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Mechanical properties of granular materials: a variational approach to grain-scale simulations

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ABSTRACT

The mechanical properties of cohesionless granular materials are evaluated from grain-scale simulations. A three-dimensional disordered packing of elastic spherical grains, bounded by a rectangular container, is loaded by incremental displacements of its boundaries. The deformation is described as a sequence of equilibrium configurations. Each equilibrium configuration is found by minimizing a functional related to the total work done by the system. A modification of the conjugate gradient algorithm is used to obtain this minimum. This approach results in an efficient computational procedure, which is also used to generate a dense initial arrangement.

The loads developed at the contacts between the grains are computed using the contact theories of Hertz [1] for normal compression and Mindlin and Deresiewicz (M-D) [2] for other components, e.g. shear and torsion. We present here results of simulations using two different sets of contact laws: (a) frictionless, accounting for normal forces only, and (b) frictional, accounting for loads due to intergranular friction in addition to the normal forces.

By micromechanical analysis we demonstrate mechanisms responsible for hysteresis, strain hardening, and stress-induced anisotropy. Macroscopically, our results capture the nonlinear and path-dependent response observed in experiments. We verify our physics-based model against published experimental data [3–5], using similar grain properties. All material parameters used in simulations are obtained from published experiments. Our moduli predictions agree with the data, aside from the shear modulus evaluated using the frictionless contact model, see Fig. 1. The good agreement between predicted and measured moduli is achieved with no adjustments of parameters.

These results confirm that the normal contact forces play an important role in determining the overall response , and that grain-scale elasticity is suitable to describe many features of the inelastic response of granular materials. The bulk modulus, for example, mainly depends on the normal contact forces, which are adequately described by the elastic Hertzian model. Nevertheless, our frictionless model underestimates the shear modulus. Thus, we conclude that appropriate account for intergranular friction, such as provided by our frictional contact model, is required to evaluate the response to shear loading.

We apply our model to quantify the effect of hydrate dissociation in marine sediments. Hydrates are modeled as load-bearing solid particles within the pores. To model dissociation, we reduce the solid fraction by shrinking the hydrate grains. The effect of the related excess pore pressure is modeled by expanding the sample to account for the decrement of effective stress, and compressing the grains. A series of possible scenarios is simulated, showing degradation in sediment strength as a reduction in the macroscopic elastic moduli. This trend agrees qualitatively with published experimental data [6]. Further dissociation might lead to loss of solid support of the skeleton, causing seafloor landslide and subsidence. To predict such instabilities and their impact on offshore platforms, our model can be used to provide constitutive relationships for large-scale simulations. To quantitatively verify our predictions, more experimental data is required.

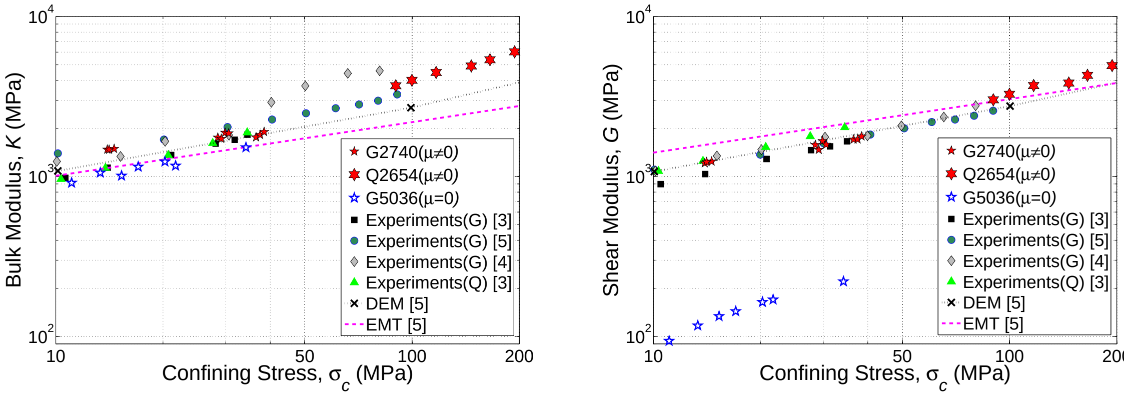

Figure 1: The effective bulk (left) and shear (right) modulus *vs.* the confining stress σ_c, evaluated from simulations using frictional ($\mu \neq 0$) and frictionless ($\mu = 0$) contact models on samples of 5036 and 2740 glass beads (G5036 and G2740) and 2654 quartz grains (Q2654). Also shown are published results of acoustic experiments in glass beads [3–5] and sands [3], in addition to Discrete Element Method (DEM) and effective medium theory (EMT) predictions [5].

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