Bayesian calibration of microCT-based DEM simulations for predicting the effective elastic response of granular materials

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ABSTRACT

A novel approach is presented for calibrating discrete element method (DEM) simulations of granular materials based on the sequential Bayesian parameter estimation over the experimental stress–strain responses. An initial DEM configuration is reproduced starting from microscopic computed tomography (microCT) images by quantitative assessments of particle morphologies and configuration, which are offered by the image processing techniques suitable for fine particles with material imperfections.

The aim of this work is twofold: i) to establish a calibration procedure which estimates the posterior probability for the micro-mechanical parameter sets given the macroscopic measurements; and ii) to numerically predict the elastic response of an assembly of Hertzian glass spheres along a given stress path, given that the structure is inferred by micro-CT images.

We first introduce the feature-based watershed algorithm, which performs image filtering, geodesic reconstruction, feature-based segmentation, watershed separation and particle analysis on the microCT images of a glass bead packing at an isotropic pressure p = 5 MPa. The resulting particle morphologies and configuration are imported in the DEM code and represent the basics of the numerical packing. However the contact force network must be superimposed to the geometric structure for a complete definition of the granular sample. That is inferred via a Monte Carlo inversion: the interparticle friction coefficient and the size of the periodic cubic cell only are adopted as free parameters, and the sets that reproduce the initial bulk stress and void ratio with high accuracy are selected for a sequential Bayesian parameter estimation. The Bayesian estimation results in a posterior probability density function of the selected parameter sets, which is updated at each measurement step using the macroscopic data.

We apply the presented approach to calibrating the microCT-based DEM simulation of glass bead packing, which is further subjected to an isotropic loading path, following the experimental test. As validation step, pressure and shear velocities are calculated numerically at various pressure levels along the compression path, in a similar fashion as for the physical samples. DEM simulations using the parameter set with the highest posterior probability are in good agreement with the experimental data.