rock sample, where the region of the location of fracture initiation and propagation until failure are known a priori. The DEM is used to simulate the middle portion of the beam while elastic continuum elements are used for the remaining portions of the rock. Also, models considering full DEM discretisation are considered and comparing the results between DEM, DEM-FDM models, the advantages and disadvantages of each method are outlined.

2. Model description

The beam size is $0.45 \times 0.05 \times 0.1$ m, the size of the discrete area is $0.08 \times 0.05 \times 0.1$ m, the porosity is 0.38, and the density is 2600 g/cm^3 (Figure 1a). In the DEM models, the spherical particles are uniformly distributed, the maximum and minimum particle size is 1.67 mm and 2.5 mm, respectively. The average particle size (d_{50}) is 2.1 mm. Contact interaction is described using the parallel bonded model, and the relevant parameters of the model can be found in Nguyen et al. (2017). The elastic parameters used for the continuum portions of the model were selected by matching the elastic response of the bonded assembly retrieved by means of numerical UCS (Uniaxial Compression Strength) tests. As detailed in Figure 1b, loading is achieved by imposing a prescribed displacement at the top of the beam. The supports are modelled by fixing the translational displacements whilst keeping rotations free. The nodes on the right support were not fixed in the x direction to allow for sliding of the beam upon deflection. The sample generation process for the DEM-FDM coupled models is as follows: First the left and right parts of the beam are generated by continuum elements. Subsequently, two coupling walls attached to the surface of the elements are generated. Finally, discrete particles are generated to fill in the middle portion of the beam. After imposing boundary conditions, loading is applied as described above.

Figure 1: a) the schematic diagram of the mode, b) DEM-FDM coupled model discretization

3. Results

Figure 2 shows model results of the elastic response of the beam in terms of load-midpoint displacement up to a displacement of 1 mm (case 1) and Figure 3 represents the beam deflection when the midpoint reaches this final displacement. The numerical results (coupled DEM-FDM, DEM and FDM) are compared with the theoretical deflection of a Timoshenko beam (Przemieniecki, 1985).

Table 1 The comparison of the running time of each method.

Method	Elastic	Failure
	Model running time	
DEM	46min	2h30min
FDM	4.5min	/
DEM-FDM coupling	32min	1h56min

The good match between all curves suggests that the coupling method is effective in the elastic regime. Note that a rigorous calibration of the DEM contact parameters to attain equivalent elastic response at the continuum scale is required. The now validated DEM-FDM coupling is then employed to investigate the mechanical response of the beam until failure (case 2). As shown in Figure 4, bonds break in the middle part of the beam where the DEM is used. Figure 5 shows the post-peak mechanical response of the beam. Here, the DEM and DEM-FDM coupled models have very similar responses. Figure 6 shows the number of broken bonds for the same models. The good match of such micromechanical evolution is the underlying reason for the similar post-peak responses in Figure 5. Finally, the computational efficiency of each method has been compared. Table 1 shows the required time of the above simulations. It should be noted that the loading rate for the plastic models is lower than the one used for the elastic ones (0.2m/s and 0.005m/s, respectively). The reason is that when the bonds begin to break, that is, when the model starts yielding, a smaller load-rate is required to maintain the simulation in a quasi-static state. Compared with DEM, the coupled model does have a higher computational efficiency for both the elastic and post-peak cases as the number of particles is decreased.

Figure 2: The comparison of load-displacement relationship in case 1.

Figure 3: The comparison of deflection in case 1.

Figure 4: The broken bonds in the coupled model (red & blue bonds - broken by tension and shear, respectively).

Figure 5: The comparison of load-displacement relationship in case 2.

Figure 6: The number of broken bonds in case 2.

4. Conclusions

In this paper the accuracy and the efficiency of DEM-FDM coupling, is investigated by simulating 3-point bending tests of a beam-shaped rock sample. Such a coupling method was deemed to be appropriate as the region of the location of fracture initiation and propagation until failure were known a priori. The coupled model (DEM-FDM) and the fully discrete (DEM) models showed good agreement during both elastic and post-peak loading conditions. Comparing the running time of these various models, it is found that DEM-FDM coupled models are about 30% more efficient than the full DEM ones.

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