Public summary of PhD-thesis of Jiadun Liu
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A FEM-DEM model for granular materials

Granular materials, such as rock, sand and soil, are abundantly present in nature. Their mechanical behavior can be simulated by using the finite element method (FEM) or the discrete element method (DEM). FEM can solve large-scale engineering problems by ignoring the discrete nature of granular materials. On the contrary, DEM takes into account the micro-structure of granular materials and its evolution by simulating each particle explicitly. However, DEM is not suitable for large-scale engineering problems since the large number of particles would lead to impractical computational times. Researcher Jiadun Liu proposed a new FEM-DEM model for granular materials that integrates the merits of FEM and DEM.

In the new FEM-DEM model, the macro-scale problem is simulated over the whole domain by using FEM, whereby at each material point (or integration point) the effective stress response due to the imposed deformation is obtained as a volume average over a micro-scale granular packing modeled by DEM. The deformation can be imposed on the granular packing via different micro-scale boundary conditions, whereby it is important to account for consistency of energy at the micro- and macro-scales, to include the effect of *both* particle displacements and particle rotations, and to generalize the formulation within the theory of large deformations. Novel numerical algorithms have been developed to apply these boundary conditions in a numerically robust and accurate fashion.

The multi-scale FEM-DEM model is implemented by using the open-source FEM code ESyS-Escript and the open-source DEM code ESyS-Particle, and is parallelized by using the module MPI in mpi4py. The multi-scale framework is applied to study in a systematic manner the role of individual micro-structural characteristics on the effective macro-scale response. The effect of particle contact friction, particle rotation, and initial fabric anisotropy on the overall response is considered, as measured in terms of the evolution of the effective stress, the volumetric deformation, the average coordination number and the induced anisotropy. The trends observed are in accordance with notions from physics, and observations from experiments and other DEM simulations presented in the literature. Hence, we may say that the present framework provides an adequate tool for exploring the effect of micro-structural characteristics on the macroscopic response of large-scale granular structures.

The applicability and limitations of the multi-scale FEM-DEM model in solving wave propagation problem are studied on a set of benchmark numerical examples. The model is validated for a one-dimensional string of particles, comparing the multi-scale solution with DNS results. In addition, two-dimensional microstructures are considered, which reveal that the applicability of the method is dependent of the constitutive assumptions made at the micro-structural level. While for bond-elastic interactions the FEM-DEM solution and the DNS solution agree well, for compressive-elastic interactions the differences may become significant. This aspect constitutes a limitation of the method that should be addressed in future research.

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