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Title: Micro-inspired continuum modeling using virtual experiments

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Motivation: One major challenge for understanding granular behavior is to be able to predict its evolution under cyclic loading. Granular properties are altered over time if soils are subjected to different combinations of cycles and amplitudes. Projecting these changes by linking micro-scale modifications and macroscale constitutive models would provide a vital insight into foundation and soil response. This is particularly important for applications related to periodic loads such as earthquake and coastal engineering.

Objectives: a) Simulate cyclic loading conditions on particles with arbitrary shapes using the level discrete element method (LS-DEM) that match results from experimental setups such as triaxial, ring shear and hollow cylindrical apparatus (HCA) with the same testing conditions.

b) Apply the findings on the project to generate fabric descriptors that link microstructure information obtained from discontinuum simulations and constitutive models to describe continuum macroscopic behavior, relating micro and macro descriptors such as fabric tensor and hardening modulus.

Methodology: Laboratory experiments aided with computed tomography were obtained for both monotonic and cyclic triaxial tests in sands. These experiments were converted into inputs for the level set discrete element method (LS-DEM) that allowed to replicate the experiment digitally with a one-to-one relation with experimental grains. From simulations critical fabric quantities were obtained and additional virtual experiments with different loading and boundary conditions were developed to get even more information related to fabric. These fabric descriptors can then be utilized to link to macroscopic quantities and models.

Results: a) It was shown that LS-DEM is not only able to capture very accurately monotonic triaxial shear or compression experiments but also cyclic triaxial loading. In other words, simulations faithfully reproduced experimental results. Cyclic loading requires a stricter control of boundary conditions in the simulation to avoid measurements errors.

b) Under periodic loading, it is possible to observe the cyclic evolution of fabric descriptors using LS-DEM. Global quantities such as the coordination number and void ratio tend to oscillate over time but, in general, converge to a more compact configuration in comparison to monotonic loading, as observed in Figure 1. This effect is augmented if the number of cycles and amplitude are increased.

Conclusions: Based on the results of this project it was possible to observe the importance of shape on simulation of triaxial testing, as it was proven it has a significant impact on volumetric and deviatoric strains. Hence, numerical models such as LS-DEM can be applied to model more accurately the behavior of soils with irregular shapes and elongated proportions rather than using spherical or polyhedral geometries. Thus, enhanced RVE's can be utilized to calibrate constants of constitutive models and aid granular material, continuum mechanics and geotechnical researchers.

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As a result of the fact explained above, fabric effects can be detected with more sensitivity, particularly for cyclic loading conditions. Arbitrary-shaped grains from CT scans of actual triaxial test are re-accommodated in a more impactful way (compared to spheres or polyhedral) that significantly changes the kinematic and kinetic descriptors of fabric. So, using these digital grain avatars in combination with in-situ cyclic loading scenarios can help forecast performance of soils in terms of micro-scale fabric information. This information can be linked to experimental observations to directly tie macroscale performance that can then predict soil subsidence and settlement of foundations. Both professional engineers and soil mechanicians can be greatly benefitted by these enhanced understanding.

Future directions: a) Execute additional experiments with apparatuses other than the standard triaxial machine and for a greater number of cycles, to obtain high resolution X-ray computer tomography data that can be then used to improve the LS-DEM model to better capture cyclic changes on granular materials. As well, its recommended to examine the effect of sample preparation (e.g., dry tamping, pluviation, etc.) and sample bedding angle on cyclic fabric evolution using DEM simulations to provide more information on fabric descriptor tensors.

b) Combine information of contact normal and contact force tensors, as well as particle alignment and void tensors, from simulations and experimental results to develop a fabric descriptor that is representative of these experiments and can be used to predict granular fabric evolution via "virtual" experiments.



Figure 1. Evolution of void ratio and coordination number under cyclic loading

Keywords: continuum modeling, discrete element simulations, dilatancy, granular fabric, cyclic loading.