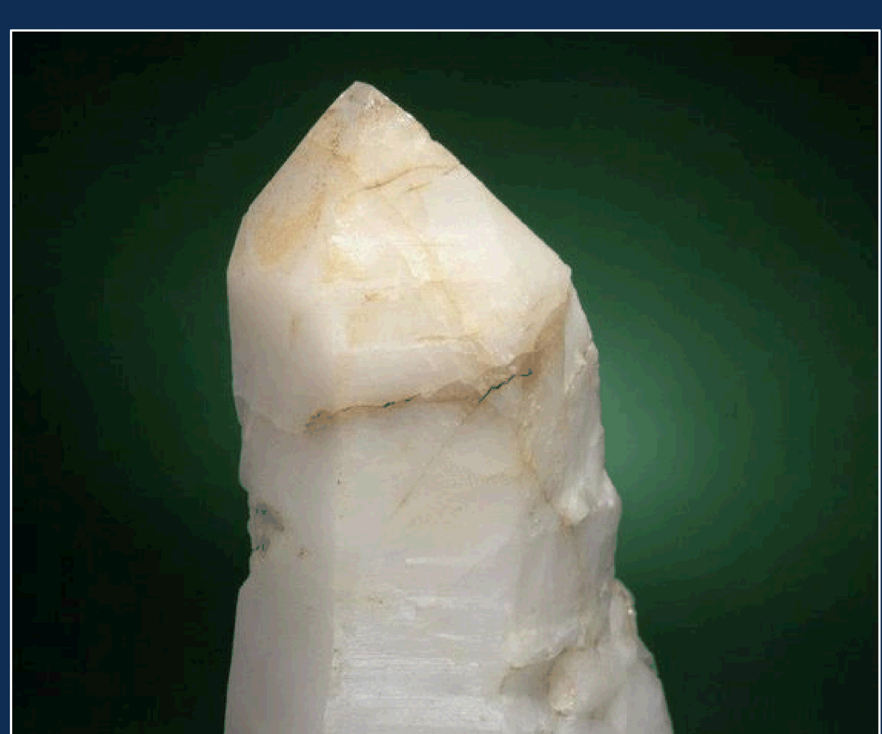
SAND2016-9669D



Exceptional service in the national interest

Chemical-Mechanical Modeling of Subcritical-to-Critical Fracture in Geomaterials

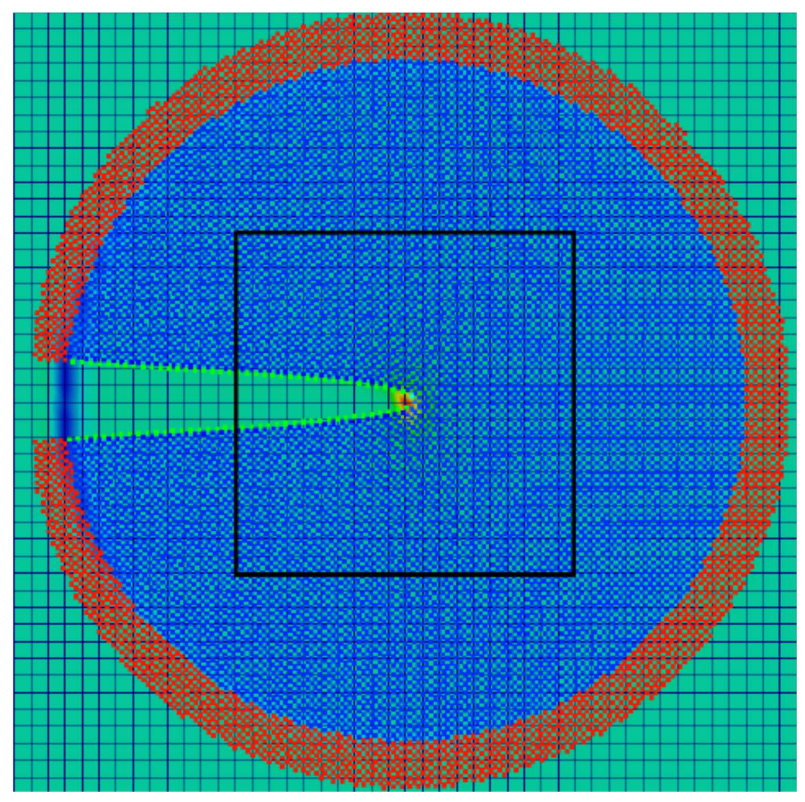
Louise Criscenti (PI), Reese Jones, Jessica Rimsza, Ed Matteo, Tom Dewers, Susan Altman (PM)

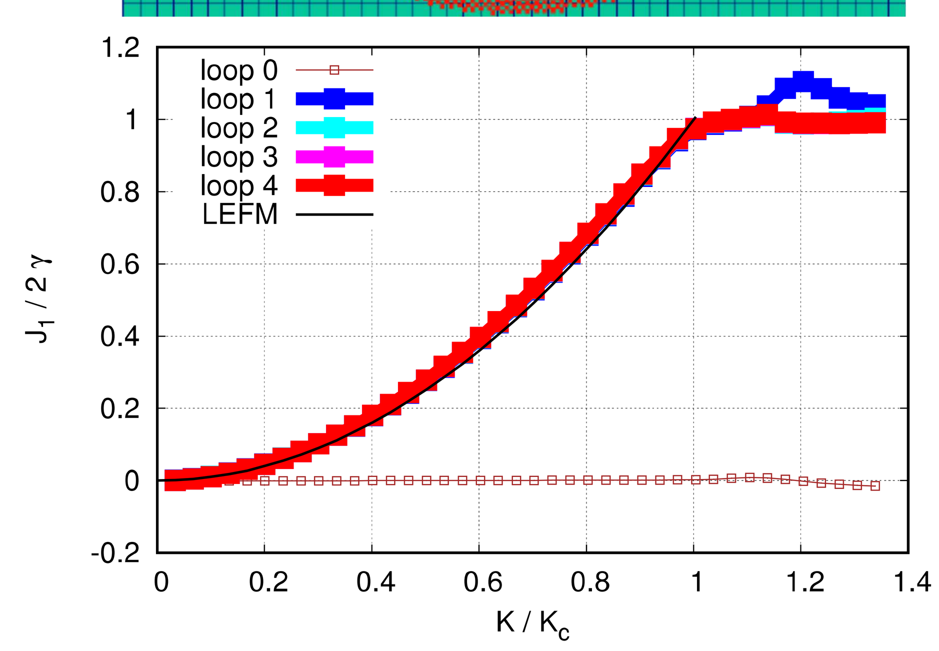
Objectives

- Develop a fundamental, atomistic-level understanding of the *chemical-mechanical* processes that **control subcritical cracks** in low-permeability geomaterials.
- Link atomic-scale insight to macroscale observables.
- Address how chemical environment affects mechanical behavior.

Atomistic to Continuum Scale Modeling

- A slit is inserted through bonds crossing a half plane
- A far-field continuum displacement boundary is applied on an annulus of atoms.
- Stress, displacement, and energy density fields are coarse-grained on a grid.
- Eshelby stress is formed and the J-integral (fracture toughness) is evaluated on the contour.

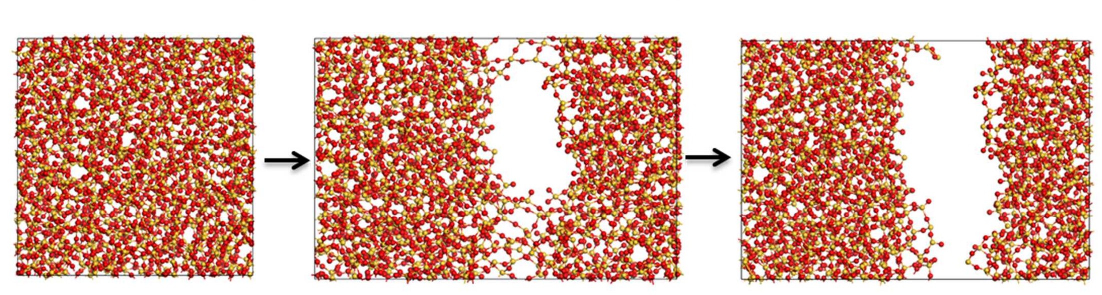




Initial Fracture Studies with REAXFF

Investigate fracture in amorphous silica:

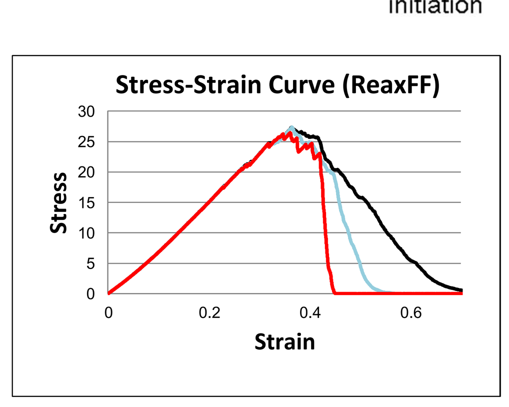
- SiO_2 is present in sandstone and shales .
- ReaxFF potentials are well parametrized for Si/O/H systems.
- Data is available [Dove, 1995] from constitutive equations to compare/validate ReaxFF simulation results .
- ReaxFF data, including efficiency, enthalpy of reactions, velocities, stress, strain, surface energies and etc., are used to develop algorithm to add chemistry to the J-integral .
- Comparison with ClayFF will provide benchmark for the development of ReaxFF for Clays.



ε=0
Dense Silica

ε~0.35
Void nucleation and fracture initiation

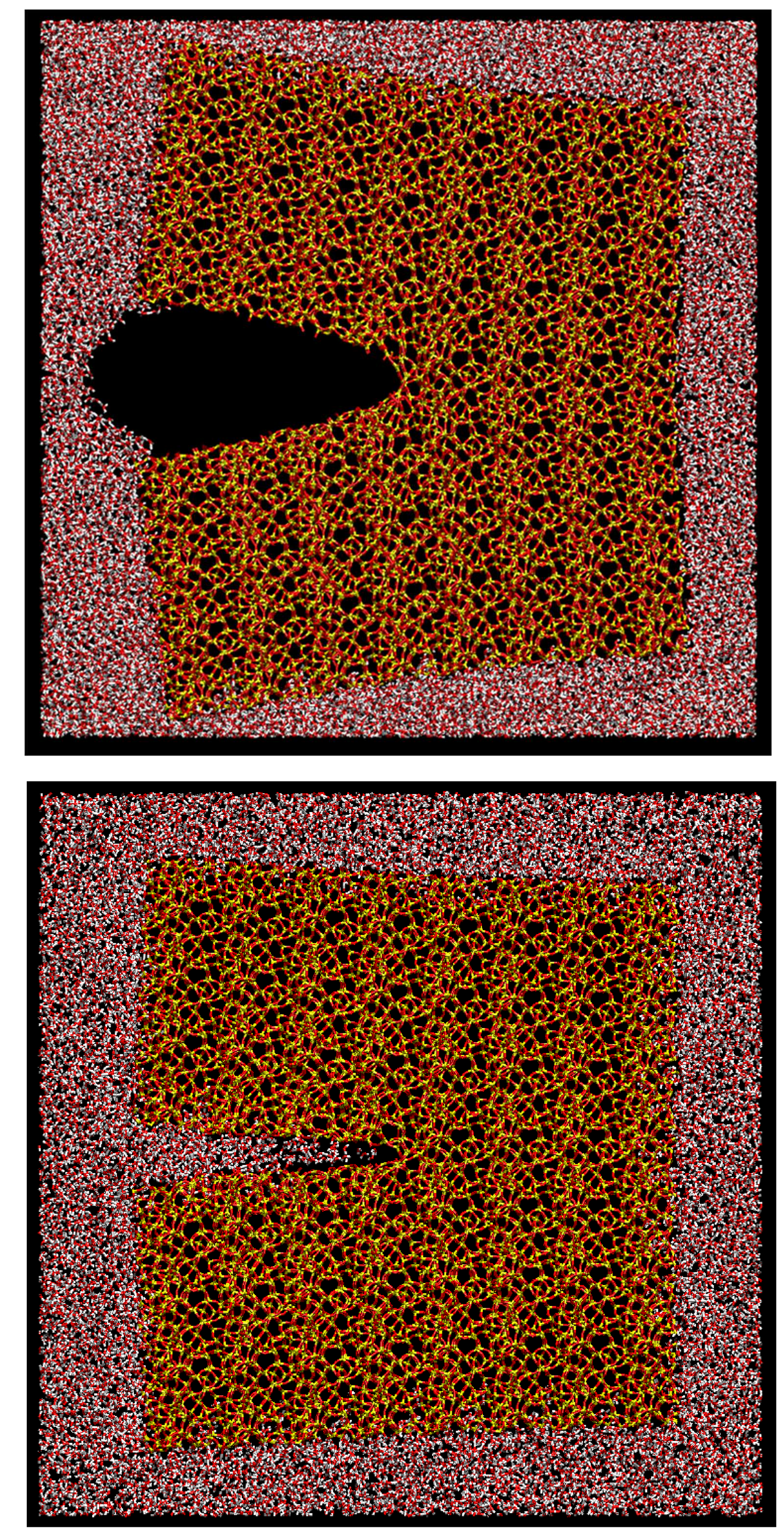
ε~0.4
Fracture



ReaxFF Elastic Constants*
E=76.1±0.3 GPa
K=55.2 ±5.2 GPa
G=21.8±0.8 GPa
v=0.32±0.02

ClayFF Elastic Constants*
E=108.5±0.6 GPa
K=65.6 ±0.5 GPa
G=47.1±0.9 GPa
v=0.21±0.02

Ongoing Simulation Studies

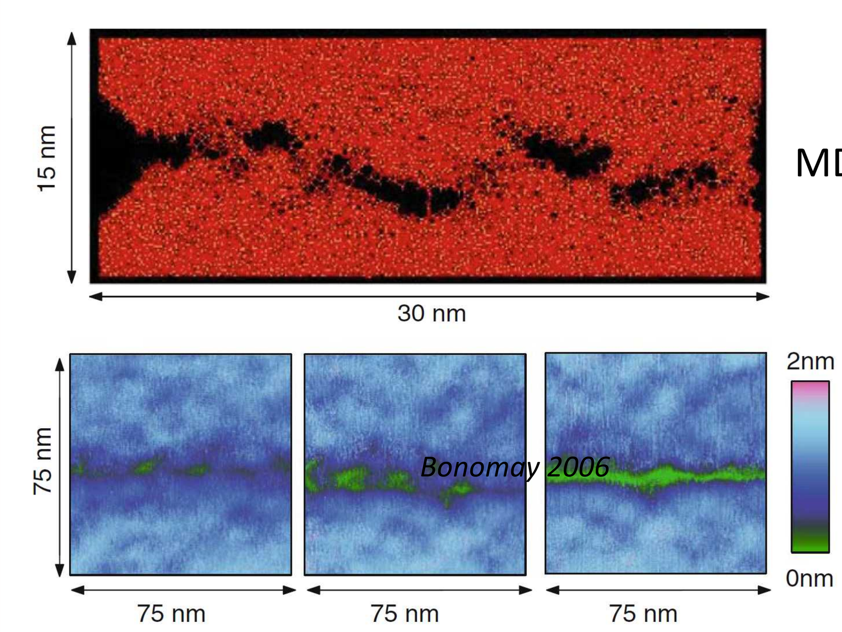


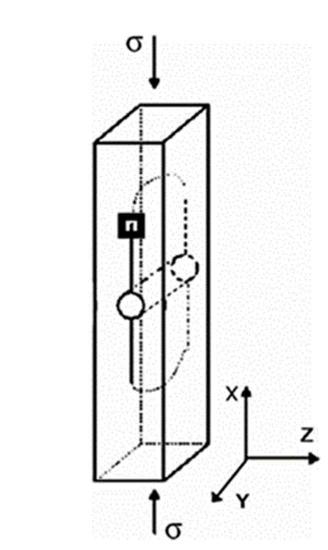
Amorphous Silica and Water

- Water should infiltrate a slit crack from observation.
- Simulation protocols are being developed for opening slit cracks and allowing water infiltration.
- A coupled process is implemented by opening the crack a set amount and allowing the system to relax for an extended period of simulation time (1 ns), resulting in water infiltration.
- Using one approach, the water appears to avoid going into the crack which is not what is observed experimentally.
- There may be kinetic or mechanistic limitations for water infiltration at these scales.
- Examples here are with Tersoff Force Field + TIP3P Water.

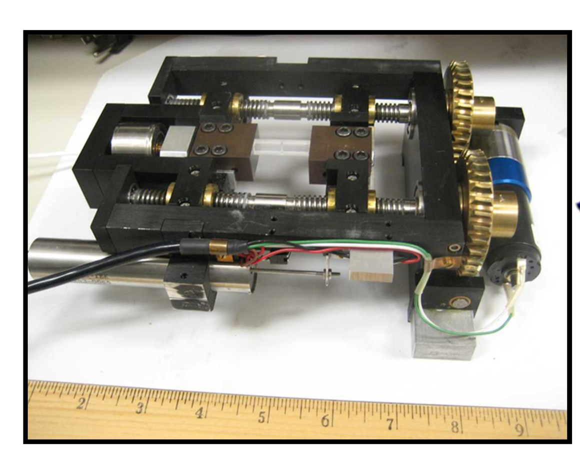
Expansion of Experimental Plan

Objective: to obtain experimental data at the atomistic scale

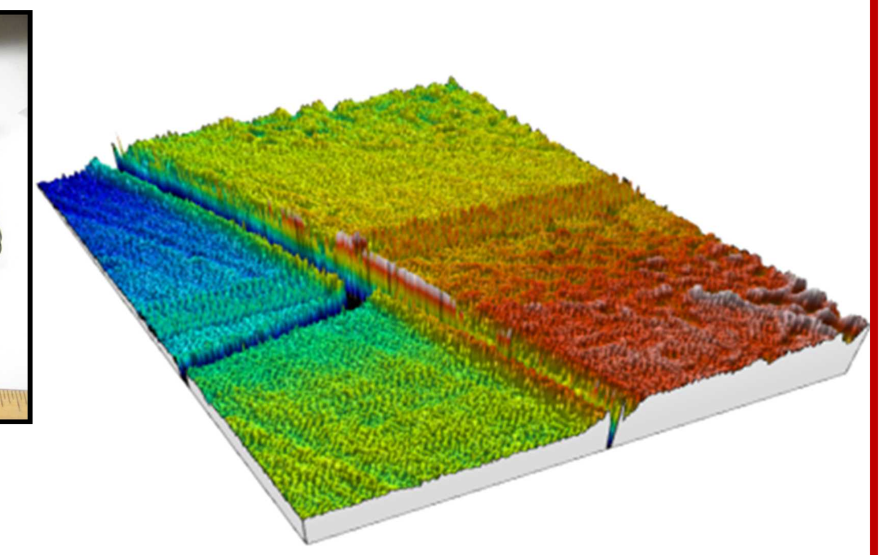




DCDC = Double Cleavage Drilled Compression



Load Frame



First crack imaged with Nanovea optical profilometer

Future Work

- Computational:
  - Develop computational approach to use REAXFF to generate cracks with water
  - Add salts to water and investigate how salt changes crack surface structure and impacts fracture toughness
- Experimental:
  - Brainstorm and test designs for loading samples submerged in liquid
  - Acquire results for loading in varying solution compositions

Built on LDRD Laboratory Directed Research and Development

Sandia National Laboratories is a multi-mission laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

PENNSTATE
U.S. DEPARTMENT OF ENERGY
NNSA National Nuclear Security Administration