ISEN Report

Energy recovery and fracture in granular rocks: towards a new generation of multi-scale simulators

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Background and Objectives

Most of the world’s energy comes from fossil fuels hosted in the shallow crust. Modern extraction technologies depend on the ability to extract such fuels in effective, safe and sustainable manner. In relation with this challenge, this project has formulated novel multi-scale modeling techniques to understand the response of rocks to drilling, fracturing and production.

The study has focused on high-porosity granular rocks, such as sandstones and carbonates. Given their considerable porosity and their microstructural characteristics, these rocks are indeed frequent hosts of hydrocarbons and ideal reference to develop multi-scale models for rock-like materials. For this purpose, these rocks have been studied from different perspectives, using discrete methods to capture the microscopic origin of deformation/failure mechanisms, as well as continuum mechanics to address the complex phenomenology of their heterogeneous deformation response.

Results

We have formulated a new discrete model for granular rocks. The model has been developed in the context of Lattice Discrete Particle Models (LDPM), a numerical approach that can simulate the mesostructure of quasi-brittle materials by a three-dimensional assemblage of polyhedral particles. Such models reproduce a wide range of mechanical processes, including cohesive fracturing, strain softening in tension, strain hardening in compression, compaction due to pore collapse, frictional slip and rate effects. LDPMs have allowed us to reproduce the microstructure of granular rocks by considering directly the grain size distribution of their solid skeleton (Fig. 1). The main challenge has been the formulation of the micro-scale constitutive laws governing the interaction between adjacent particles. To validate the effectiveness of these laws, we have calibrated the LDPM to capture the response of Bleurswiler sandstone, which for this purpose has been selected as a model material. Some of the results obtained by LDPM are presented hereafter. The results indicate that a realistic description of the granular microstructure together with a mechanically consistent set of constitutive laws enables the reproduction of a number of key macroscopic processes, such as the transition from dilative to contractive response, as well as from brittle/heterogeneous failure to ductile/homogeneous compaction. All such effects are reproduced by ensuring both quantitative and qualitative agreement with the macroscopic patterns observed in deformation experiments, thus corroborating the predictive capabilities of the new LDPM formulation for granular rocks (Fig. 2).
Figure 1. Grain size distribution adopted for the simulation of Bleurswiller sandstone

Figure 2. Simulation of triaxial compression response at both low and high confining pressures

Figure 3. Yield cap predicted numerically by the LDPM formulation
These preliminary findings show that the newly developed discrete method for rock is capable to capture some of the concepts from the theory of plasticity that are routinely used in the domain of geomaterial characterization (e.g., the concept of yield locus; Fig. 3). Such features can be used to derive homogenized laws and study the interaction between inherent micro-scale heterogeneities and emergent macro-scale heterogeneities (e.g., faults and strain localization zones). For this reason, such inelastic processes have been studied in this project also via continuum modeling. This has been done with reference to a variety of high-porosity rocks subjected to axisymmetric deformation paths under laboratory conditions (Fig. 4). To simulate realistically the formation of strain localization zones we have considered material models able to capture processes such as the hardening due to densification and the deterioration due to the breakage of grains and/or cement bonds (Fig. 5). In addition, different geometric patterns of rock heterogeneity have been considered, with the purpose to study their effect on the creation of a hotspot for strain concentration and consequent specimen failure.

Figure 4. Finite element mesh for triaxial compression tests with random spatial heterogeneity.

Figure 5. Simulated distribution and propagation of compaction zones in triaxial compression tests.

This FEM-based study has highlighted the remarkable interaction among local heterogeneity (e.g., spatial and statistical variability of cement and grain size distribution), process induced
heterogeneity (e.g., strain localization zones, layers of heterogeneous compaction) and site-specific conditions (e.g., frictional contacts, layering). As a result, it has pointed out the mandatory need to consider fine-scale heterogeneities in the formulation of continuum laws for engineering applications in the domain of energy recovery. Such an objective can be met by further integrating the discrete/continuum methods formulated in this project, i.e. by combining failure analyses and micro-inspired continuum laws.

**Project Participants**

ISEN funding has provided partial support for two postdoctoral collaborators, Dr. Congrui Jin, who has collaborated to the modeling efforts based on LDPM techniques, and Dr. Ferdinando Marinelli, who has conducted numerical analyses of failure processes based on continuum mechanics. In addition, the project has supported the activities of two graduate students, Reed Laverack and Shiva Esfahani, providing them with the opportunity to develop expertise in the theoretical and numerical study of failure processes in porous rocks.

**Publications resulting from this ISEN project**

The results of this ISEN project have originated the following publications. The support of ISEN has been acknowledged in all publications:


**External proposals submitted as a result of this ISEN project**

**Title:** Grain Size Effects in Sediment Compaction: An Augmented Continuum Theory Based on Grain-Scale Fracture Mechanics  
**PI:** Giuseppe Buscarnera  
**Sponsoring Agency:** Petroleum Research Fund – American Chemical Society (PRF - ACS)  
**Budget:** $110,000  
**Status:** Pending

Additional funding sources are being explored, especially within the basic science program of NSF.