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Assessing the fracture strength of geological and related materials via an atomistically based J-integral

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Exceptional service in the national interest

Technological motivation

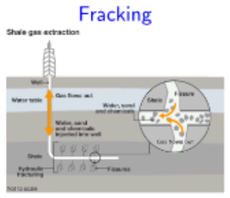
Goals:

- Develop fundamental understanding of the *chemical-mechanical* mechanisms that **control subcritical cracks** in low-permeability geomaterials
- Link atomic-scale insight to macroscale observables and directly address how chemical environment affects mechanical behavior.

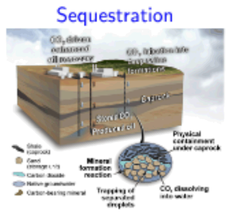
Why Atomistic Simulation?

- Cracks start at the *atomistic scale* by the *breaking of bonds* at the rock-fluid interface.
- Crack tip formation & crack propagation is influenced by fluid and surface *chemistry* (e.g., development of surface charge & adsorbed species along fracture surface).

Fracking



Sequestration



large-scale problems with mechanical and chemical forces acting on cracks

Approach

Generally speaking, this work is based on the **simple premise**:

- *consistent* fields from atomistic simulation
- application of continuum theory

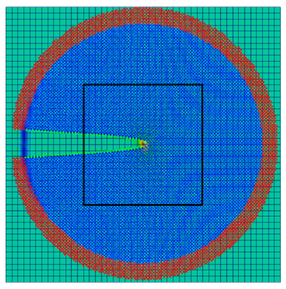
} → nanoscale results

i.e. first, connect atomistic data to continuum fields in a manner and a **scale** consistent with the conservation balances; then, use continuum theory to analyze the process.

There are many technologically relevant examples of the validity of this approach down to the length-scale of nanometers and hundreds of atoms.

In particular, atomistic simulation is particularly suited to the analysis of configurational forces since they typically have atomic details.

Method: 1-way coupling



1. A slit is inserted through bonds crossing a half plane
2. A far-field continuum displacement solution is applied on an annulus of atoms (red)
3. stress, displacement, and energy density fields are coarse-grained on a grid (green)
4. Eshelby stress is formed and the J-integral is evaluated on the contour (black)

Ingredients

- atomistics provides a first-principles description of the crack surface and other defects structure and energetics
- continuum provides far-field surrogate model and theory for interpretation

Background

(1) **Connection between particle & continuum mechanics**:

- [Irving&Kirkwood 1950] **Correspondence of particle trajectories & continuum fields through the balance laws**
- [Hardy 1982] Extension of I&K to smooth kernels
- [Zimmerman 2010] Referential/material frame extension well-suited to solids

(2) **Theory of configurational forces**:

- [Eshelby 1951] **Foundations of configurational forces**
- [Rice 1968] Application to fracture
- [Wu 2001] Application to diffusion

(3) **Application to atomic systems**:

- [Jones 2010] Path-independent, $T = 0$ atomistic **J**-integral
- [Jones 2010] Finite T, quasistatic **J**-integral
- [Zimmerman 2013] Application to ductile metals

(1) Eshelbian mechanics: J integral

The energy release rate *relative* to a process with motion χ_t, $\mathbf{F} = \partial_{\mathbf{X}}\chi_t$, and a *fixed reference configuration* $\mathbf{X}$ is:

$$\dot{\Pi}(\varphi_t, \chi_t, \mathbf{F}) - \dot{\Pi}(\mathbf{X}, \chi_t, \mathbf{F}) = \int \partial_{\mathbf{X}}\Psi \cdot \dot{\varphi}_t \, dV$$

where $\varphi_t(\mathbf{X})$ is a map describing the *configurational change* in the reference configuration, and

$$\partial_{\mathbf{X}}\Psi = \nabla_{\mathbf{X}}\Psi(\mathbf{X}, \mathbf{F}(\mathbf{X})) - \partial_{\mathbf{X}}W(\mathbf{X}, \mathbf{F}) : \nabla_{\mathbf{X}}\mathbf{F} = \nabla_{\mathbf{X}} \cdot \mathcal{S}$$

is *work conjugate* to the configurational change φ_t.

$\mathcal{S}$ is the Eshelby stress and the **J**-integral is the resultant force

$$\mathbf{J} = \int_{\partial\Omega} \mathcal{S}\mathbf{N} \, dA = \partial_{\mathbf{X}}\Pi$$

conjugate to the motion of the crack tip $\dot{\varphi}_t$.

(1) Eshelbian mechanics: Eshelby stress

The Eshelby stress can be defined explicitly as

$$\mathcal{S} = \Psi\mathbf{I} - \mathbf{F}^T\mathbf{P}$$

where

- Ψ is the (Helmholtz) free energy,
- $\mathbf{F} = \nabla_{\mathbf{X}}\chi$ is the deformation gradient,
- $\mathbf{P}$ is the 1st Piola-Kirchhoff stress

notice these are an **energy-conjugate triplet**.

At zero temperature equilibrium, the **J**-integral reduces to

$$\mathbf{J} = \int_{\partial\Omega} \mathcal{S}\,\mathbf{N} \, dA = \int_{\partial\Omega} \Psi\mathbf{N} - \mathbf{F}^T\mathbf{P}\mathbf{N} \, dA = \int_{\partial\Omega} W\mathbf{N} - \mathbf{H}^T\mathbf{P}\mathbf{N} \, dA$$

where W is the internal energy, $\mathbf{H} = \nabla_{\mathbf{X}}\mathbf{u}$ is the displacement gradient, and $\mathbf{N}$ is the outward unit normal.

(2) Consistent coarse-grained fields: momentum

In order to construct the necessary fields, take Newton's law

$$m_\alpha \ddot{\mathbf{u}}_\alpha = \mathbf{f}_\alpha$$

with mass m_α, displacement $\mathbf{u}_\alpha$ and force $\mathbf{f}_\alpha = \partial_{\mathbf{x}_\alpha}\Phi$, and localize with kernel $\psi = \psi(\mathbf{X})$ where $\psi_\alpha \equiv \psi(\mathbf{X}_\alpha - \mathbf{X})$ is an averaging weight

$$\sum_\alpha m_\alpha \ddot{\mathbf{u}}_\alpha \, \psi_\alpha = \sum_\alpha \mathbf{f}_\alpha \, \psi_\alpha$$

The left-hand side can be identified with a change in **momentum**

$$\mathbf{p}(\mathbf{X}, t) = \sum_\alpha m_\alpha \dot{\mathbf{u}}_\alpha(t) \, \psi_\alpha$$

and the right-hand side with a divergence of **stress**

$$\nabla_{\mathbf{X}} \cdot \mathbf{P} = \sum_\alpha \mathbf{f}_\alpha \, \psi_\alpha = \sum_{\alpha\beta} \psi_\alpha \mathbf{f}_{\alpha\beta} = \frac{1}{2} \sum_{\alpha\beta} (\psi_\alpha - \psi_\beta)\mathbf{f}_{\alpha\beta} = \ldots$$

(2) Irving-Kirkwood/Hardy formalism

To obtain the stress from its divergence, instead of a truncated expansion for $\Delta\psi = \psi_\alpha - \psi_\beta$, define an **exact relation**

$$\Delta\psi = \nabla_{\mathbf{X}}\psi \cdot \Delta\mathbf{X} + \ldots = \nabla_{\mathbf{X}} B \cdot \Delta\mathbf{X}$$

via

$$B_{\alpha\beta}(\mathbf{X}) = \int_0^1 \psi \left(\lambda(\mathbf{X}_\alpha - \mathbf{X}) + (1 - \lambda)(\mathbf{X}_\beta - \mathbf{X})\right) \, d\lambda$$

to obtain a stress (recall $\nabla_{\mathbf{X}} \cdot \mathbf{P} = \frac{1}{2}\sum_{\alpha,\beta} \mathbf{f}_{\alpha\beta} \, \nabla_{\mathbf{X}} B_{\alpha\beta} \cdot \mathbf{X}_{\alpha\beta}$)

$$\mathbf{P}(\mathbf{X}, t) = -\frac{1}{2} \sum_{\alpha,\beta} \mathbf{f}_{\alpha\beta}(t) \otimes \mathbf{X}_{\alpha\beta} \, B_{\alpha\beta}(\mathbf{X})$$

which is unique up to a solenoidal field & is similar to the **virial**.

(2) Consistent fields

The estimation of three energy-conjugate fields are necessary.

- **energy density**:

$$W(\mathbf{X}, t) = \sum_\alpha \phi_\alpha(t) \, \psi(\mathbf{X} - \mathbf{X}_\alpha) - \overbrace{\sum_\alpha \phi^X_\alpha \psi(\mathbf{X} - \mathbf{X}_\alpha)}^{W_0(\mathbf{X})}$$

  where $\phi^X_\alpha = \phi_\alpha(\{\mathbf{X}_\beta\})$ is PE in a *fixed reference configuration* $\{\mathbf{X}^\beta\}$ (perfect lattice w/ bonds deleted along crack).
- **displacement gradient** :

$$\mathbf{H} = \nabla_{\mathbf{X}}\mathbf{u} = \sum_I \mathbf{u}_I(t) \nabla_{\mathbf{X}} N_I(\mathbf{X}) \, .$$

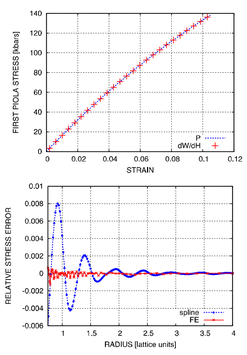
  using *interpolation* $\mathbf{u} = \sum_I \mathbf{u}(\mathbf{X}_I, t) N_I(\mathbf{X})$ of displacement

$$\mathbf{u}(\mathbf{X}, t) = \frac{\sum_\alpha (\mathbf{x}_\alpha(t) - \mathbf{X}_\alpha) \, m_\alpha \psi(\mathbf{X}_\alpha - \mathbf{X})}{\sum_\alpha m_\alpha \psi(\mathbf{X}_\alpha - \mathbf{X})}$$

  defined *mass-weighted* consistent w/ momentum density.
- **stress**

$$\mathbf{P}(\mathbf{X}, t) = -\sum_{\alpha<\beta} \mathbf{f}_{\alpha\beta}(t) \otimes \mathbf{X}_{\alpha\beta} B_{\alpha\beta}(\mathbf{X})$$

Results: Consistency and Accuracy



The coarse-grained fields satisfy

$$\mathbf{P} = \nabla_{\mathbf{F}}\Psi$$

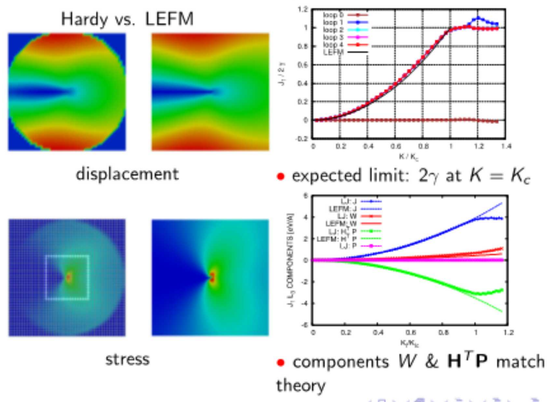
i.e. there is (thermodynamic) **consistency** between the energy, stress and deformation measures ($\mathbf{P}$ −, $\nabla_{\mathbf{F}}\Psi$ +)

Also our use of *partition of unity*/FE kernels

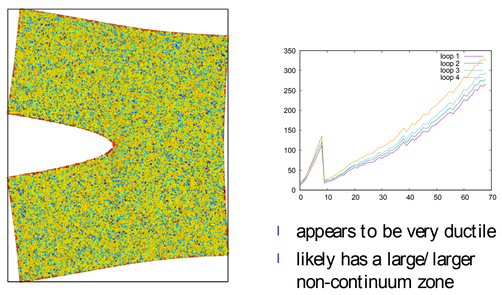
$$\psi_\alpha(\mathbf{X}_I) = N_I(\mathbf{x}_\alpha)$$

(and interpolation) can lead to faster and more *accurate* estimates than with traditional kernels.

Idealized crack with displacement boundary conditions



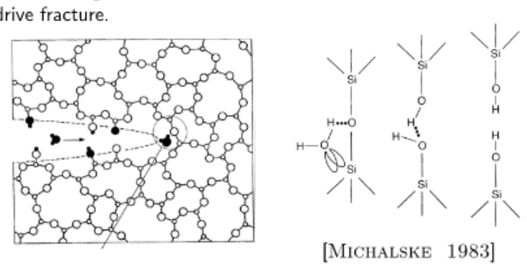
Amorphous materials: silica glass



- appears to be very ductile
- likely has a large/larger non-continuum zone

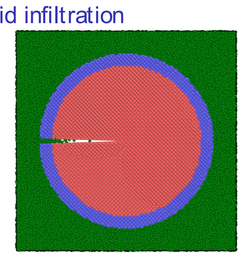
Chemistry

The interaction of the crack and a fluid can change the apparent fracture toughness. Chemical as well as mechanical influences can drive fracture.



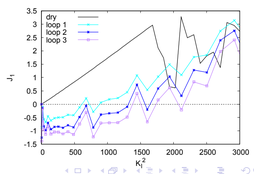
[Michalske 1983]

Fluid infiltration



- access to crack tip is limited by steric & diffusion consideration
- [Orowan 1944] surface adsorption can reduce surface energy
- pressure can do work on the leaves of crack and reduce the effective J

We see suppression of fracture and path dependence due to increased contribution by fluid exposure. The J integral needs to augmented to handle significant surface energy and stresses.

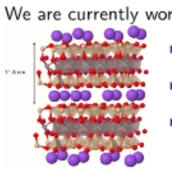


Current work

This atomistic-continuum approach

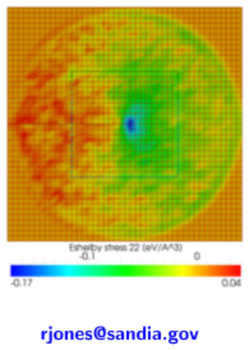
- shows path-independence
- good agreement with theory
- rational implementation
- extensible to many types of fracture

We are currently working on:



- reacting fluids
- pH effects
- mineral & clay structures

using potentials like ReaxFF.



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