Micro- to macro-scale modeling of multi-physics in fractured rocks

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ABSTRACT

In this work, we present numerical models and results for multi-physical analyses that address the distinct geometric and physical features of fractures from micro- to macro- scales. Different geometric representations of fractures are used for each scale, and physical laws are applied as appropriate. Our model overcomes the computational challenges associated with intersections and shearing and the contact dynamics along rough fracture surfaces, interfaces, and corners treated with discontinuum approaches at the grain scale. We have conducted simulations to analyze how a network of discrete fractures responds to fluid injection. Further, we investigate how single fractures with realistic asperity geometries are altered due to compaction and pressure solution. We used continuum and discontinuum approaches to analyze the compaction of rock containing discrete rough fractures. These examples show that it is important to properly address the complex geometry and multi-physics of fractures to understand and control the evolving surface and subsurface geosystems.

1. Introduction

Based on geometric features, fractures can be categorized into three different scales: dominant fractures with a certain width and roughness, discrete thin interfaces, and microscale grain assemblies and asperities (Hu et al., 2017a; Hu and Rutqvist, 2020a, 2020b). At reservoir scales, fractures are usually very thin (e.g. microns to millimeters) relative to their length (meters). They often arbitrarily oriented and intersecting with each other, and form a network. When a single fracture is examined more closely, it is often rough, and may be filled with minerals and connected to smaller fractures in the surrounding rock. Zooming into the microscale, a single fracture becomes a rough channel with asperities made up of a number of tightly contacting mineral grains.

In this work, we present numerical models and results for multi-physical analyses to address the distinct geometric and physical features of fractures from micro to macro scales. We will introduce the numerical approach in Section 2 where different geometric representations of fractures are used for each scale, and physical laws are applied as appropriate. In Section 3, we show a number of examples including how networks of discrete fractures respond to coupled hydro-mechanical (HM) processes such as loading and injection, how single fractures are compacted where the geometry and distribution of asperities play key roles, and how geometric and physical abnormal features (e.g., sharp corners, deformation zones) control the subsequent chemical-mineralogical transformation (diagenetic) processes of granular geosystems.

2. Approach

Previously, we have developed comprehensive model capabilities to simulate coupled HM processes in porous, fractured and granular systems at different scales based on the numerical manifold method (NMM, Hu and Rutqvist, 2020a, 2020b, 2021). The modeling capabilities involve different governing equations, constitutive relationships, HM couplings, and approaches for addressing intersections and shearing of interfaces at different scales. Radiating from the direct coupling of conservation of solid momentum and conservation of fluid mass, discontinuum mechanics with the calculation of dynamic contacts is applied for the discrete fracture networks and microscale asperities and grains. In addition, different and indirect couplings apply with different constitutive behavior and physical laws.

In order to conduct coupled mechanical-chemical (MC) analyses at multiple scales, we linked NMM to a reactive transport code Crunch. Crunch is well-known for modeling reactive transport developed by Steefel since 1990s (Steefel and Lasaga, 1994; Steefel et al., 2015). In this new MC model (Hu et al., 2021), rigorous algorithms have been developed to address the challenges associated with evolving geometry (as a result of deformation and contact change, and chemical reaction) and complex physics.

3. Modeling Fractures at Multiple Scales

3.1. Coupled Hydro-Mechanical Responses to Borehole Injection in a Discrete Fractured Porous Rock

The first example involves coupled hydro-mechanical (HM) responses to borehole injection in a discrete fractured porous rock (Hu et al., 2017). We simulate fluid injection from a vertical borehole (diameter 0.1 m) at the center of a fractured model domain now scaled to size of 1 × 1 m. This example represents near borehole coupled HM effects that take place during injection. The initial total stress is assumed to be 35 MPa and 30 MPa, in the two horizontal directions, respectively. The initial fluid pressure is 5 MPa. All boundaries have fixed pressure head. The injection pressure is increased by stages: 2MPa from 1000 to 4000 seconds, 4MPa from 4000 to 7000 seconds, and 6 MPa after 7000 seconds. For the rock matrix, the Young's modulus is 10GPa, Poisson's ratio is 0.3, and the permeability coefficient is 1× 10^{-10} m/s. For the discrete fractures, the initial mechanical apertures is 0, the residual aperture is 10μm and the friction angle is 0.

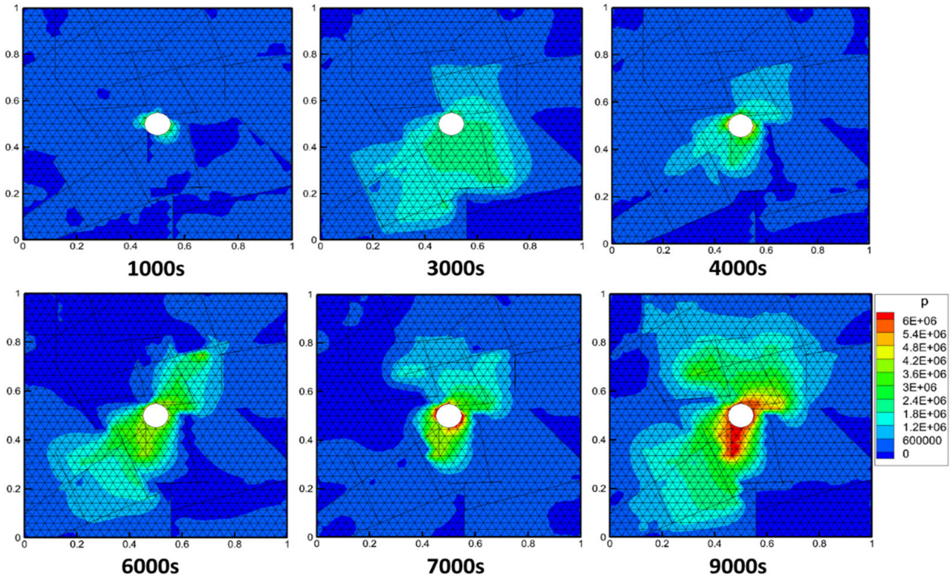


Figure 1. Simulated evolution of the injection-induced fluid pressure (Unit: Pa)

Figure 1 shows the simulated evolution of the injection-induced fluid pressure. The pressure first builds up in the rock matrix near the borehole, then increases in the fracture network with the increase of the injection pressure. Then it is released with the opening of some fractures. This behavior is repeated with each pressure step and finally, the increased pressure develops in a large part of the domain because of the increased fracture apertures around the borehole. This example involves the opening of fractures due to pressure increase within the fractures, as well as pore-elastic expansion of rock matrix that tends to close the fractures. From this example, we show that both direct and indirect coupling can be important to consider for the design of efficient energy recovery.

3.2. Compaction of Fractures Impacted by Geometry and Distribution of Asperities

In this example, we calculated mechanical compression of rough fractures with explicit representation of the asperities with later confinement (Hu and Rutqvist, 2020b). Here we show two cases with different profiles of asperity geometry and distribution: (1) evenly distributed smaller asperities, and (2) non-evenly distributed asperities with two major asperities. The sizes of the domains are the same: 10 mm × 5 mm. The Young's modulus is 4GPa and the Poisson ratio is 0.3. The Young's modulus of the two columns on the left and right sides is 40GPa.

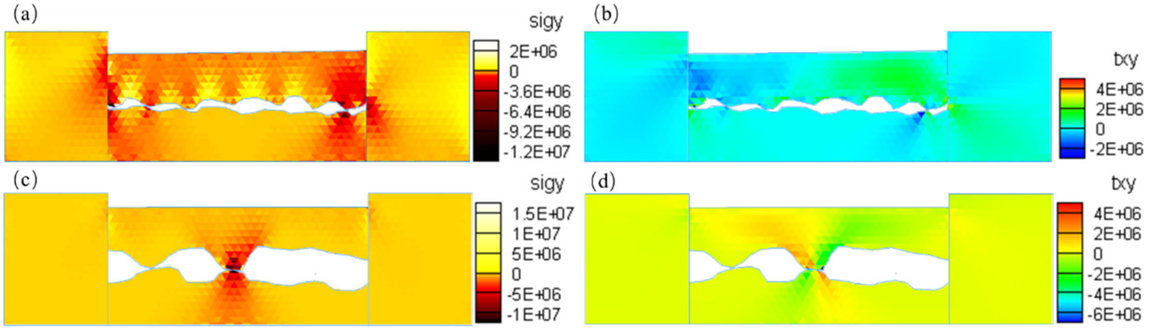
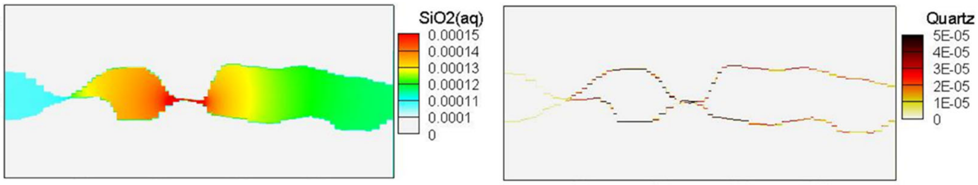


Figure 2. Calculated normal (left) and shear (right) stresses (Pa) of a compressed fracture when reaching equilibrium

Figure 2 shows vertical (left) and shear (right) stresses. When equilibrium is reached, the average value of closure for case (1) is 0.8mm and for case (2) is 0.5mm. We observed that both the vertical stress and the shear stress concentrate at the contacting areas evenly through the fracture for case (1), whereas for case (2) the dominant contacting asperities govern the closure as well as stress concentration.



Silica concentration (mol/L) Precipitation rate $(mol/m^3/s)$

Figure 3. Calculated silica concentration (mol/L, left) and precipitation rate (mol/m³/s, right)

Extracting the converged stress for the case (2) profile, we used NMM-Crunch code to calculate enhanced dissolution as a result of pressure solution, diffusion, and precipitation. As shown in Figure 3, at the high-stress contacting major asperity, pressure solution occurs with enhanced reaction rate and solubility, causing the dissolution of silica. The dissolved silica forms a gradient in chemical potential and concentration from the contacting area to the rest of the fracture channel and precipitates at the rough free surfaces where stress is relatively low. When equilibrium is reached, the diffusion rate is balanced with the precipitation rate on the rough free surfaces, suggesting a balance between the pressure solution and precipitation.

3.3. Modeling Compaction of Discrete Rough Fractures with Continuous and Discontinuous Approaches

In this example, we used an image of a network of rough fractures and applied two different models to simulate its mechanical behavior induced by compaction (Hu and Rutqvist, 2021). These two models are: (1) a continuous model where the fractures are represented as porous and deformable zones with a softer material than the rock matrix, and (2) a discontinuous model where the fractures are represented as discontinuous rough surfaces. In both models, the asperities are explicitly represented. The model domain for this example is 10m × 8m. For each model, a vertical loading of 0.42 MPa is applied on the top. The other three boundaries are fixed. For both models, the Young's modulus is set to 4GPa and the Poisson's ratio is 0.3. In the continuous model, the solid material within the fractures surfaces is assumed to have a Young's modulus of 4 MPa, which is three orders of magnitude lower than the surrounding rock matrix. The Poisson's ratio is the same as the rock matrix. In the discontinuous model, the loading and confinement columns are assumed to have a Young's modulus of 4GPa. The fractures, represented as rough interfaces, have a friction angle of 30°.

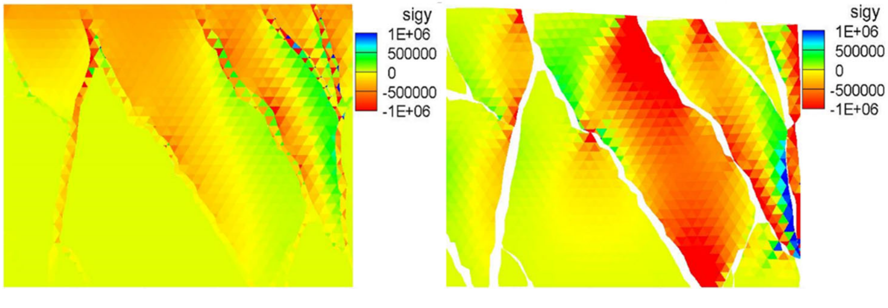


Figure 4. Calculated vertical stress (Unit: Pa) with the continuous (left) and discontinuous rough interface (right) models

The vertical stress calculated by the two different models is shown in Figure 4. From this example, we concluded that because the discontinuous model captures the dynamical changes of contacts with large displacements on the right and the stress re-distribution as a result of the dynamic changes of contacts, the results appear to be quite different than those obtained from the continuous model. We show that when rough fractures are not filled with minerals and when a number of rough fractures form a blocky system, dynamic contacts play an important role in the geometric, multi-physical evolution of the system.

4. Conclusions

Fractures at different scales have different geometric and physical features. Based on their distinct geometric features, we categorized fractures into three different scales: dominant, discrete fracture, and discontinuum asperity scales. In this study, we used different geometric representations of fractures and developed numerical models with different governing equations and constitutive relationships to study coupled processes in fractures at different scales. Our models are able to handle the computational challenges with accurate representations of intersections and shearing of fractures at the discrete fracture scale, and rigorously treat dynamic contacts along rough fracture surfaces, interfaces, and corners at the discontinuum asperity and microscopic scales. We presented analyses involving injection-induced hydro-mechanical changes within a discrete fractured porous rock, closure and pressure solution within single fractures impacted by geometry and distribution of asperities at the microscale, and compaction of a discrete rough fractured rock with continuous and discontinuous approaches. We show that:

- The opening of fractures due to pressure increase within a discrete fracture network and pore-elastic expansion of rock matrix that tends to close the fractures are competing mechanisms that are both important to consider for the design of efficient energy recovery;
- At the asperity scale, major asperities govern closure and stress distribution and pressure solution;
- Accurate representation of geometric features of fractures at different scales is essential.

By properly addressing the the complex geometry and multi-physics of fractures, our multiscale modeling capabilities can be useful for advancing fundamental understanding and optimizing energy recovery and storage in fractured rocks.

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References

Hu M, Wang Y, Rutqvist J. 2017. Fully coupled hydro-mechanical numerical manifold modeling of porous rock with dominant fractures. Acta Geotechnica 12(2), 231–252.

Hu M, Rutqvist J. 2020a. Numerical manifold method modeling of coupled processes in fractured geological media at multiple scales. Journal of Rock Mechanics and Geotechnical Engineering 12(4), 667-681.

Hu M, Rutqvist J. 2020b. Microscale mechanical modeling of deformable geomaterials with dynamic contacts based on the numerical manifold method. Computational Geosciences 24, 1783–1797.

Hu M, Rutqvist J. 2021. Multi-scale coupled processes modeling of fractures as porous, interfacial and granular systems from rock images with the numerical manifold method. Rock Mechanics and Rock Engineering. https://doi.org/10.1007/s00603-021-02455-6

Hu M, Steefel CI, Rutqvist J. 2021. Microscale mechanical-chemical modeling of granular salt: Insights for Creep. Journal of Geophysical Research: Solid Earth. https://doi.org/10.1029/2021JB023112

Steefel CI, Lasaga AC. 1994. A coupled model for transport of multiple chemical species and kinetic precipitation/dissolution reactions with application to reactive flow in single phase hydrothermal systems. American Journal of Science 294, 529-592.

Steefel CI, Appelo CAJ, Arora B, Jacques D, Kalbacher T, Kolditz O, Lagneau V, Lichtner PC, Mayer KU, Meeussen JCL, Molins S. 2015. Reactive transport codes for subsurface environmental simulation. Computational Geosciences 19, 445-478.