

# **Coupled Flow and Mechanics in Porous and Fractured Media**

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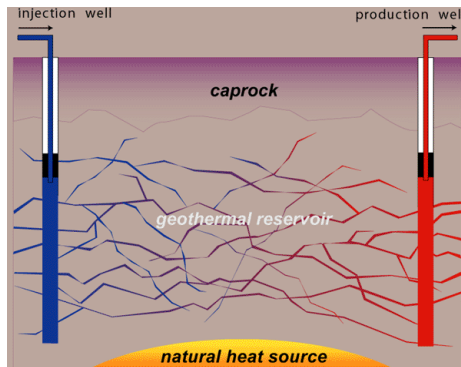


# Outline

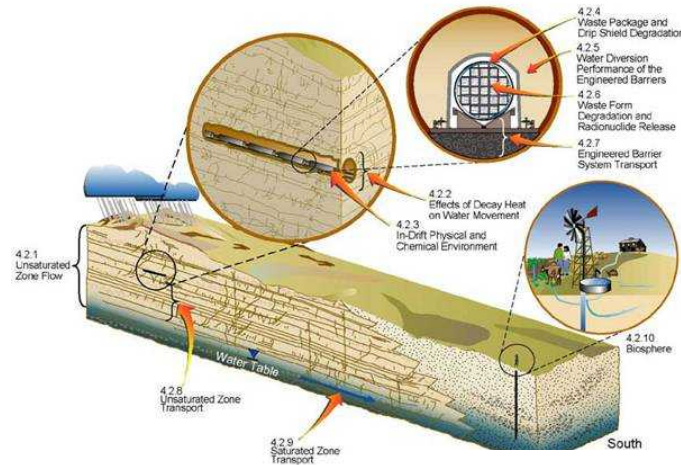
- 1. Motivation: Geosciences at Sandia National Laboratories**
- 2. Sierra software system**
  - i. Geoscience capabilities**
  - ii. Examples**
- 3. Multiphysics coupling in Sierra**
- 4. Coupled flow and geomechanics: CO<sub>2</sub> Sequestration**
- 5. Hydromechanical modeling of discrete fracture networks**

# Geoscience Applications at SNL

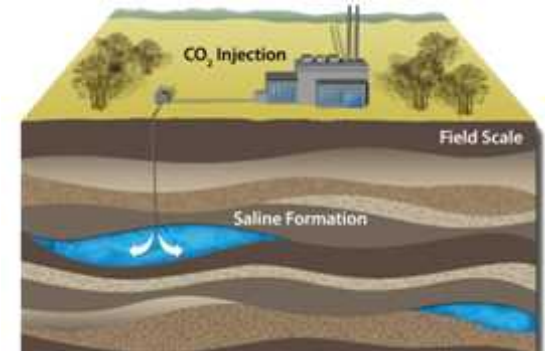
## Engineered Geothermal



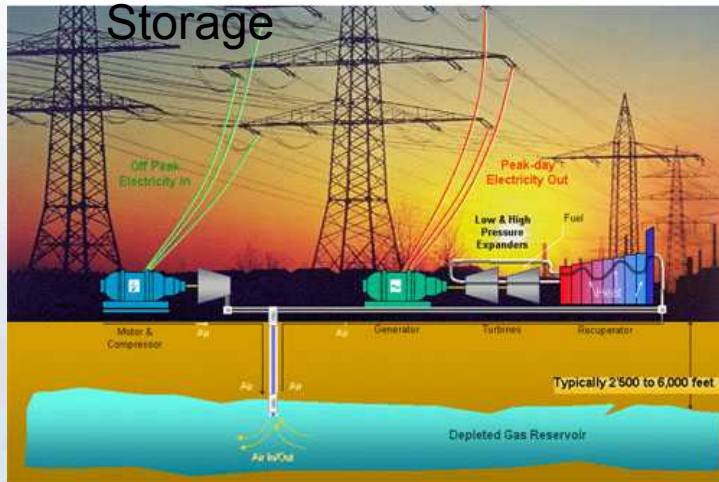
## Nuclear Waste Isolation



## CO<sub>2</sub> Sequestration

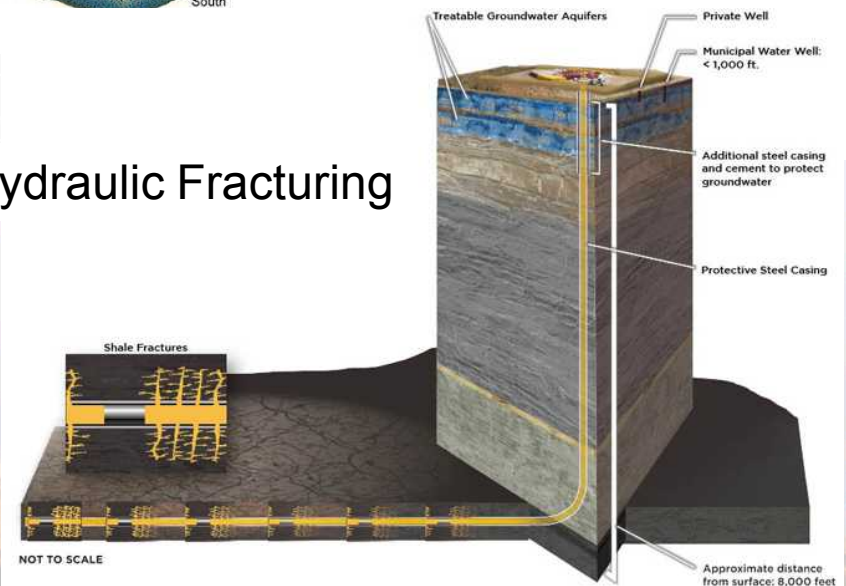


## Compressed Air Energy Storage



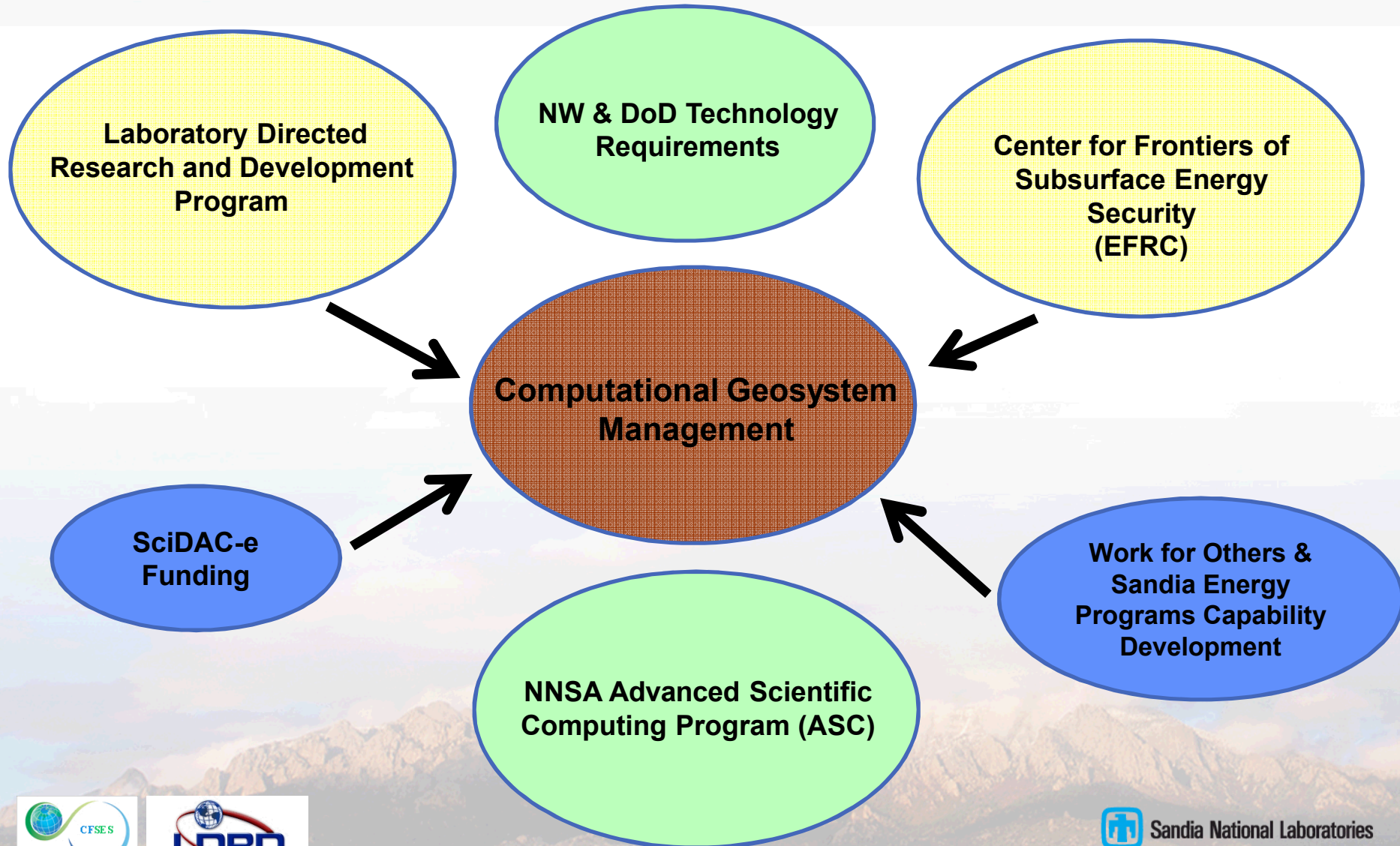
Derek Sept. 2009

## Hydraulic Fracturing



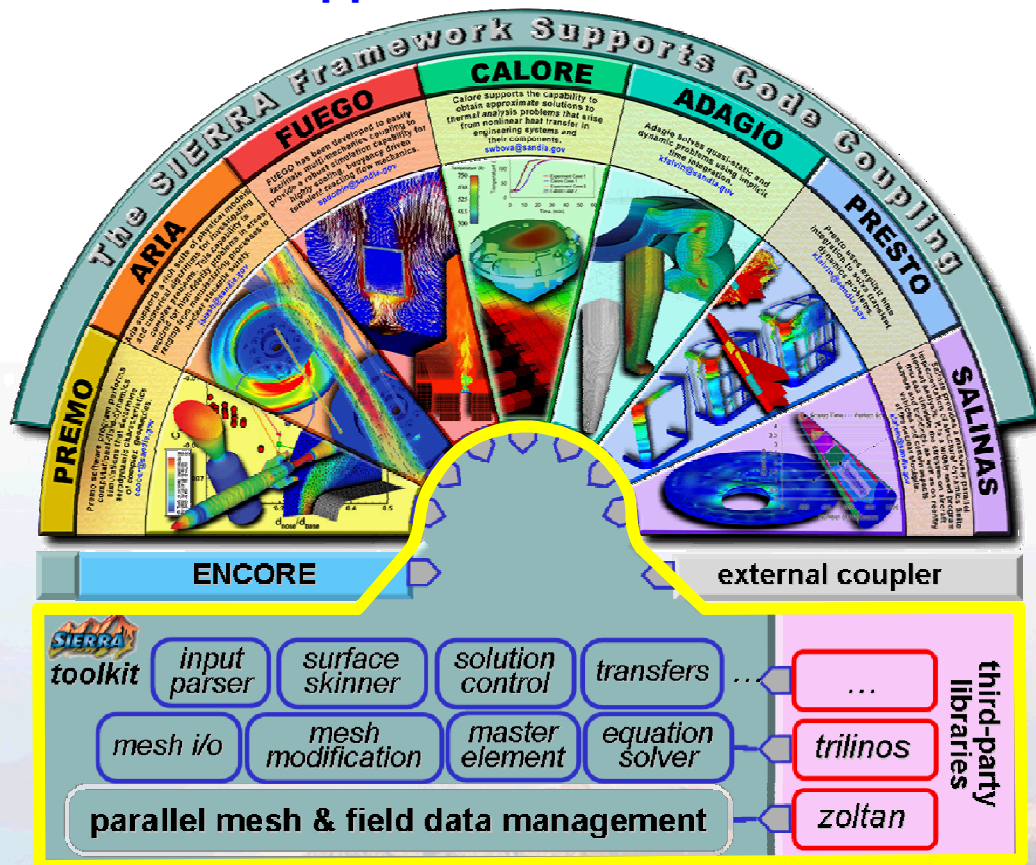
<http://www.hydraulicfracturing.com>

# Sandia Computational Geoscience Research and Subsurface Management Program



# Subsurface simulation software leverages SIERRA Mechanics Foundation

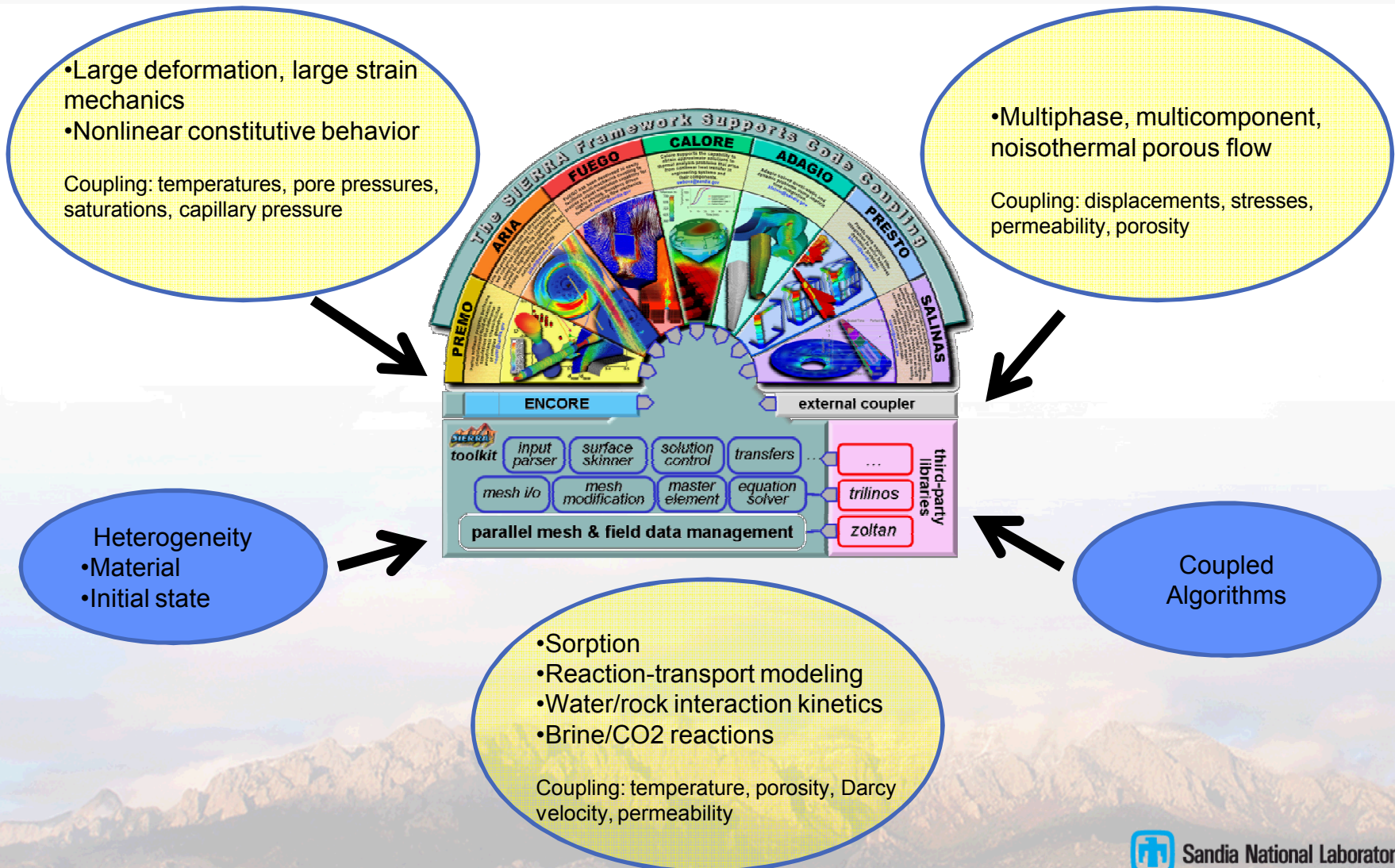
## SIERRA\_toolkit FE application code services



## Services provided to mechanics applications:

- Mesh & field data management (parallel, distributed)
- Transfer operators for mapping field variables from one mechanics to another
- Solution controller for code coupling: Arpeggio
- Includes third party libraries (e.g. solver libraries, MPI communications package)
- Accommodates heterogeneity

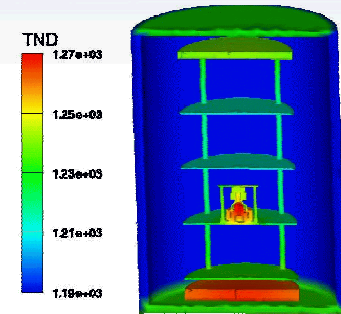
# SIERRA Mechanics Represents Enabling Capability for Coupled Geoscience Multiphysics Simulation



# SNL Thermal/Fluid Modeling Capabilities in Sierra Mechanics

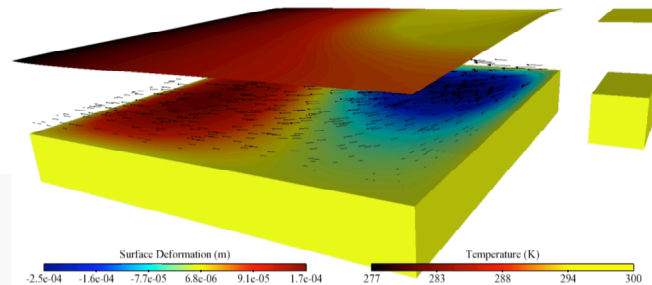
- **Aria** – Non-Newtonian, Multi-physics, and Free Surface Flows

- Fully-Coupled, Galerkin FEM (GFEM)
- Complex material response
- Level sets for surface tracking
- Flexible coupling schemes



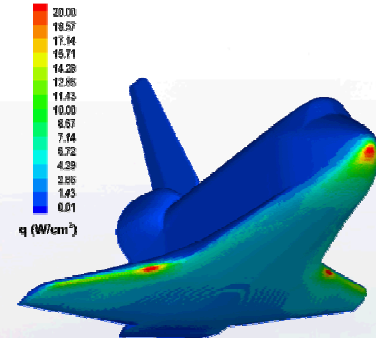
- **Calore** – Heat Transfer, Enclosure Radiation and Chemistry

- Galerkin FEM (GFEM)
- Dynamic enclosures
- Element birth death
- Contact



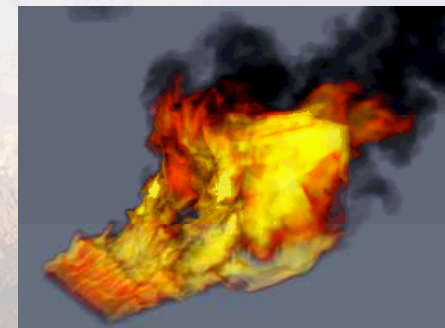
- **Premo** – Compressible Fluid Mechanics

- Fully-Coupled, Edge-Based Finite Volume (node centered)
- Subsonic through hypersonic
- Laminar and turbulent



- **Fuego** – Low Speed, Variable Density, Chemically Reacting Flows (Fire)

- Loosely-Coupled, Control Volume FEM (CVFEM)
- Eddy dissipation and mixture fraction reaction models
- RANS and LES based turbulence models
- Pressurization models



# CDFEM Capability Development Status

## **Objective:**

Implement CDFEM capability in Sierra Mechanics to track moving interfaces and capture interfacial physics between multiple materials or phases

## **Approach:**

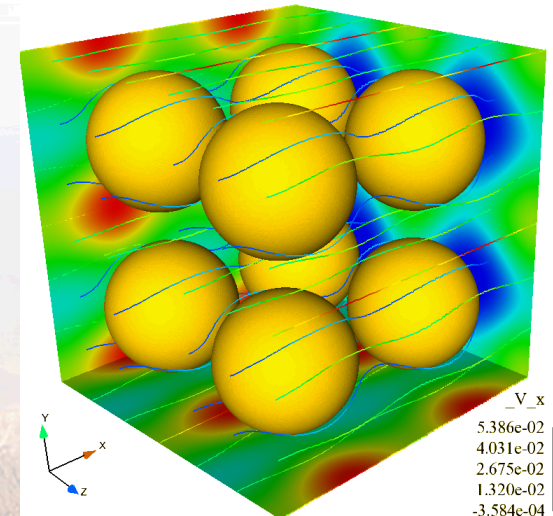
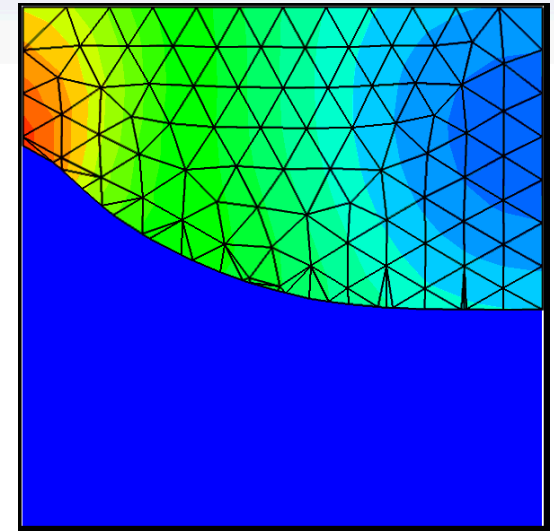
- Use level set technology to capture implicit interfaces
- Decompose non-conformal elements into conformal ones and obtain solution on conformal elements
- Use ALE technology to handle nodes that change phase

## **Accomplishments:**

- Implemented CDFEM for steady state and transient interface problems
- Capability verified to scale well in parallel
- Tested on air-water capillary flows, solid suspension flows, and thermal phase change problems
- Verified accuracy of CDFEM to be 2<sup>nd</sup> order for potential flow, conduction, two fluid viscous flow, and blunt body flow problems

## **Status:**

- Extending scheme to track interface based on various interfacial physics including reactions, phase change, and thermal degradation
- Extending capability to multiple phases (more than two)



# Overview of Porous Flow in Aria

- **Leveraged development under LDRD & EFRC**

- Targets SNL activities in energy security, conventional munitions, thermal batteries, heat pipes, ...

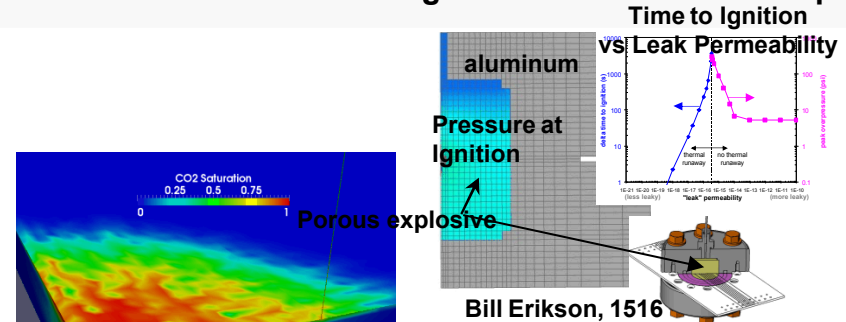
- **Current capabilities**

- Single phase heat and reactive mass flow
- Immiscible two-phase flow
- Two-phase, two-component (air & water) evaporating/condensing thermal model
- Chemically reactive flows (e.g. calcite mineralization)
- Spatially heterogeneous material and transport properties
- Couples with mechanics and other Sierra physics modules

- **Capability under development**

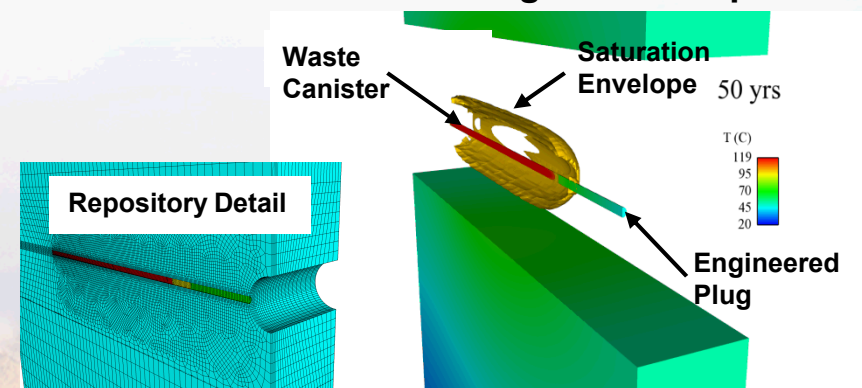
- Nonisothermal two-phase CO<sub>2</sub>-H<sub>2</sub>O-NACL EOS with general phase behavior
- Advanced discretization schemes (UT technology)

## Modeling Cook-Off in Granular Explosives



CO<sub>2</sub> saturation levels in a brine-filled reservoir represented with uncorrelated heterogeneous permeability

## Heat-Generating Waste Disposal



Development of a confining saturation envelope in ultra-low permeability clays, trapping gases within.

# Boundary and Initial Conditions

- Initial Conditions
  - Element block dependent
  - Function of coordinates
    - Linear, quadratic built-in
  - Output file from a previous solution
  - User Plug-in
- Dirichlet BCs (nodeset, sideset)
  - $f(t, x, \text{soln\_vector}, \text{expression})$ 
    - Many built-in forms
  - Plug-in
- Flux BCs (sidesets)
  - $f(t, x, \text{soln\_vector}, \text{expression})$
  - Many built-in forms
    - Third-type BCs
  - Outflow (e.g. wells)
  - Periodic
  - XFER – values set from a transfer
  - Encore function
  - Plug-in
- Distinguishing Condition (constraint)
  - Replaces original equation
  - Implemented in weak form
  - E.g. Kinematic BC with deforming mesh (ALE):

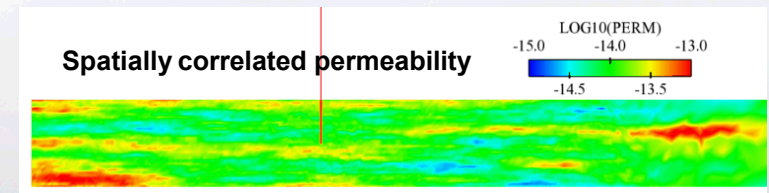
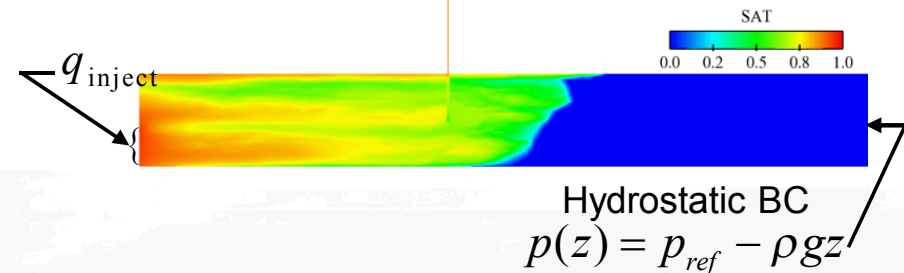
$$R^i = \int_S (\mathbf{n} \cdot (\mathbf{v} - \dot{\mathbf{x}}) - v_{leak}) N^i dS = 0$$

## Fingering of CO<sub>2</sub> Injected into a Heterogeneous Aquifer with Leaky Well

Hydrostatic IC  
 $p(z) = p_{ref} - \rho g z$

Outflow BC

$$q_\beta = \rho_\beta \frac{k_{r\beta}}{\mu_\beta} k(PI) (p_\beta - p_{ref})$$





# Aria Multiphase Porous Flow Physics

## Two-Phase Two-Component Non-Isothermal Model (water, air, energy)

- **Water** - steam tables, equilibrium thermodynamic phase partitioning
- **Air** - ideal gas, Henry's Law partitioning
- **Energy** - conduction, latent and sensible energy transfer, including binary diffusion of heat
- Evaporating/condensing flows
- **Phase appearance/disappearance** via persistent variables approach
- General specification of transport property dependence on solution vector (e.g., densities, viscosities, diffusion coeffs. depend on T, P, phase volume fraction)
- Capillary pressure, relative permeability models
- Specification of **heterogeneous property fields** (e.g. permeability, porosity, GSLIB linkage)
- Other EOS under development



# Aria Porous Flow Physics

## Two-Phase Heat and Mass Flow

### Mathematical Model

- Two-Phase Component Mass and Energy Balances:**

$$\frac{\partial}{\partial t} \begin{bmatrix} \phi(S_l \rho_l^w + S_g \rho_g^w) \\ \phi(S_l \rho_l^a + S_g \rho_g^a) \\ (1-\phi)\rho_s e_s + \phi(\rho_l S_l e_l + \rho_g S_g e_g) \end{bmatrix} + \nabla \bullet \begin{bmatrix} \mathbf{F}_l^w + \mathbf{F}_g^w \\ \mathbf{F}_l^a + \mathbf{F}_g^a \\ \mathbf{q}_e \end{bmatrix} + \begin{bmatrix} Q_w \\ Q_a \\ Q_e \end{bmatrix} \begin{array}{l} \text{water} \\ \text{air} \\ \text{energy} \end{array}$$

- Net Mass Flux:**

$$\mathbf{F}_\beta^\alpha = Y_\beta^\alpha \rho_\beta \mathbf{v}_\beta + \mathbf{J}_\beta^\alpha$$

$\alpha$  = component

$\beta$  = phase

- Darcy Velocity:**

$$\mathbf{v}_\beta = -\frac{k_{r\beta}}{\mu_\beta} \mathbf{k} \bullet (\nabla P_\beta - \rho_\beta \mathbf{g})$$

- Binary Diffusion (gas phase):**

$$\mathbf{J}_g^\alpha = -\rho_g D_g^\alpha \nabla Y_g^\alpha$$



# Aria Porous Flow Physics

## Two-Phase Heat and Mass Flow

### Mathematical Model (cont.)

- **Total Energy Flux (heat conduction, convection, binary diffusion):**

$$\mathbf{q}_e = -\lambda_T \nabla T + \sum_{\beta} \rho_{\beta} \mathbf{v}_{\beta} h_{\beta} + \sum_{\alpha} h_g^{\alpha} \mathbf{J}_g^{\alpha}$$

- **Saturation Constraint:**  $S_l + S_g = 1$

- **Mixing Rules:**  $\sum_{\beta=l,g} Y_{\beta}^{\alpha} = 1, \quad \alpha = w \text{ (water), } a \text{ (air)}$

- **Capillary Pressure:**  $P_g - P_l = P_c(S_l)$

- **Relative Permeability:**  $k_{r,\beta} = f(S_l, T, \dots)$

# Spatial Discretization

- **Unstructured Grid Finite Element-Based Discretization**
- **Finite-dimensional basis representation:**  $f(x, u) = \sum_J N_J(x) f_J(u)$
- **Residual-based implicit weak formulation:**

$$\begin{bmatrix} R_{w,I} \\ R_{a,I} \\ R_{e,I} \end{bmatrix} = \int_{\Omega} N_I \sum_J N_J \begin{bmatrix} \dot{d}_{w,J} \\ \dot{d}_{w,J} \\ \dot{e}_J \end{bmatrix} d\Omega - \int_{\Omega} \nabla N_I \bullet \begin{bmatrix} \mathbf{F}_w \\ \mathbf{F}_a \\ \mathbf{q}_e \end{bmatrix} d\Omega - \int_{\Omega} N_I \begin{bmatrix} Q_w \\ Q_a \\ Q_e \end{bmatrix} d\Omega + \int_{\Gamma} N_I \begin{bmatrix} \mathbf{F}_w \bullet \mathbf{n} \\ \mathbf{F}_a \bullet \mathbf{n} \\ \mathbf{q}_e \bullet \mathbf{n} \end{bmatrix} d\Gamma$$

## Hybrid Features:

- **Mass lumping for multiphase systems**
- **Control-volume finite element upwind scheme for convective terms**
  - Supports tensor permeability



# Nonlinear Solution Procedures

**Discretization leads to nonlinear system:**

$$\mathbf{R}(\mathbf{u}) = (\mathbf{R}_w, \mathbf{R}_a, \mathbf{R}_e)^T = \mathbf{0}$$

**Nonlinear Solve:**

– Newton Iteration

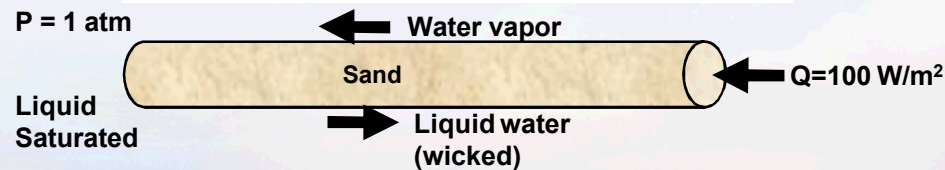
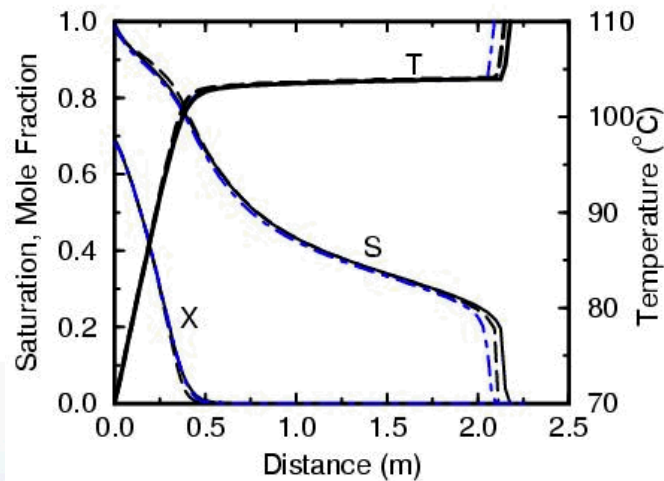
$$\mathbf{J}(\mathbf{u}^q) \delta \mathbf{u}^{q+1} = -\mathbf{R}(\mathbf{u}^q)$$

$$\mathbf{u}^{q+1} = \mathbf{u}^q + \delta \mathbf{u}^{q+1}$$

# Coupled Mass and Heat Flow Examples

## Porous Heat Pipe with Non-Condensable Gas

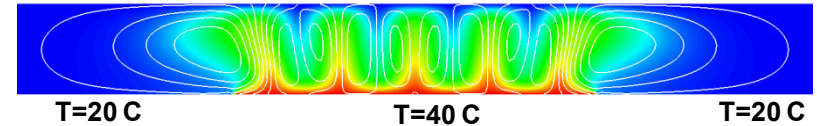
(solid – PorSalsa/upwind, dashed – TOUGH2/upwind, dash-dot – Aria/gfem)



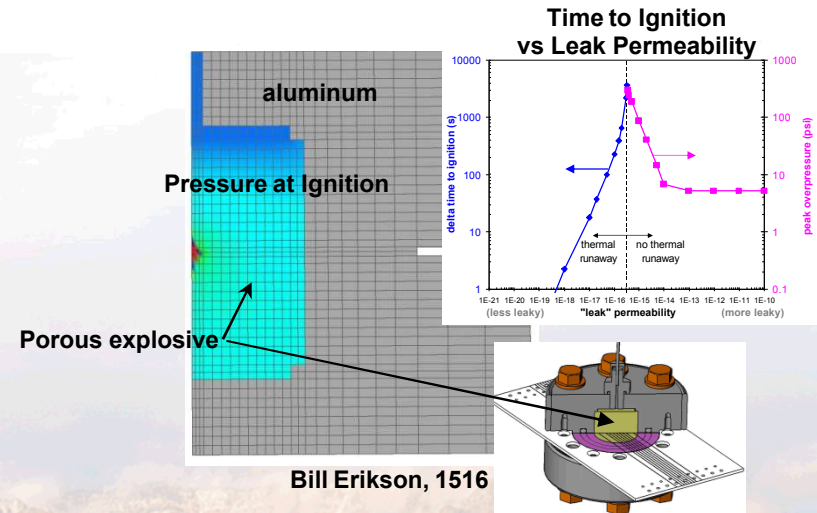
## Elder Problem

### Buoyant Convection in a Porous Layer

Ra = 150



## Modeling Cook-Off in Granular Explosives



# CO<sub>2</sub> Leakage Through an Abandoned Well

## Reference Problem Description:

- 3D model of leakage during supercritical CO<sub>2</sub> injection into a brine aquifer
- Single CO<sub>2</sub> injection well
- Two aquifers separated by an aquitard
- One leaky well, 100 m from injection well
- 500 k elements, 1200 day injection

## Assumptions:

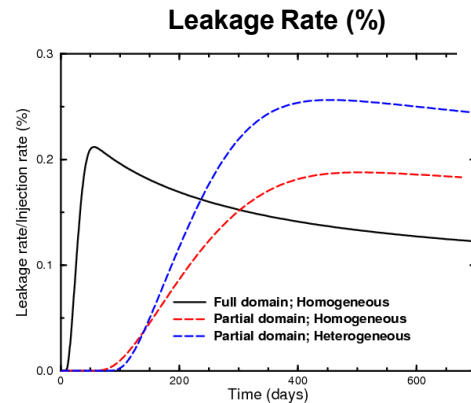
- Isothermal injection process
- CO<sub>2</sub> and brine immiscible phases
- Isotropic formation
- Neglect capillary pressure

## Results:

- Computed leakage rate and arrival times compare well with benchmark study

## Effects of Heterogeneous Permeability:

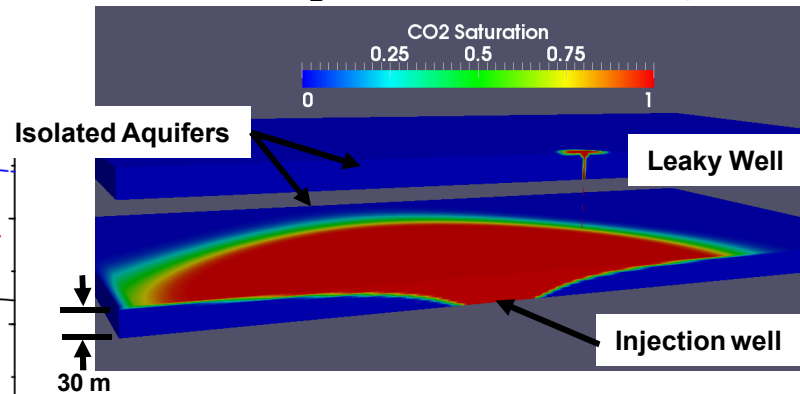
- Geologic aquifers are highly heterogeneous
- Truncated domain allows multiple realizations
- Lognormal distribution of permeability, normal distribution of porosity
- Highly non-uniform (fingering) injection in the presence of heterogeneity
- Lognormal permeability increases the leakage rate



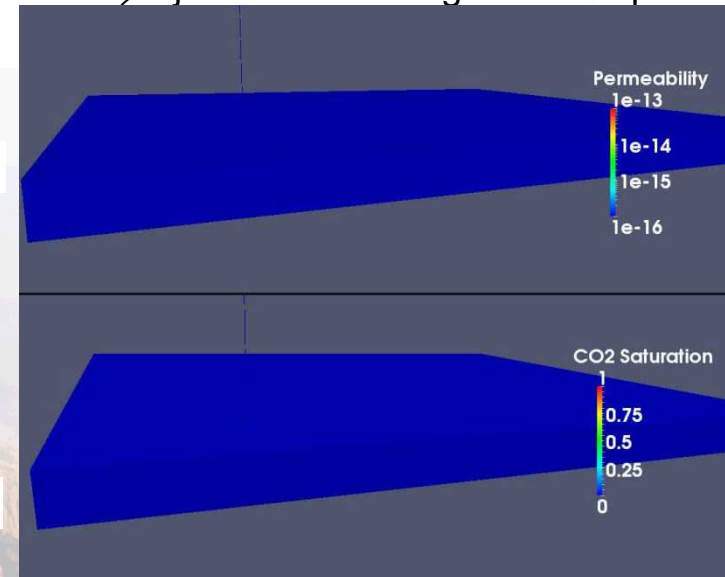
## Lognormal Permeability

## CO<sub>2</sub> Fingering with Heterogeneity

## CO<sub>2</sub> Distribution at 200 days



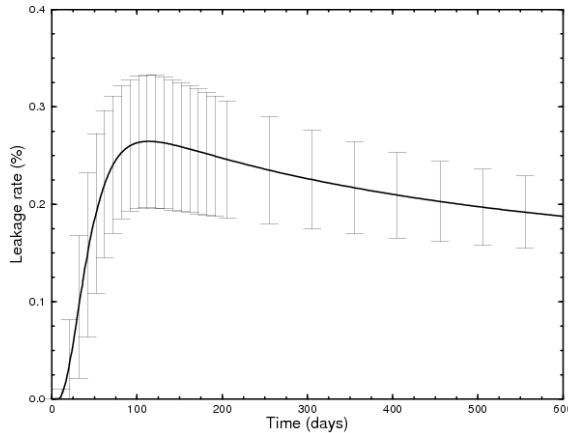
## CO<sub>2</sub> Injection in Heterogeneous Aquifer



# CO<sub>2</sub> Leakage Through an Abandoned Well

## Effects of Heterogeneity

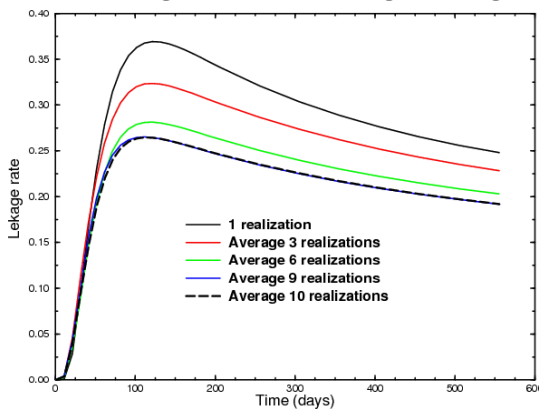
Average Leakage Rate and Std. Dev.



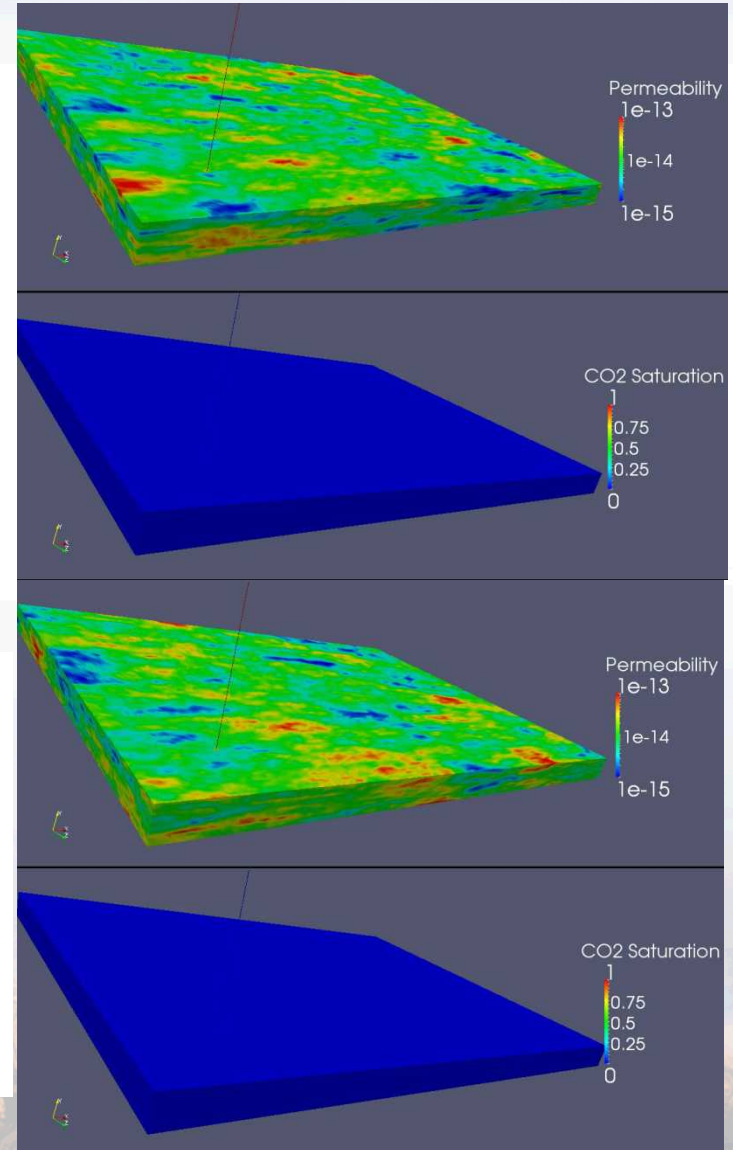
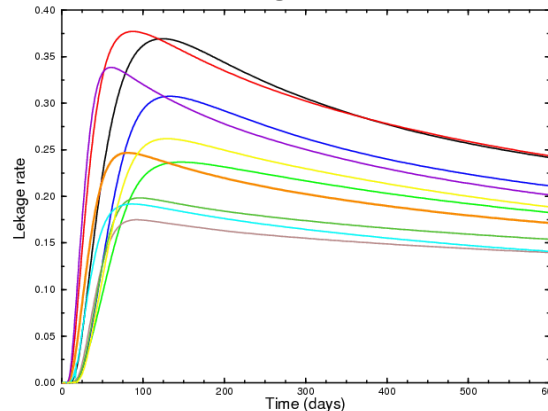
Some Results  
(10 realizations)

- Correlation between fast paths and permeability distribution is evident
- Leakage, arrival time are heavily dependent on permeability distribution
- Standard deviations are substantial
- Appears useful results can be obtained from a few realizations

Leakage Rate: Running Average

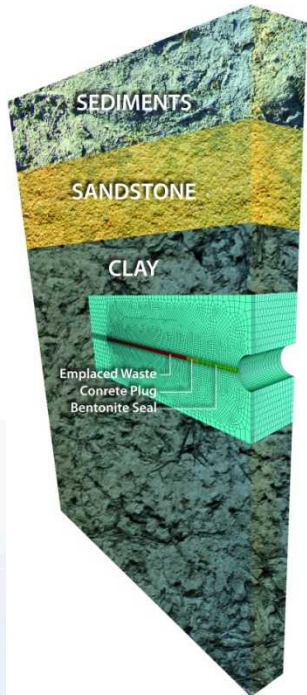


Leakage Curves

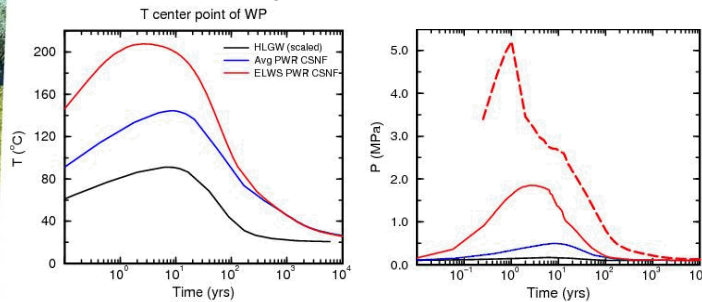


# High Level Waste Disposal in Clay

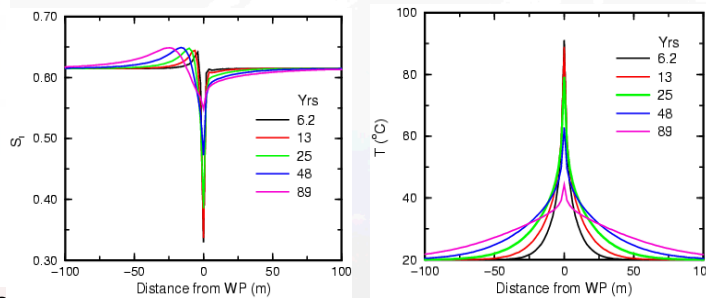
## Thermo-Hydrologic Features



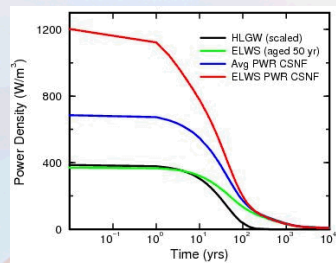
**Repository Temperature and Pressure**



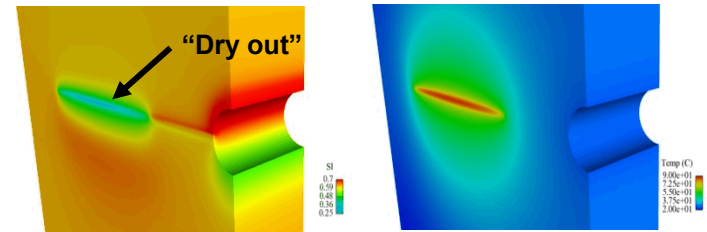
**Spatial Variation of Temperature and Pressure**



**Sample Power Densities**



High decay powers in ultra-low permeability clays can result in dry out regions and saturation envelopes.



Waste Canister

Saturation Envelope

50 yrs

T (°C)  
119  
95  
70  
45  
20

Engineered Plug

Development of a confining saturation envelope in ultra-low permeability clays, trapping gases within.

# Overview of Geomechanics in Adagio

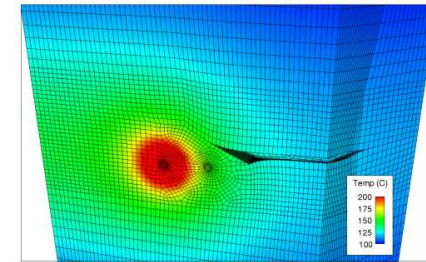
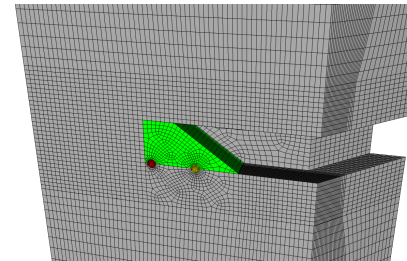
## Features:

- Large deformation, large strain kinematics
- Robust contact algorithms (both detection and application)
- Based on iterative (matrix-free) solvers with low order hourglass stabilized 8-node hexahedron element
- Efficient constitutive model implementations

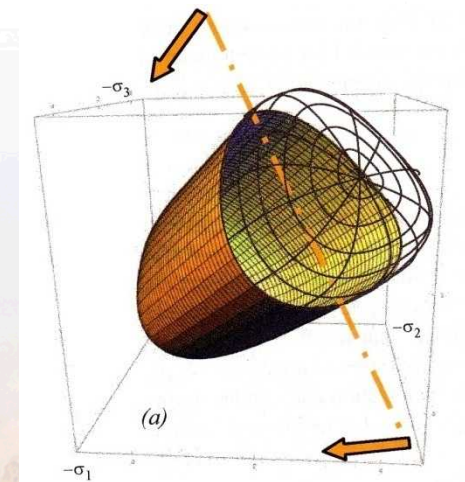
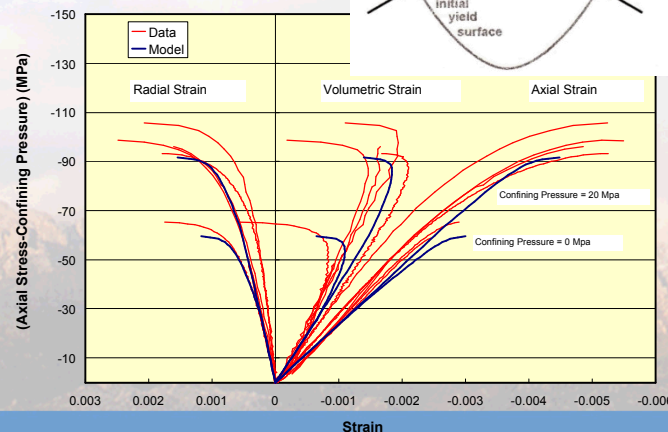
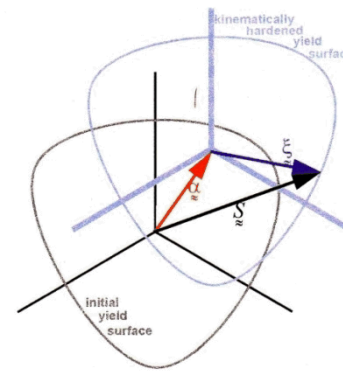
## Models for Geomechanics:

- Elastic
- Elastic/Plastic
- Soil Foam
- Power Law Creep
- MD Creep Model
- Crushed Salt Creep Model
- Clay
- GeoModel

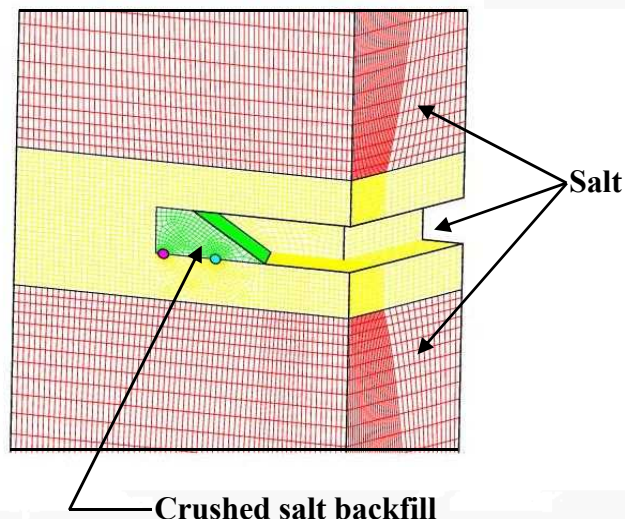
## Thermally Enhanced Creep Closure



## Undeformed and Deformed Storage Tunnels in a Heated Salt Repository



# Sierra Mechanics Simulation of Salt Repository



- Three-dimensional fully coupled thermal/mechanical analysis
- Massively Parallel Calculation - 96 processors
- Dissimilar meshes and domains for thermal and structural mechanics
- Contact surfaces used for both thermal and structural problems

## Thermal Analysis Features:

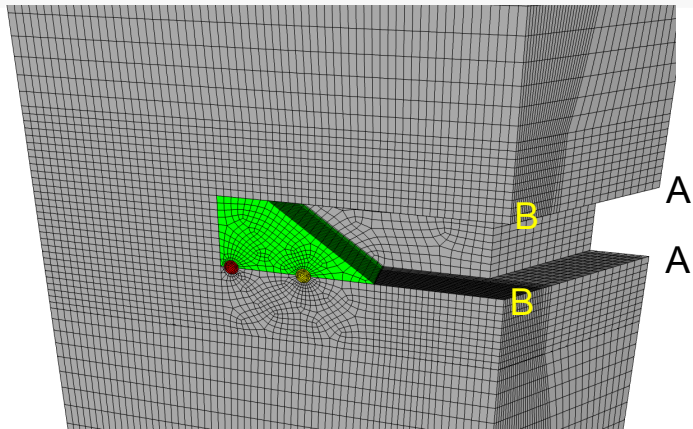
- 904736 nodes / 864927 elements
- Contact surfaces used to accommodate heat conduction between contacting surfaces (alcove and haulage way)
- Re-computation of radiation view factors for deforming heated room surfaces

## Structural Analysis Features:

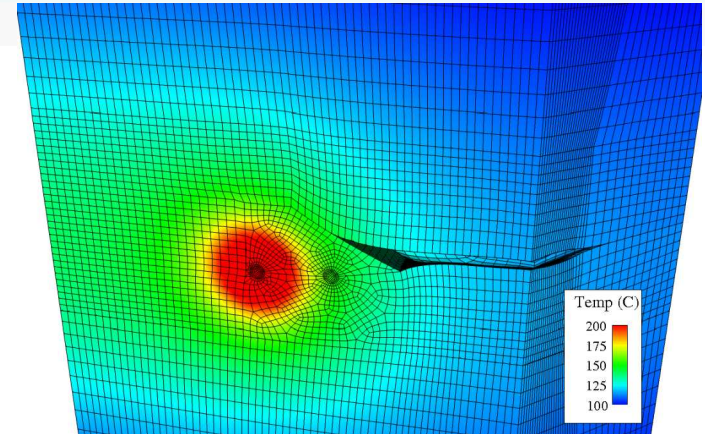
- Quasistatic analysis with 294698 nodes / 279537 elements
- Large deformation, large strain formulation
- Nonlinear power law secondary creep model for salt
- Volumetric compaction model for the crushed salt
- Contact surfaces defined to allow arbitrary roof, rib, and floor contact
- Temperature dependent material properties



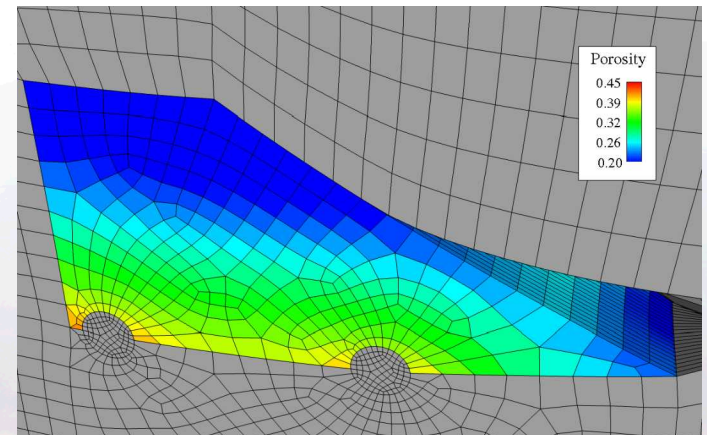
# Generic Salt Repository Closure Details



Cross-section A-A




Generic salt repository final deformed state



Corresponding porosity in crushed salt backfill

Cross-section B-B



# Solving Multiphysics Problems

## Trade-offs in Coupling Strategies

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### Full Coupling

- Provides a consistent solution
- Known convergence properties
- Expensive to solve
- Requires compatible algorithms among physics

### Tight / Loose Coupling

- Can be efficient to solve (smaller, nicer matrices)
- Allows separate meshes, time steps, discretizations
- Best de-coupling may be unknown
- May be more expensive in the long run



# Building Blocks for Coupled Equations

**Region:** a mesh and set of fields

- One or more equations, constraints, etc.
- Aria: implicitly solved equations in a single matrix
  - Newton (Analytic + AD + FD)
  - Newton Finite Difference
  - Trilinos::NOX

Multiple Regions can be coupled with “**transfers**”

- Fields are copied/interpolated between Regions
- Entire mesh or select blocks, sidesets, etc.
- Can have different discretizations ( $Q1 \leftrightarrow P0$ )
- Sequencing is user defined



# Solving Multiphysics Problems

## Solution Control Building Blocks

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- **Blocks you can use**
  - **INITIALIZE** - Defines initialization sequence, including transfers
  - **SEQUENTIAL** - Once through pass (direct-to-steady-state)
  - **TRANSIENT** - Time iterative loop, all members at same time step size
  - **SUBCYCLE** - Sub-cycling within a transient block
  - **NONLINEAR** - Nonlinear iteration of members
- **Lines you'll see in blocks**
  - **ADVANCE** - Think of this as “move one step forward”
  - **TRANSFER** - Copy/interpolation fields from one Region to another
  - **EVENT** - Custom functions defined by different Sierra components
  - **Others**, like **INDICATE**, **MARK**, **ADAPT**, ...
- **When clauses:**
  - **Allow conditional execution of lines, e.g.,**  
`Advance Aria_Region when "CURRENT_STEP % 10 == 0"`
  - **Custom functions can be created and plugged in**



# Input File Structure Reveals Execution Hierarchy

Domain

Procedure

Region

```
Begin Sierra job_name
  Define Materials
  Define "Finite Element Model":
    Mesh & Materials
  Define Linear Solvers
```

```
Begin Procedure procedure_name
  Define Solution Control
  (e.g., time stepping)
```

```
Begin Aria Region region_name
  Nonlinear Solver Settings
  Equation Definitions
  Boundary Conditions
  Sources
  Post-processors
  Output File Definition
```

End

End

End

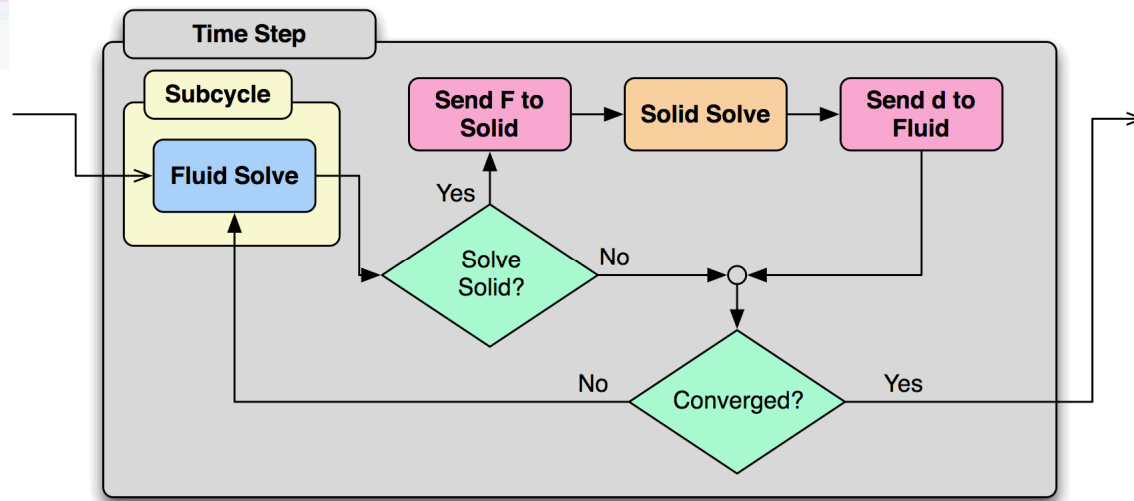
**Procedure:** solution control instructions

- multiple procedures allowed within a domain

**Region:** a mesh and set of fields

- multiple regions allowed within a procedure

# Conditional Loose Coupling with Nonlinear Iteration and Subcycling



```

Begin System Main
  Use Initialize MyInit
  Begin Transient MyTransient
    Begin Nonlinear MyNonlinearLoop
      Begin Subcycle MySubcycle
        Advance AriaRegion
      End
      Transfer ForceAriaForceAdagio when "Solve_Solid()"
      Advance AdagioRegion when "Solve_Solid()"
      Transfer DispAdagioDispAria when "Solve_Solid()"
    End
  End
End
    
```

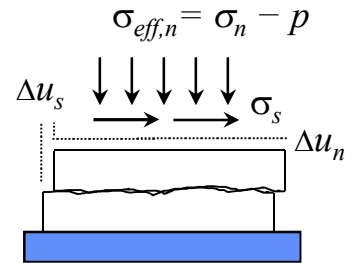
# Coupling Multiphase Flow and Geomechanics

**Effective stress principle:**  $\bar{\sigma}_{eff} = \sigma^T + \alpha p_{eff}$  e.g.,  $p_{eff} = p_w S_w + p_n S_n$

- effective stress is used the constitutive models
- equilibrium is based on total stress – balance of external forces

**Porosity maps from deformation gradient:**  $\frac{1 - \phi_0}{1 - \phi} = \det \mathbf{F}(\mathbf{u})$

- deforming grids in flow and mechanics
- permeability models can depend on porosity or other damage criteria



# Coupled Flow and Geomechanics Injection into an Reservoir/Caprock System

## Motivation

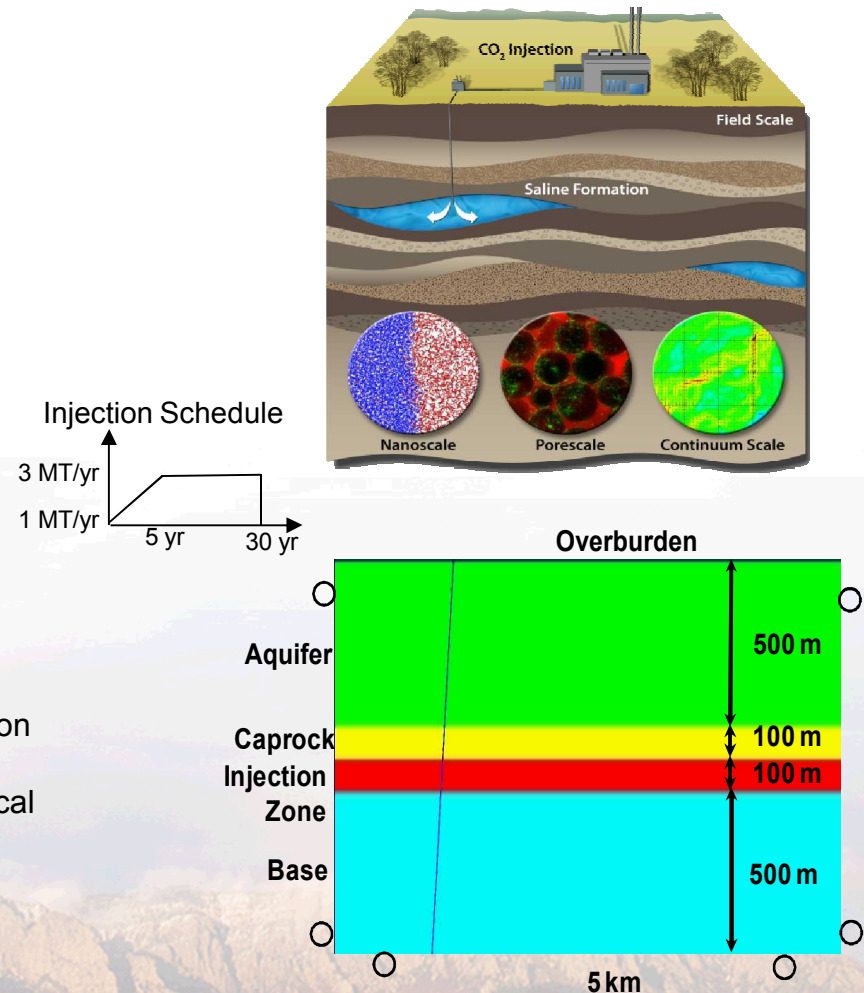
Global consumption of fossil fuels has significantly increased levels of atmospheric CO<sub>2</sub>, a greenhouse gas. Carbon capture and storage (CCS) is a promising mitigation strategy. CCS consists of capturing and sequestering CO<sub>2</sub> emissions from large “point sources”, for example, coal-fired power plants.

We are developing multiscale multiphysics simulation tools for investigating both the short and long term coupled chemical and mechanical processes encountered during subsurface CO<sub>2</sub> sequestration.

## Problem Features and Goals

- Injection of large volumes of supercritical CO<sub>2</sub> into a layered brine reservoir-caprock system at greater than 1km depth.
- High pressures can damage either the injection reservoir (e.g. plastic deformation), or the confining caprock (fracture generation or activation)
- We use a coupled multiphase flow and geomechanics numerical models to determine conditions for failure of the caprock due to injection pressures, flow rates, permeabilities, thus determining operation limits for design of safe CO<sub>2</sub> injection.

## Problem Schematic



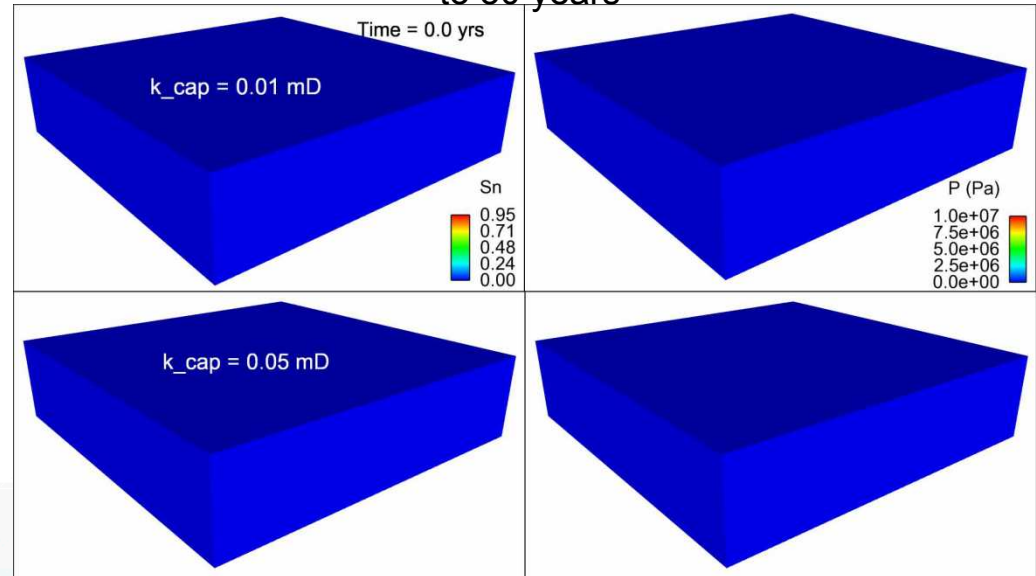
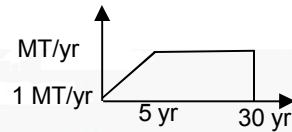
# Coupled Flow and Geomechanics

## Flow, CO<sub>2</sub> transport and Deformation

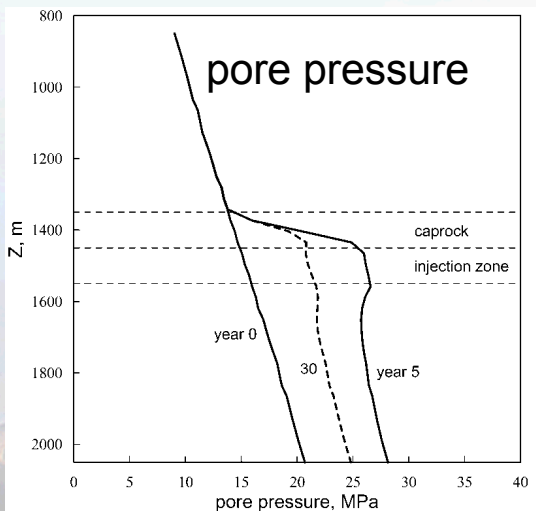
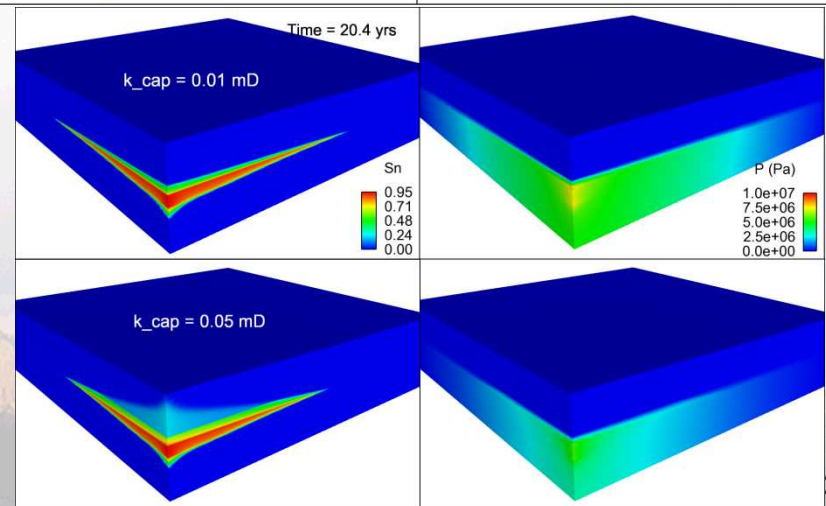
CO<sub>2</sub> saturation, Overpressure & Displacement  
to 50 years

### Results

- “gravity-override” for injected lighter, less viscous CO<sub>2</sub>
- higher overpressure, further penetration with low permeability caprock
- 50  $\mu$ D caprock leaks during injection. Buoyant leaked CO<sub>2</sub> rises and pools at the upper impermeable surface



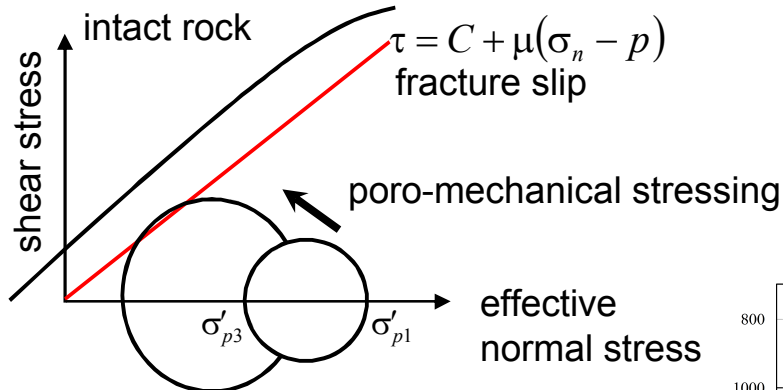
20 yrs



# Coupled Flow and Geomechanics

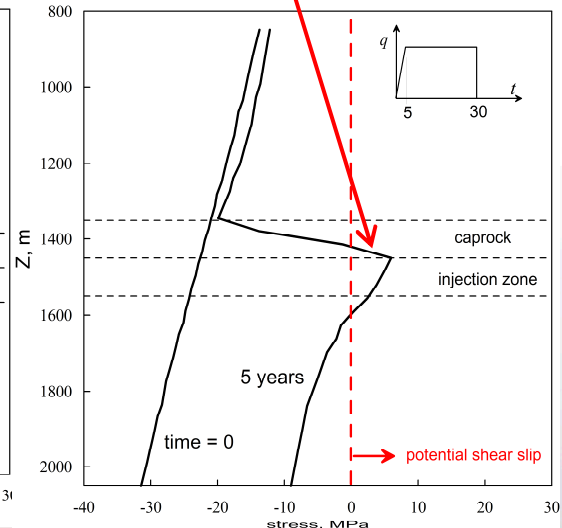
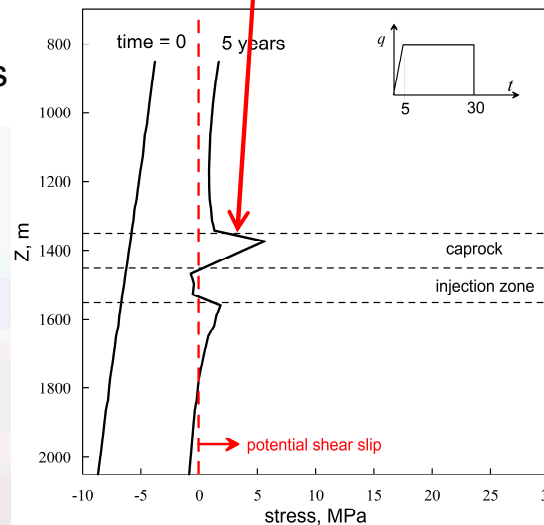
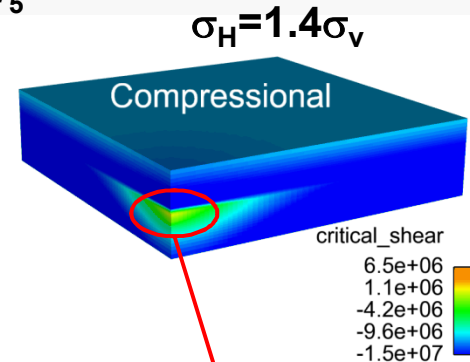
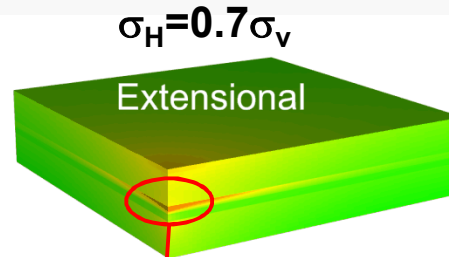
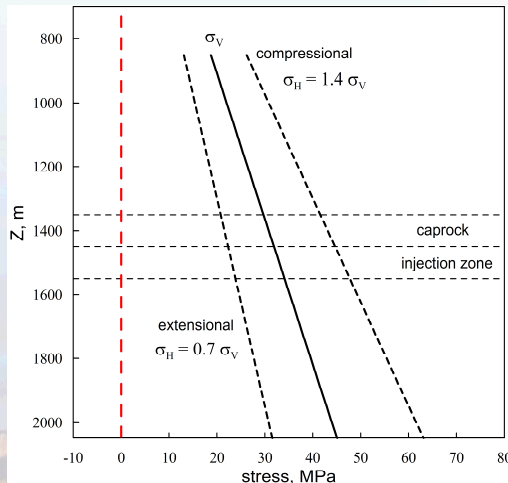
## Effect of Regional Stress State

### Linear Mohr-Coulomb



Critical Shear

$$\sigma'_{p1} - 3\sigma'_{p3} > 0$$



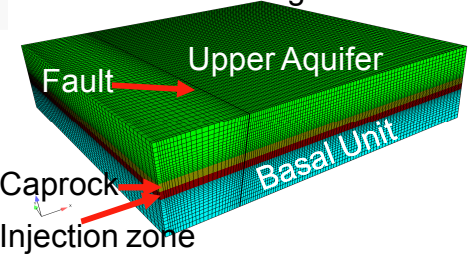
Extensional regional stresses are more dangerous to caprock integrity

# Coupled Flow and Geomechanics

## Hydromechanical Effects of Faults

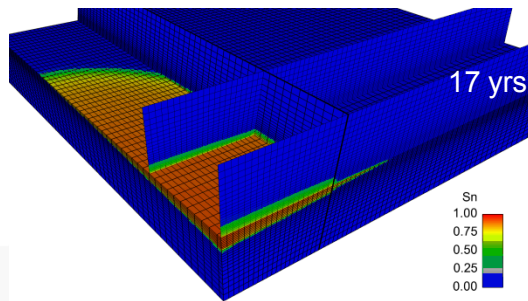
Some faults could go undetected and may pose a risk to sequestration of CO<sub>2</sub> by reactivation due to injection pressures. This study considers possible hydromechanical effects due to a low and high permeability fault.

Discrete Geologic Model



Low Permeability Fault

Interior view of CO<sub>2</sub> Saturation



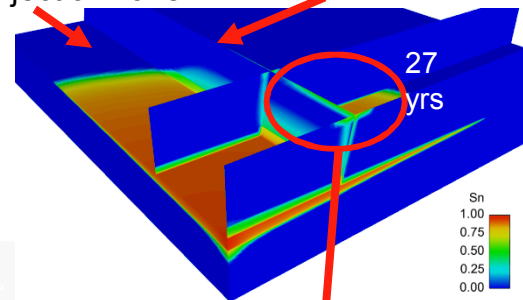
17 yrs

S<sub>n</sub>  
1.00  
0.75  
0.50  
0.25  
0.00

High Permeability Fault

Top of injection zone

Fault plane

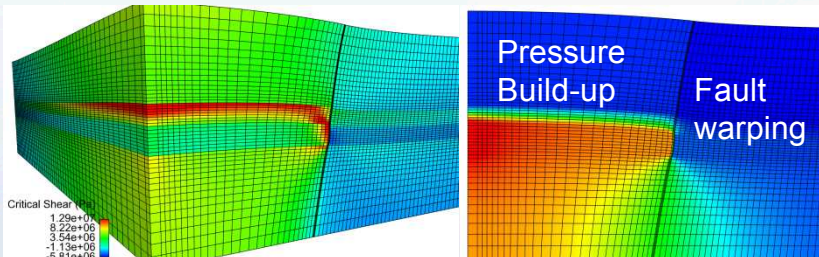
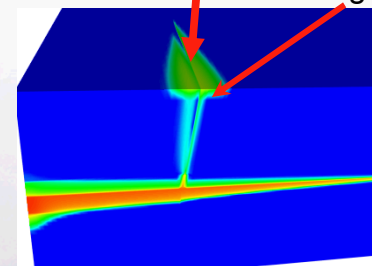


27 yrs

S<sub>n</sub>  
1.00  
0.75  
0.50  
0.25  
0.00

Exterior view

Leaking Fault



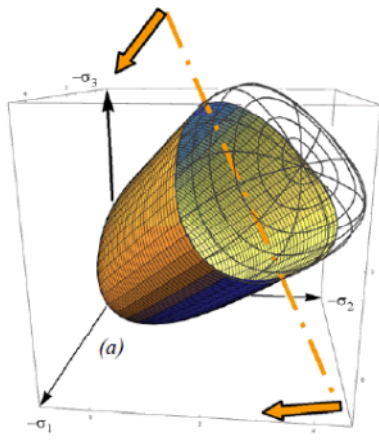
**Low permeability** fault impedes CO<sub>2</sub> injection, diverts flow along fault and builds pressure behind the fault, thereby shearing/warping the fault and inducing critical shear failure in both the caprock and fault.

**High permeability** fault creates a pathway for leakage of CO<sub>2</sub> through the caprock, ultimately pooling at the top of the upper aquifer, which is capped by an impermeable boundary.

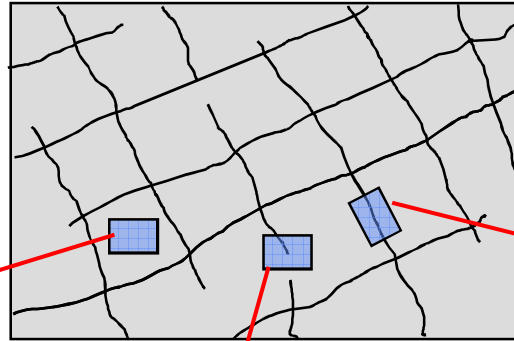
# Hydromechanical Coupling in Fractured Rock

## bulk constitutive properties

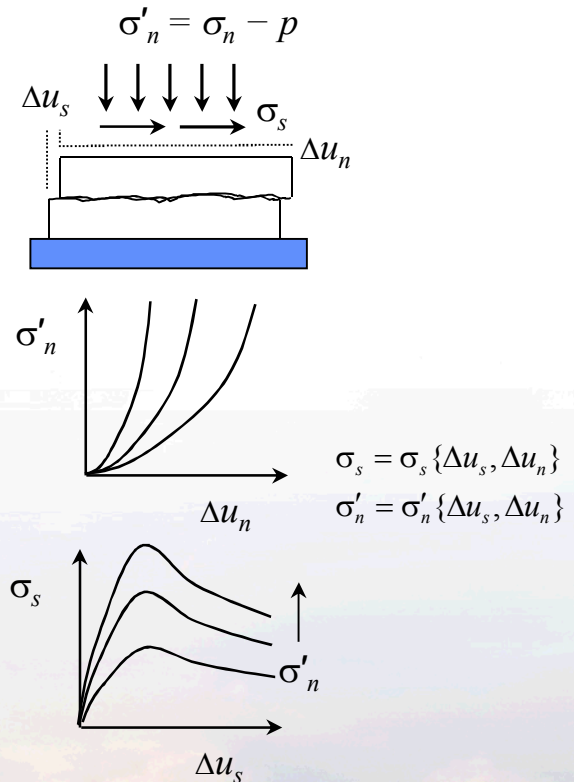
(Sandia GeoModel  
Fossum & Brannon, 2004)



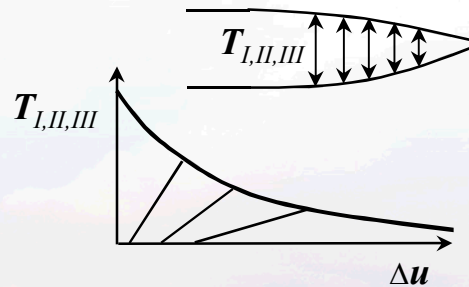
## Fractured Porous Rock



## fracture contact properties

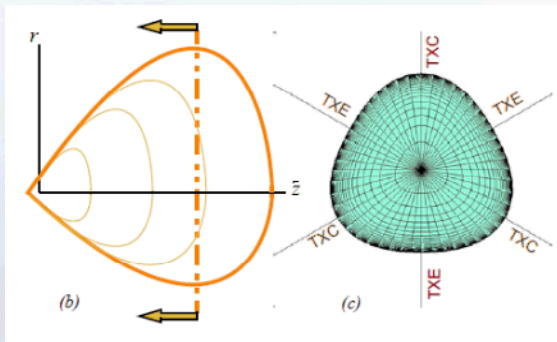


## crack-tip cohesive properties

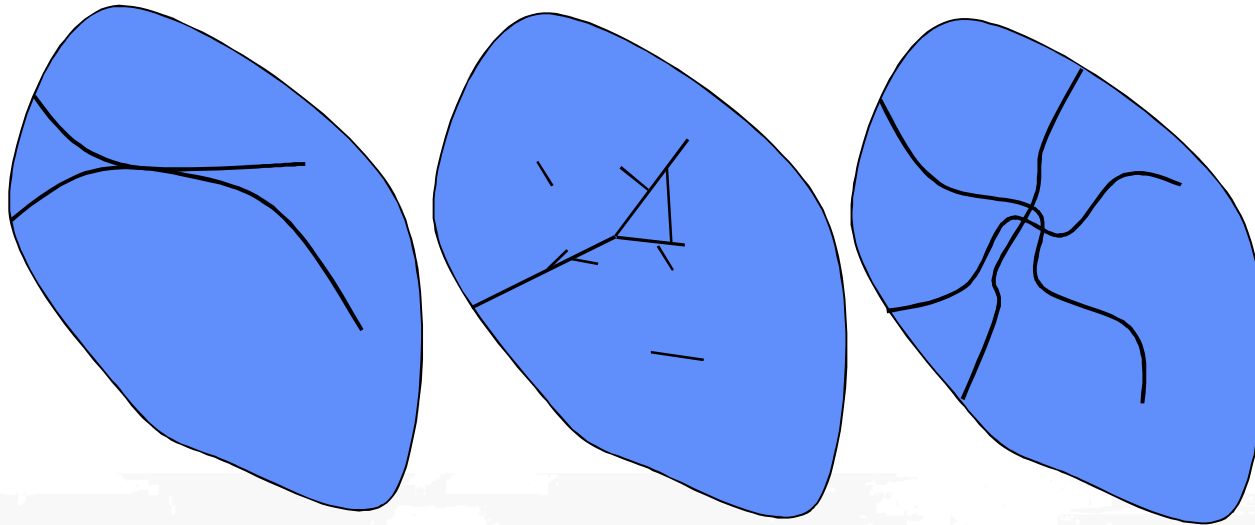


## additional challenges

- scale dependence
- history dependence
- precipitation
- dissolution



# Computational Challenges to Allowing Cracks to Grow Arbitrarily

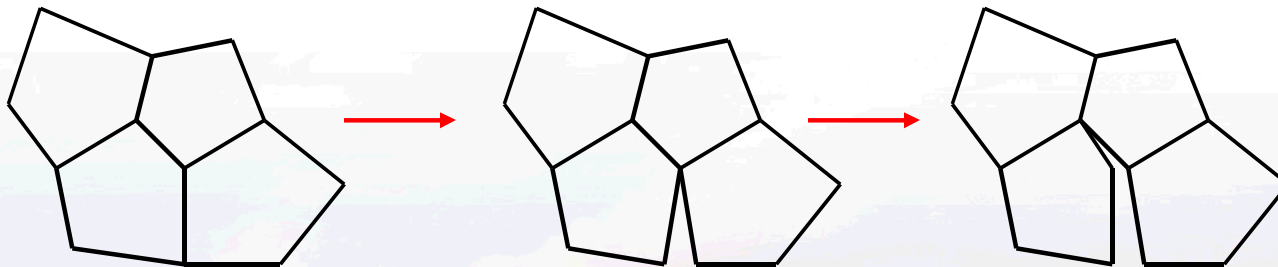


- Do we restrict branching?
- Do we restrict initiation?
  - from surface only?
  - from crack tips only?
  - from existing cracks only?
- Constraints on turning angles?
- Constraints on crossing angles?
- Constraints on minimum fragment size?

What about 3D?

# Computational Approach

- Random Voronoi tessellation (mesh)
- Polyhedral finite-elements
- Fracture only allowed at element edges.
- *Dynamic* mesh connectivity
- Insert cohesive tractions on new fracture surfaces.

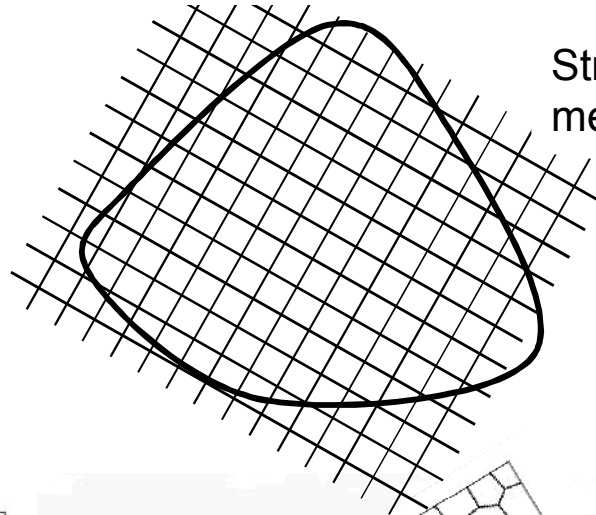
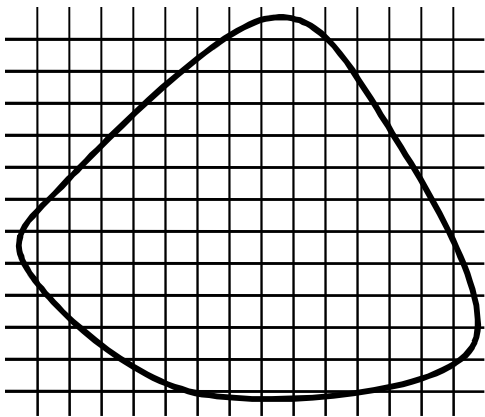


dynamic insertion of cohesive tractions based on . . .

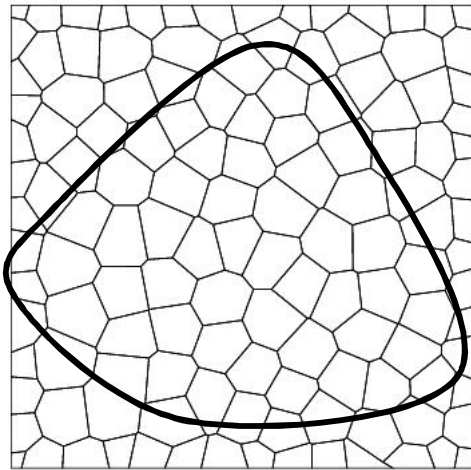
Pandolfi, A. and Ortiz, M. (2002) 'An efficient adaptive procedure for three-dimensional fragmentation simulations,' *Engineering with computers*, 18, 148-159.

# Eliminating Mesh Induced Crack Bias

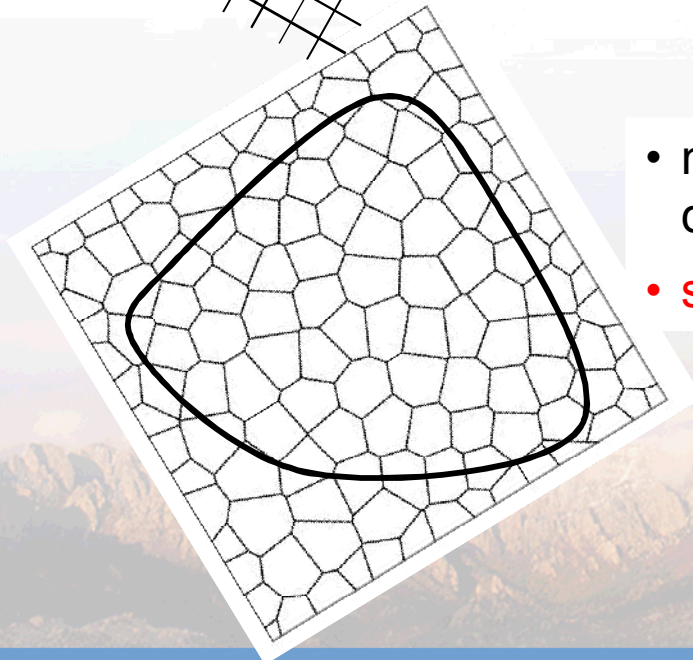
If cracks can grow only at element edges, then need to eliminate any directional bias in crack growth.



Structured grids can result in strong mesh induced bias (nonobjective).

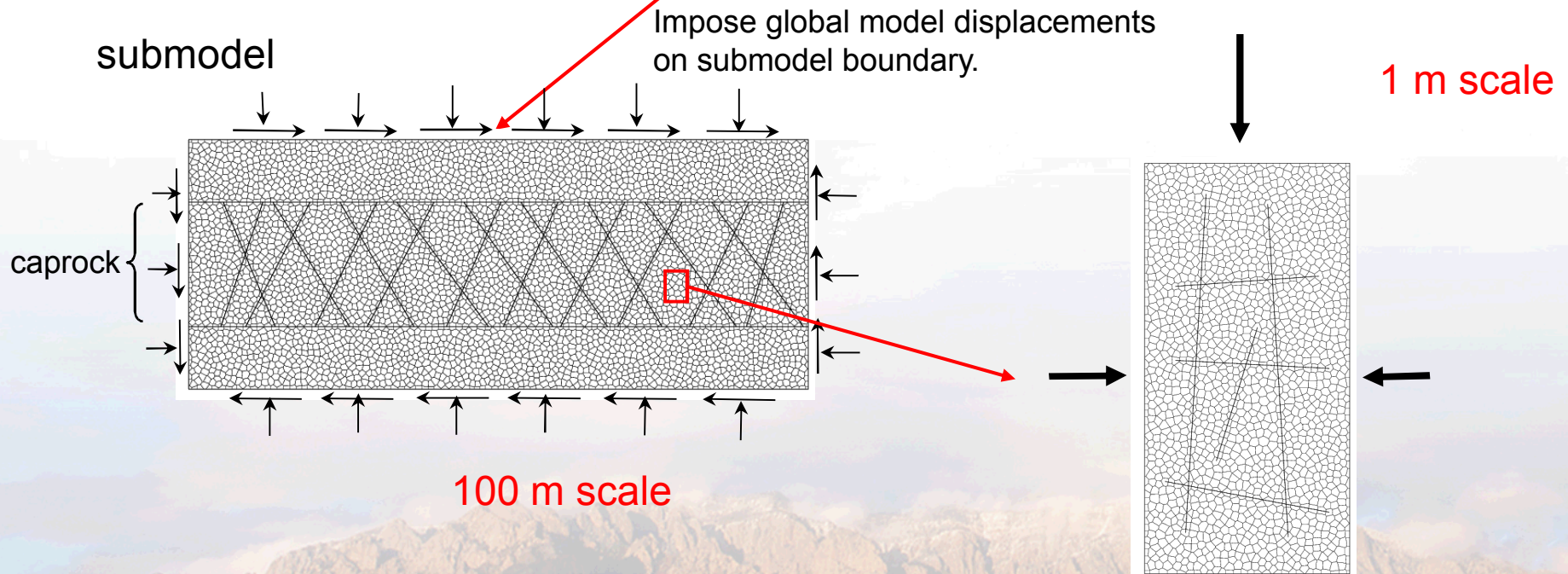
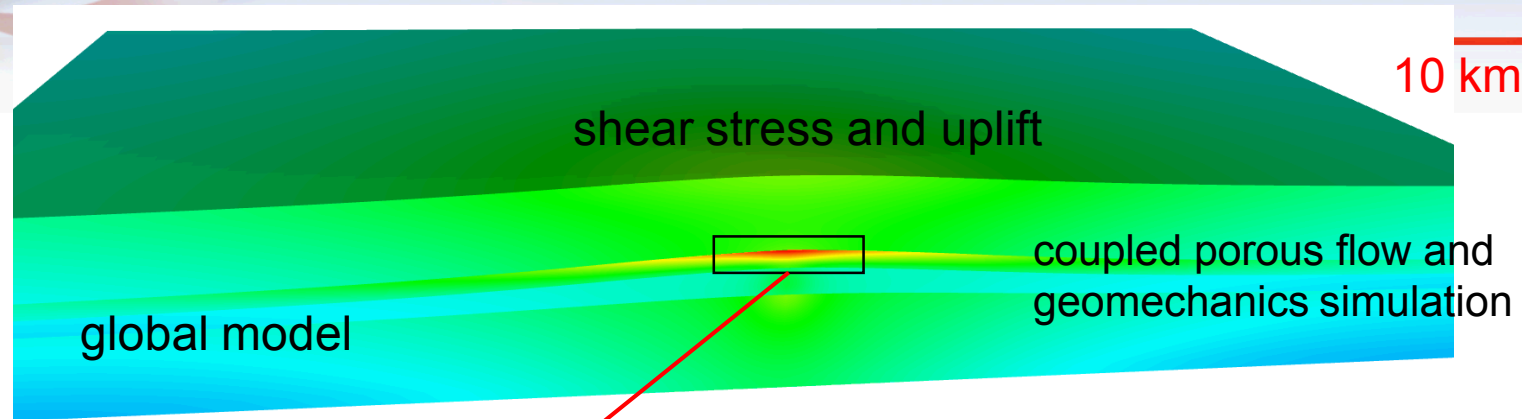


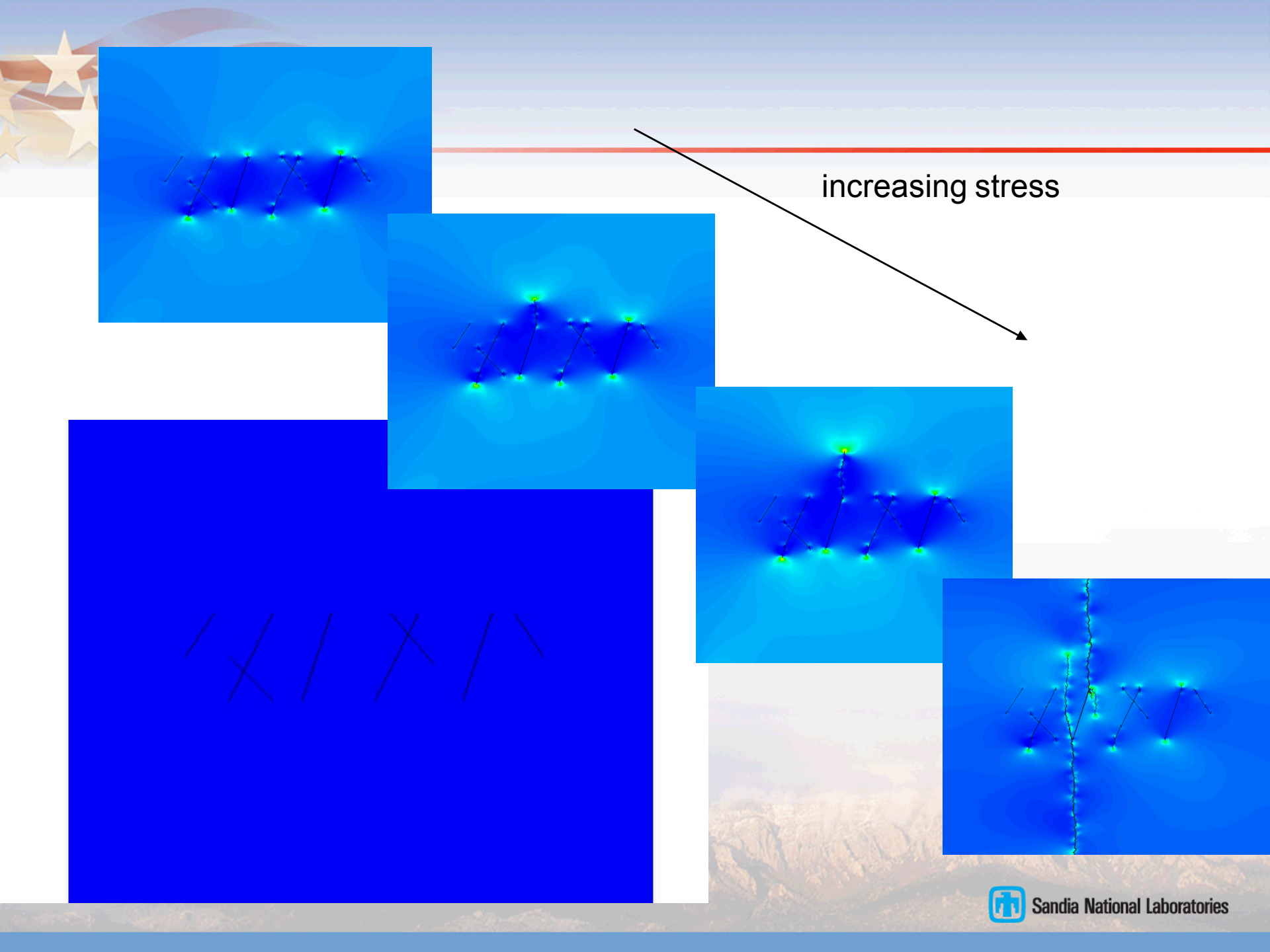
Voronoi tessellation of  
with random seeding



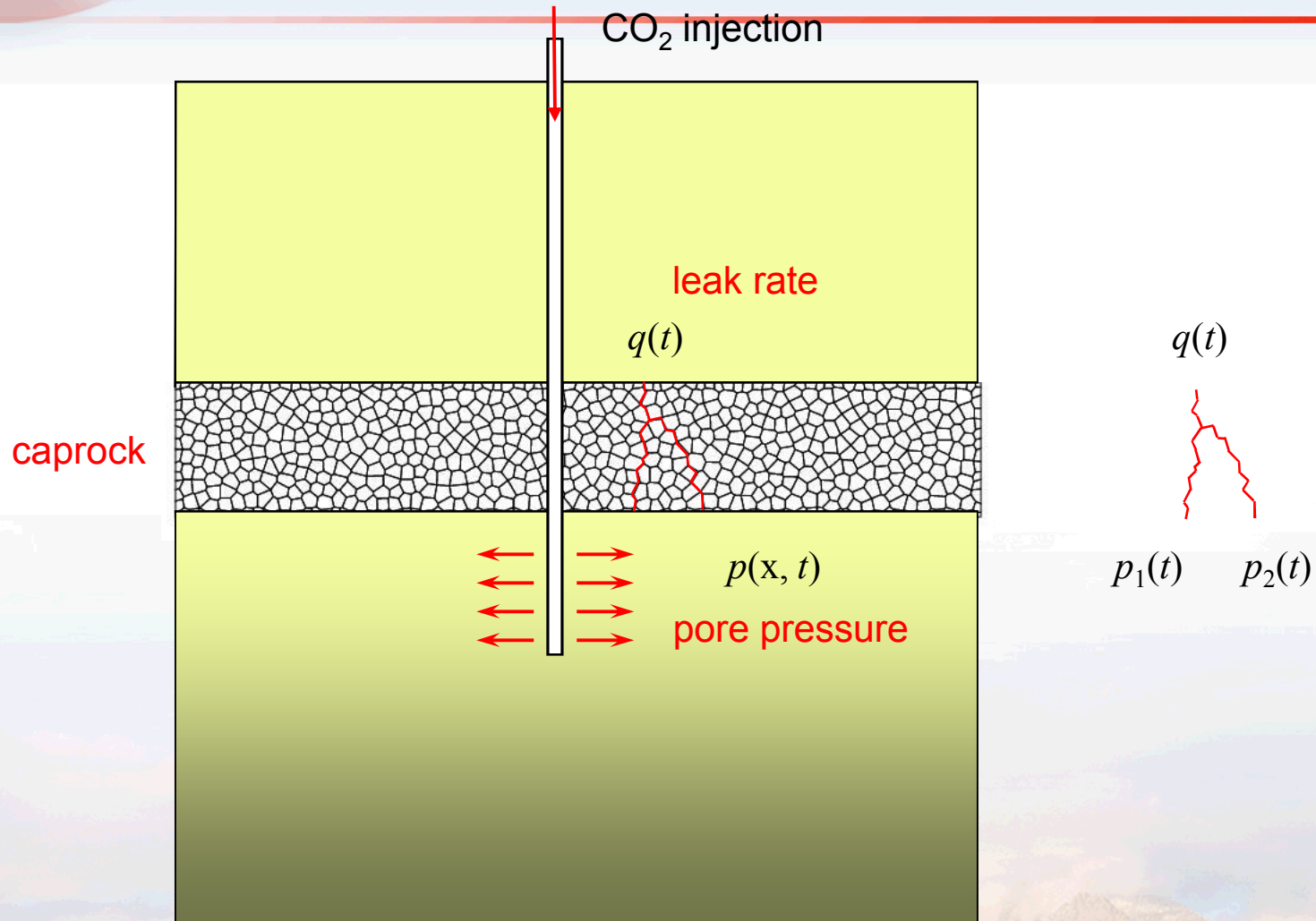
- need to use 'random' discretizations
- statistically isotropic

# Multiscale analysis of caprock integrity during CO<sub>2</sub> injection



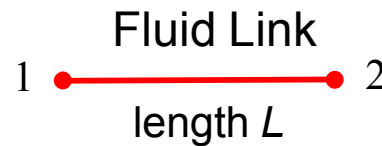
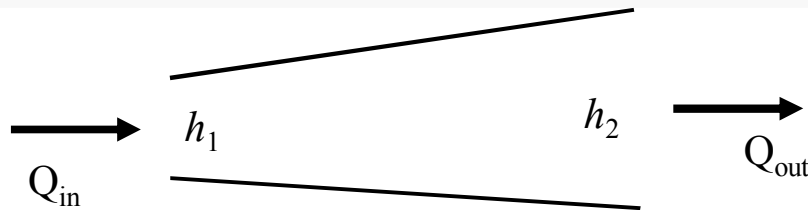


# Fluid Flow in 2D Discrete Fracture Networks



# Fluid Flow in 2D Discrete Fracture Networks

Solve fluid network to get nodal pressures and flow rates.

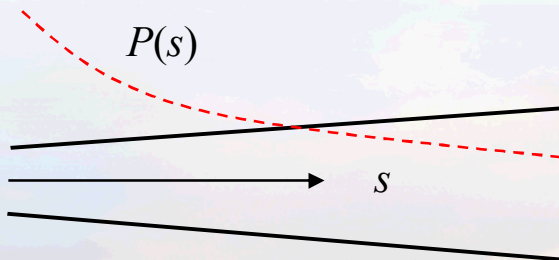


$$\begin{Bmatrix} Q_1 \\ Q_2 \end{Bmatrix} = \frac{T}{\mu} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \begin{Bmatrix} P_1 \\ P_2 \end{Bmatrix}$$

Reynold's lubrication equation

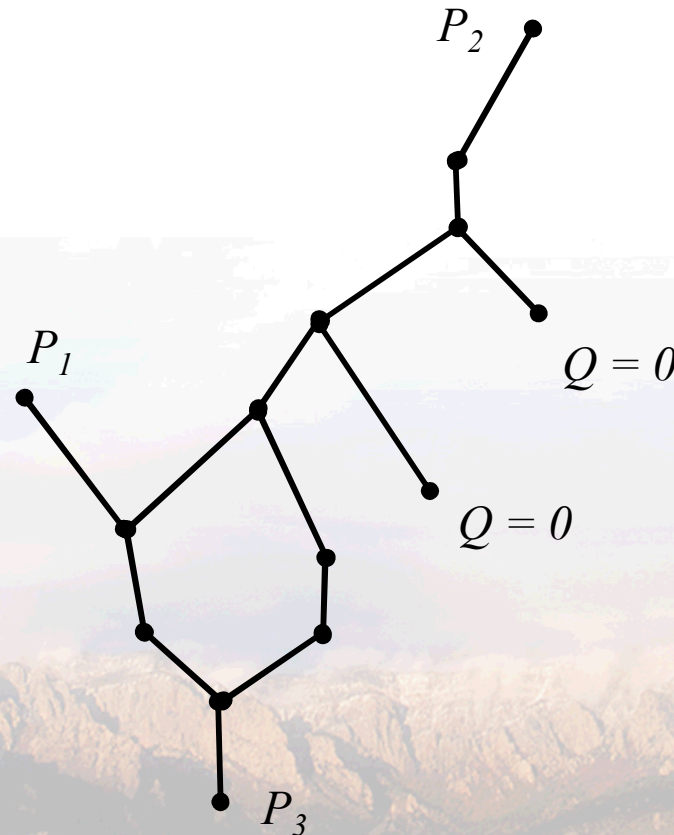
$$\nabla(\rho \mathbf{Q}) = 0$$

$$\mathbf{Q} = -\frac{h^3}{12\mu} (\nabla p - \rho g h)$$

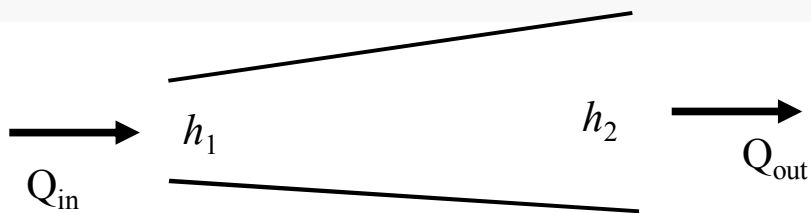


$$T = \frac{h_1^2 h_2^2}{6L} \frac{1}{h_1 + h_2}$$

$Q$  = flow rate  
 $P$  = pressure  
 $\mu$  = viscosity  
 $T$  = transmissibility



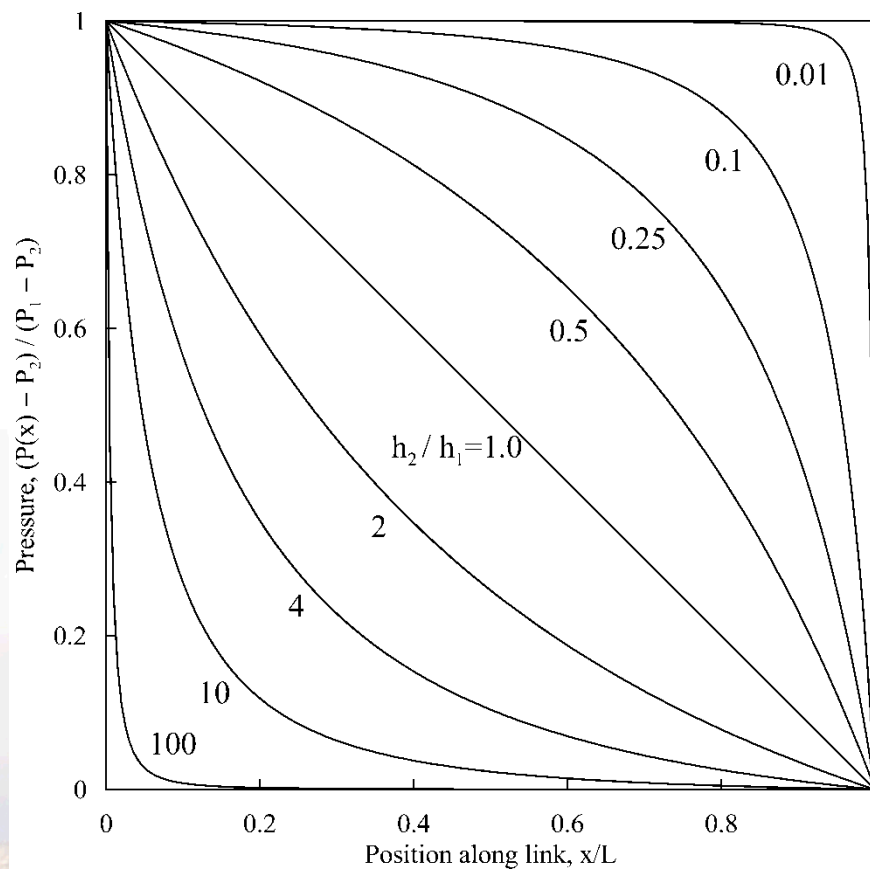
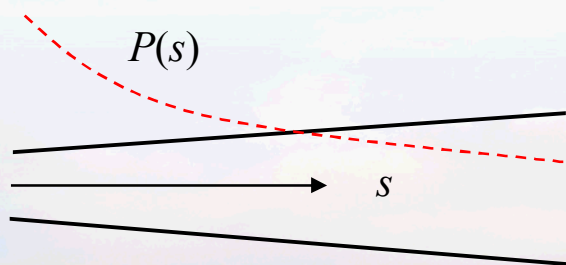
# Fluid Flow in Discrete Fracture Networks



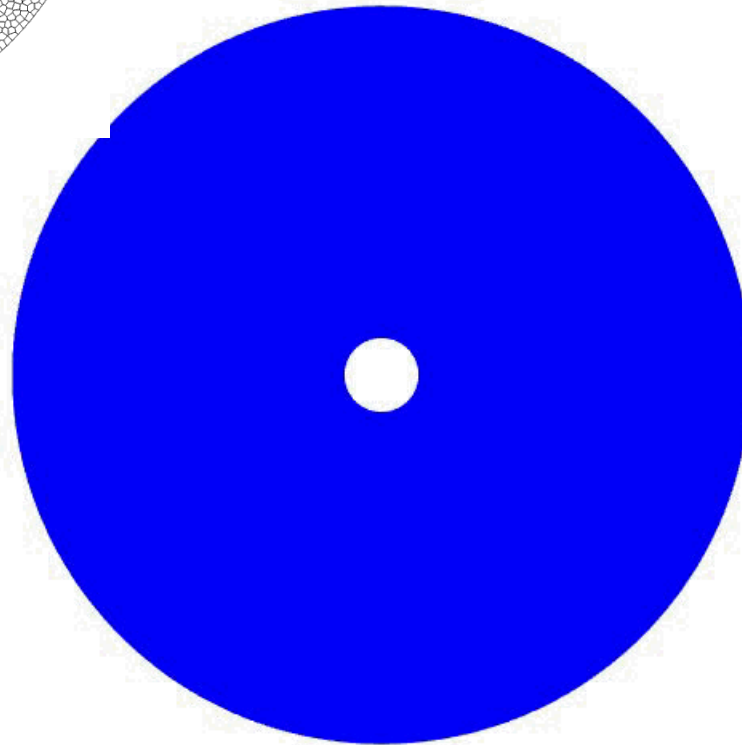
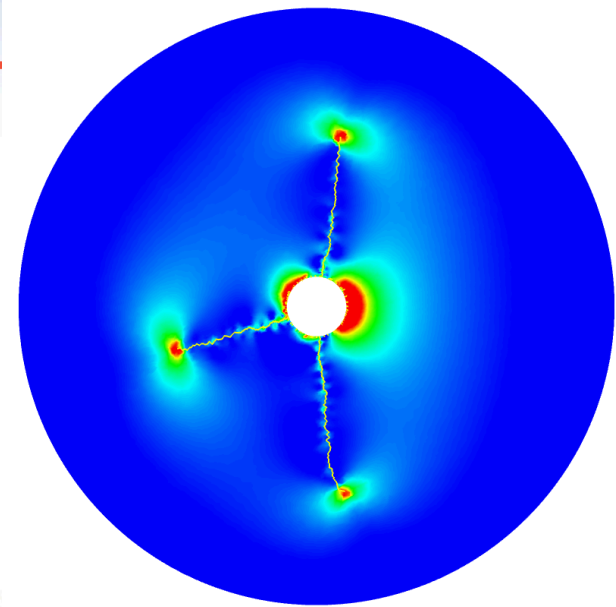
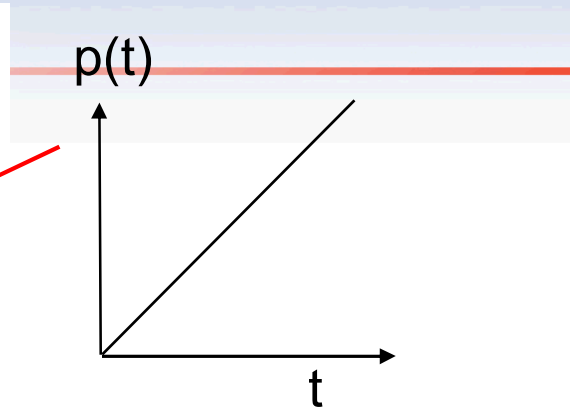
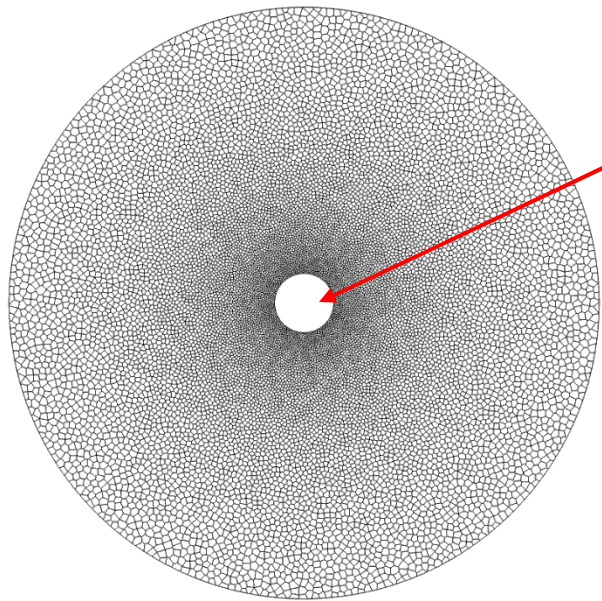
Reynold's lubrication equation

$$\nabla(\rho \mathbf{Q}) = 0$$

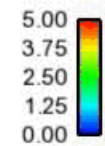
$$\mathbf{Q} = -\frac{h^3}{12\mu}(\nabla p - \rho gh)$$



# Hydraulic Fracture Simulation



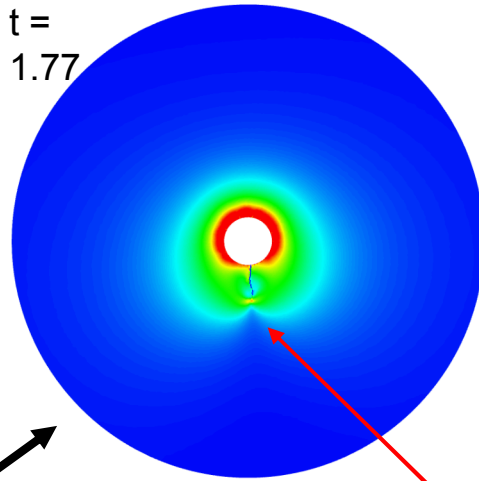
max\_p



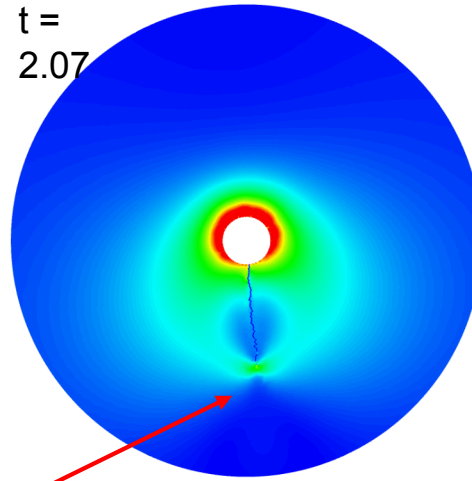
# Hydraulic Fracture Simulation

fluid pressure  
up to crack tip

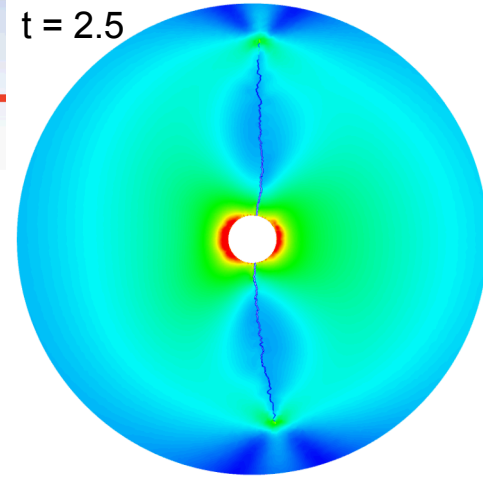
$t = 1.77$



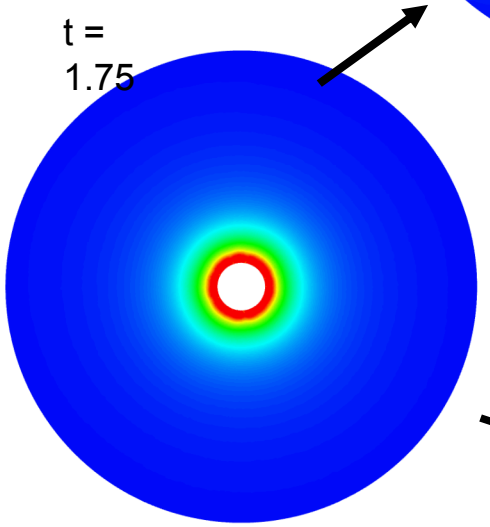
$t = 2.07$



$t = 2.5$



$t = 1.75$

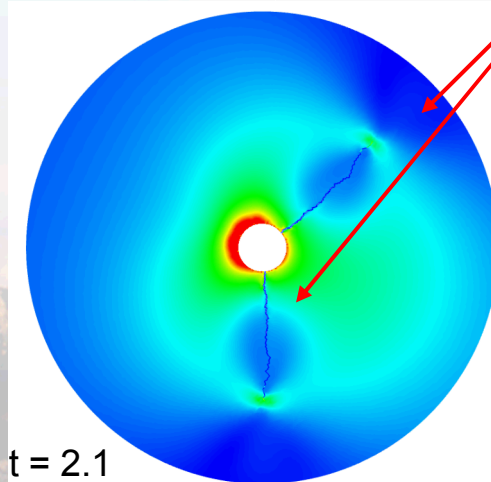


Initial crack delays  
initiation of  
secondary crack.

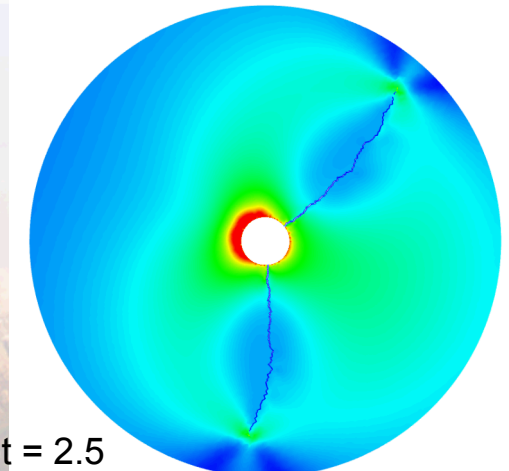
Both cracks  
propagate  
simultaneously.

fluid pressure up  
to cohesive tip

$t = 2.1$

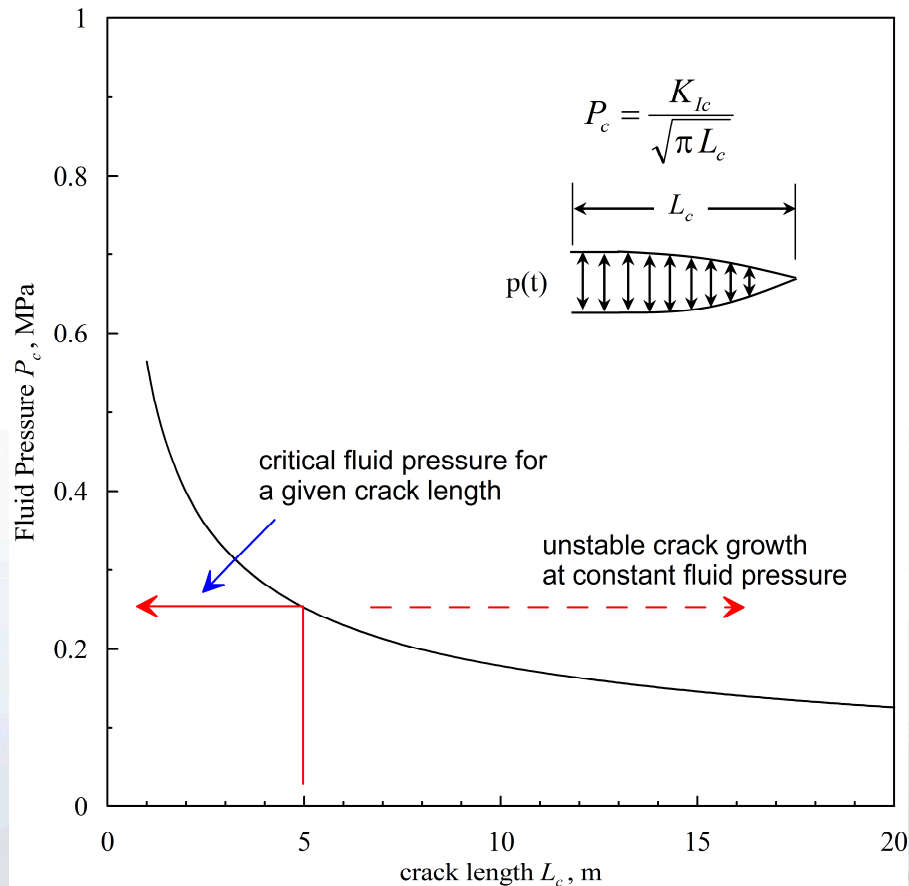


$t = 2.5$



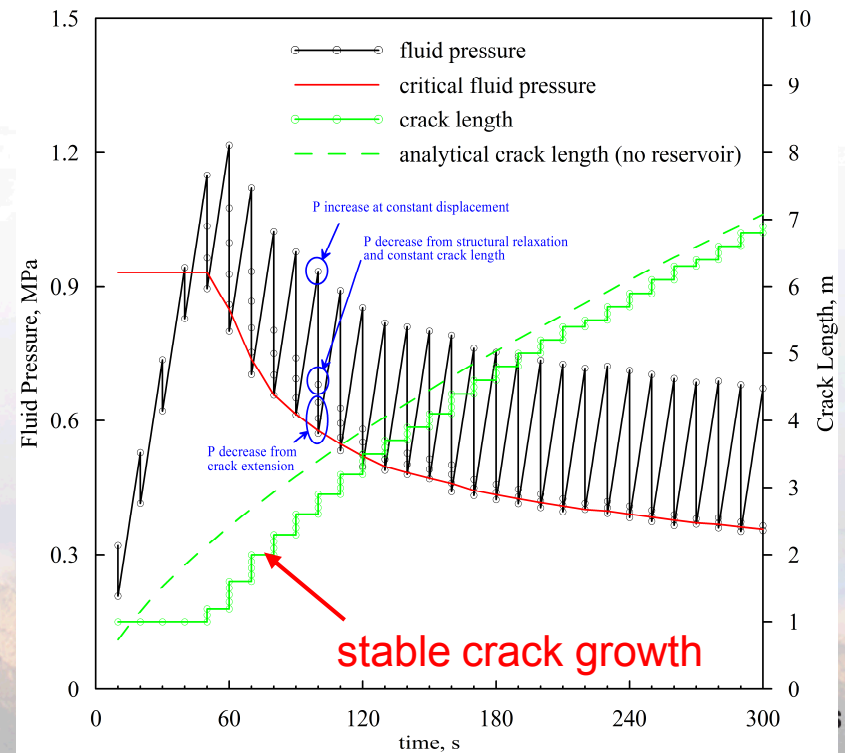
# Hydraulic Fracture Simulation

- Constant fluid pressure causes unstable crack growth.
- Use fluid-mass control.



```

do
  increment fluid mass,  $\Delta m$ 
  equilibrate at constant crack length,  $a$ .
  while ( $K_I > K_{Ic}$ )
    increment crack length,  $\Delta a$ .
    equilibrate at constant crack length,  $a + \Delta a$ .
  end while
end do
    
```





# Future Directions

- **Models of perm(stress, porosity, damage)**
- **Multiphysics coupling of dynamic discrete fracture network generation**
  - **One-way coupled (continuum → discrete) dynamic discrete fracture**
  - **Flow physics on shells**
  - **3D Vornoi mesh in Sierra**
- **Thermal CO<sub>2</sub>-NACL-H<sub>2</sub>O phase behavior**
- **Geochemistry**



# Backup Slides

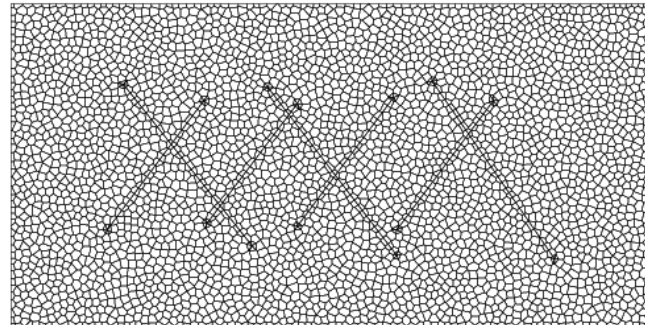
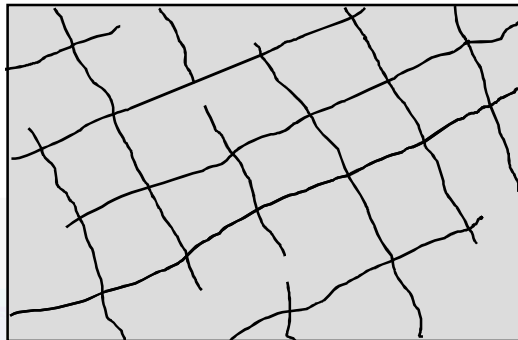
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# MeshingGenie (Trilinos)

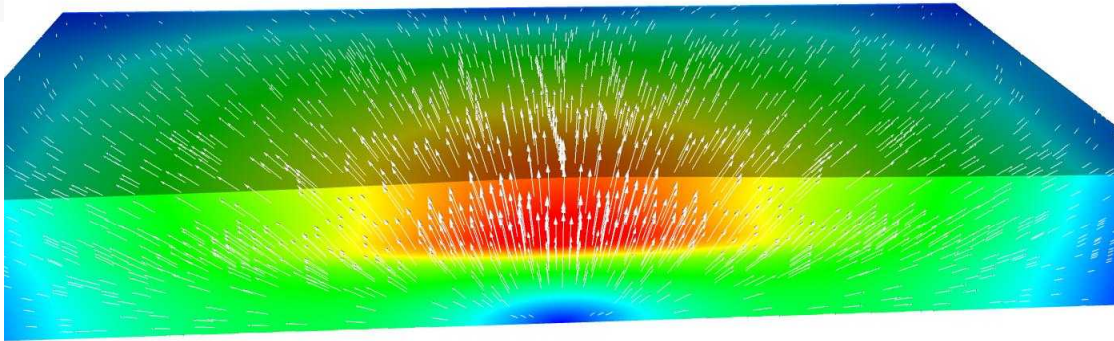
(Ebeida, M., Knupp, P., Vitus Leung, Sandia National Laboratories)

Fractured Rock



# Injection Induced Uplift

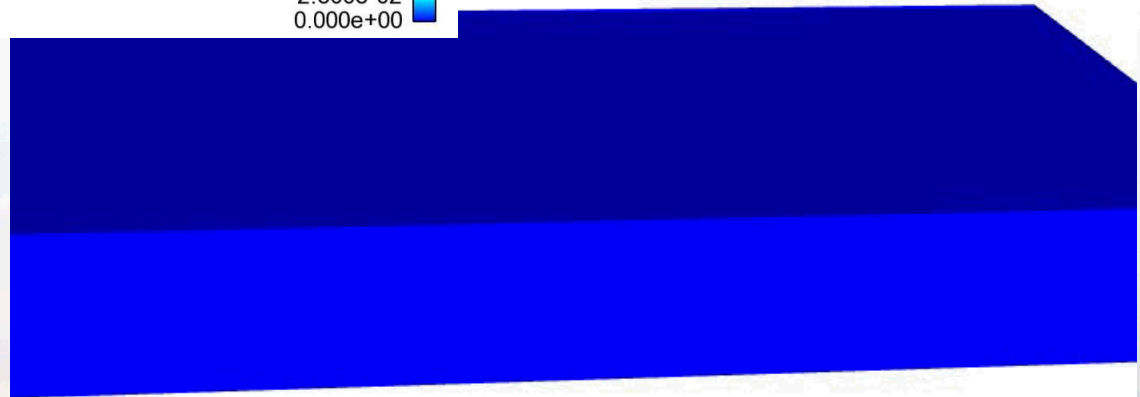
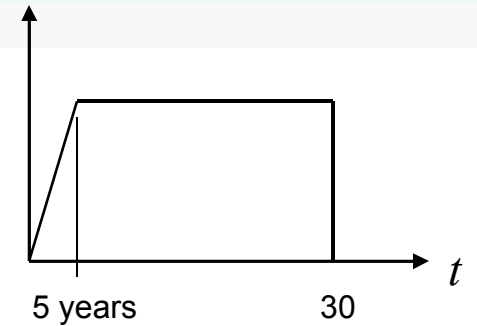
5.32 years



displacement field x 1000 at year 5

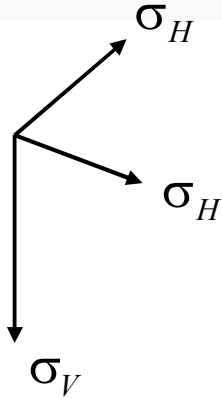
displ\_vec  
1.000e-01  
7.500e-02  
5.000e-02  
2.500e-02  
0.000e+00

injection rate



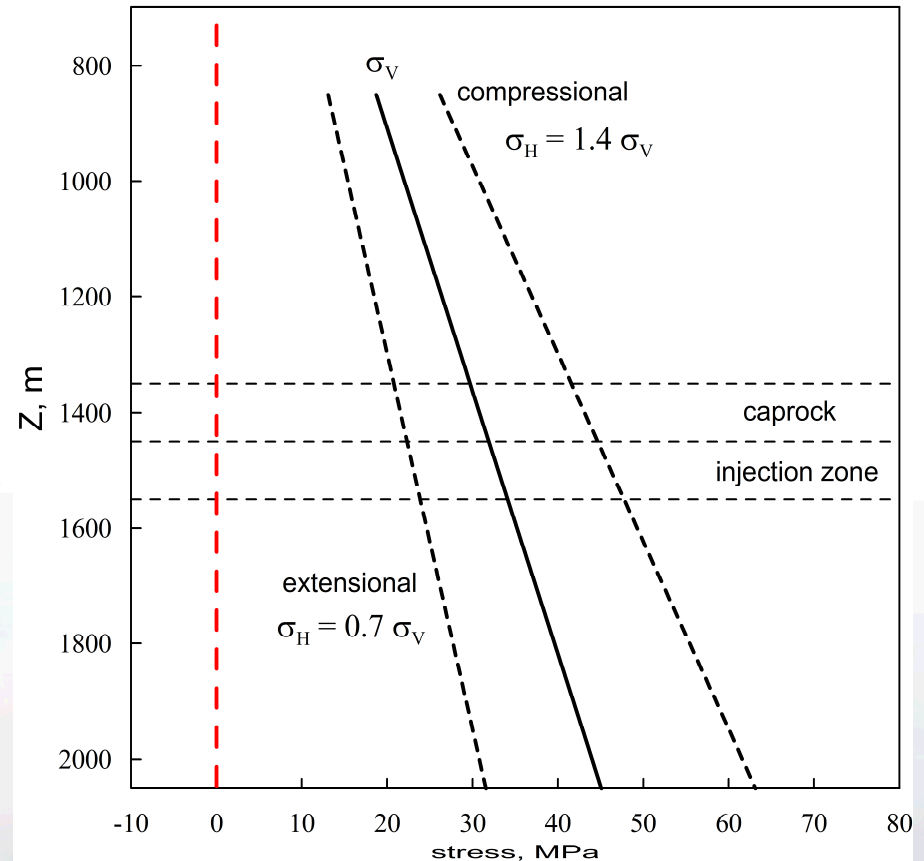
displ\_vec  
1.000e-01  
7.500e-02  
5.000e-02  
2.500e-02  
0.000e+00

# Initial Stress State



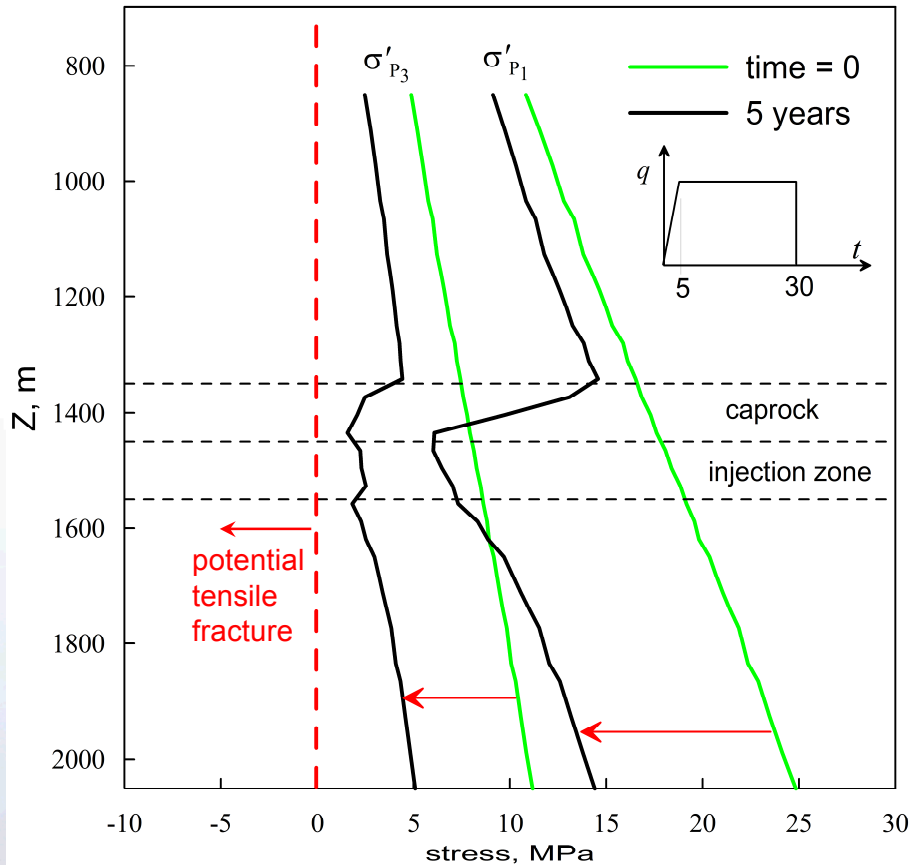
Look at two initial stress regimes

1. extensional  $\sigma_H < \sigma_V$
2. compressional  $\sigma_H > \sigma_V$



# Extensional Initial Stress

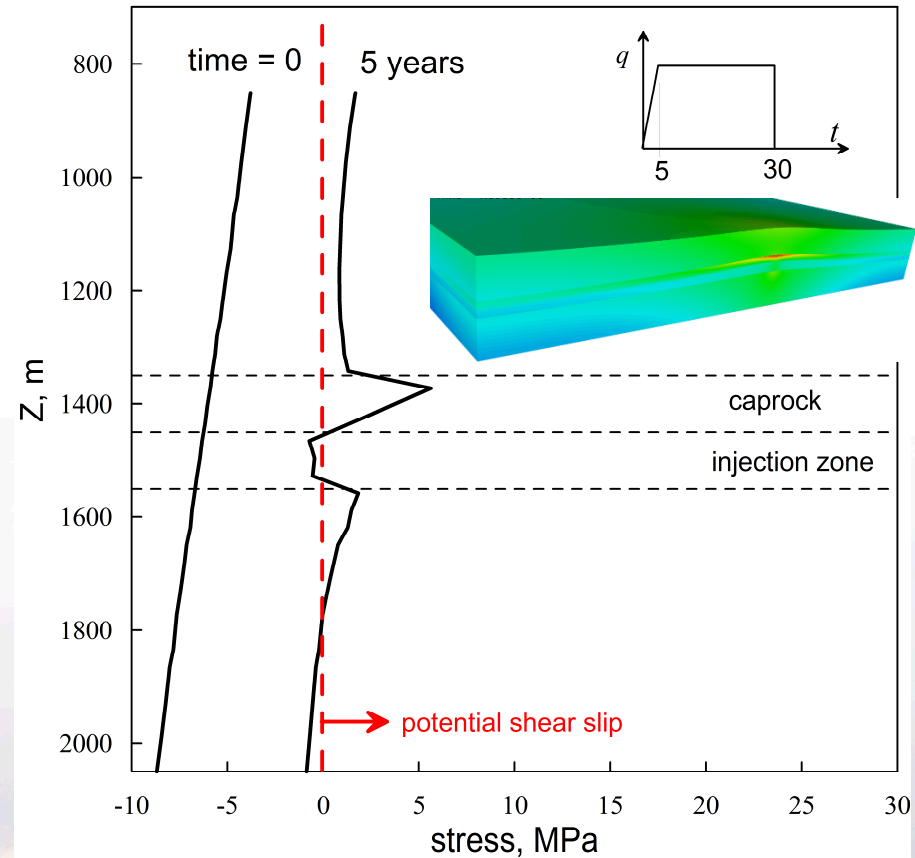
effective principal stresses



effective principal stress

critical shear

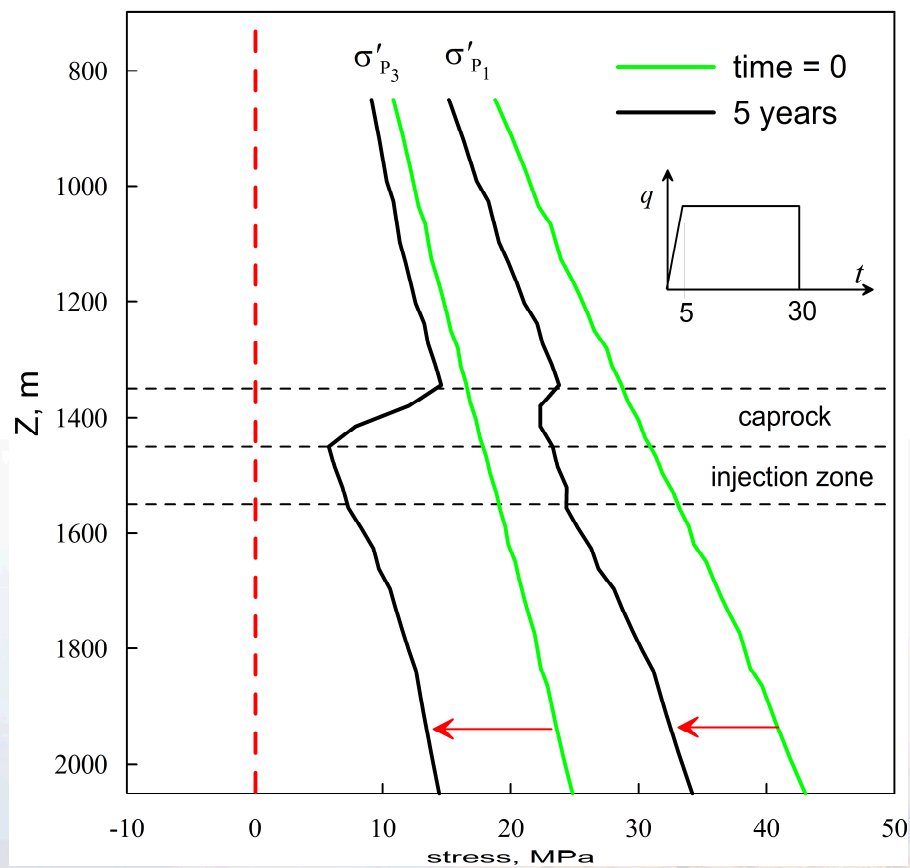
$$\sigma'_{p1} - 3\sigma'_{p3} > 0$$



critical shear stress

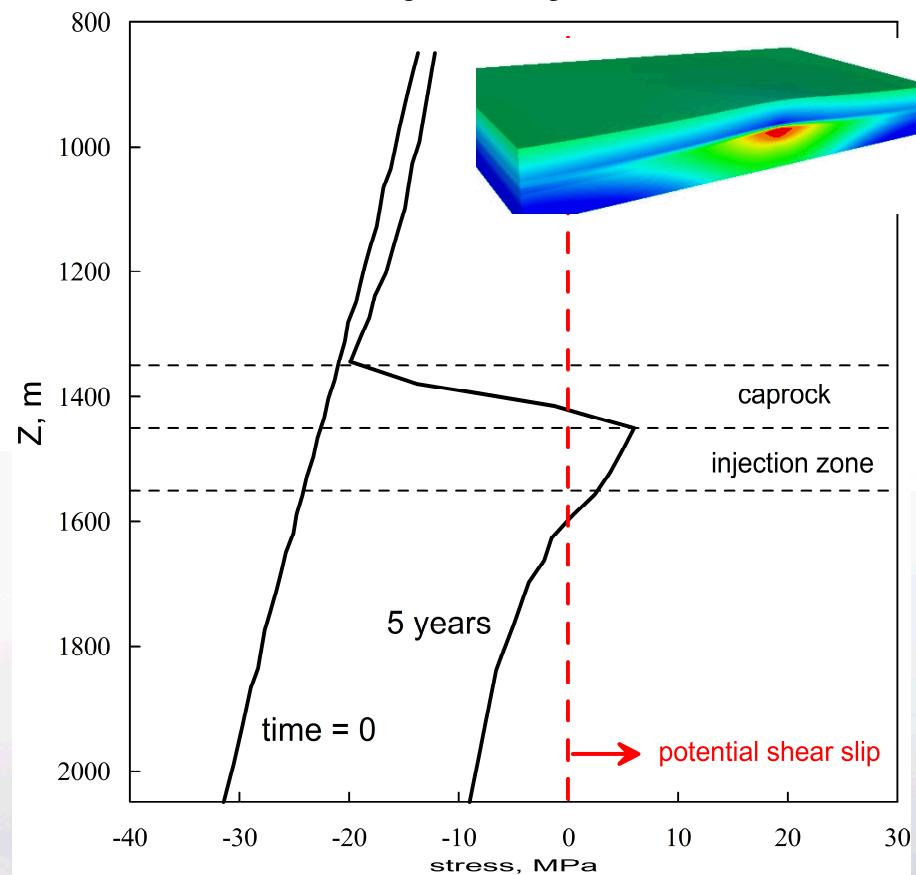
# Compressional Initial Stress

effective principal stresses



critical shear

$$\sigma'_{p1} - 3\sigma'_{p3} > 0$$



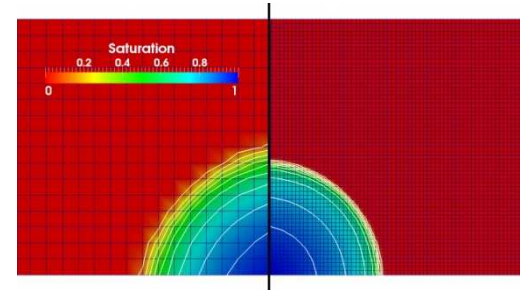
# Aria Multiphase Porous Flow Physics

## Two-Phase Immiscible Flow

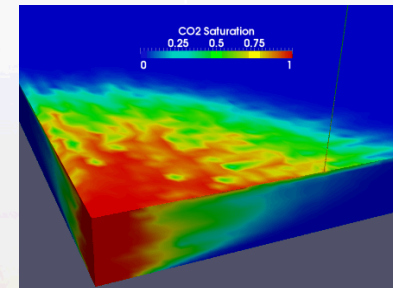
- Compressible (fluids and/or formation), buoyancy effects
- General dependence of thermophysical and transport properties on solution vector
- Capillary pressure (optional)
- Relative permeability
- Specification of heterogeneous transport property fields (e.g. permeability, porosity)
- Can be coupled to energy equation

### Benchmark Problem

Displacement of oil by water flood without capillary pressure or gravitational effects.



Grid effects using upwind CVFEM scheme



Injected CO<sub>2</sub> saturation levels in a brine filled reservoir represented with heterogeneous permeability

# Aria Porous Flow Physics

## Immiscible Flow

### Mathematical Model

- **Two-Phase Immiscible Mass Balances:**

$$\frac{\partial(\rho_w \phi S_w)}{\partial t} = \nabla \cdot \left( \rho_w \frac{k_{rw}}{\mu_w} \mathbf{k} \cdot (\nabla p - \rho_w \mathbf{g}) \right) + Q_w$$

$$\frac{\partial(\rho_n \phi S_n)}{\partial t} = \nabla \cdot \left( \rho_n \frac{k_{rn}}{\mu_n} \mathbf{k} \cdot (\nabla p + \nabla p_c - \rho_n \mathbf{g}) \right) + Q_n$$

- **Thermophysical property models (new models are easily incorporated):**

$$\rho_w = \rho_{w,0} (1 + \kappa_{Tw} (p - p_o))$$

$$\rho_n = \rho_{n,0} (1 + \kappa_{Tn} (p_n - p_{n,o}))$$

$$p_n = p + p_c(S_w)$$

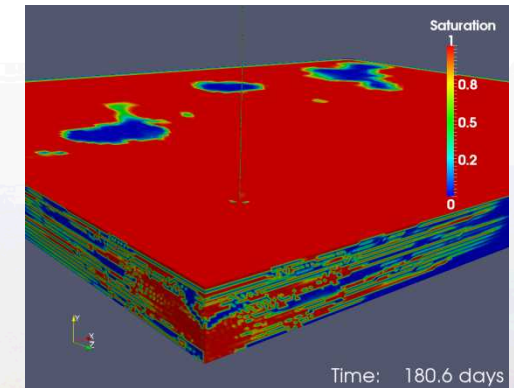
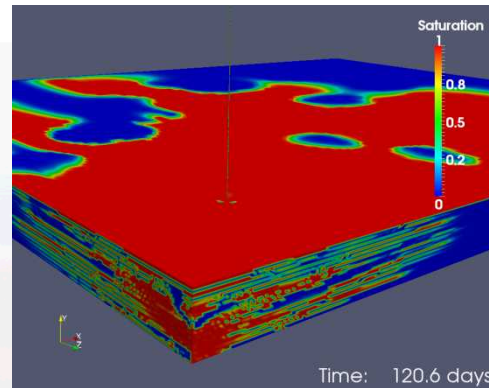
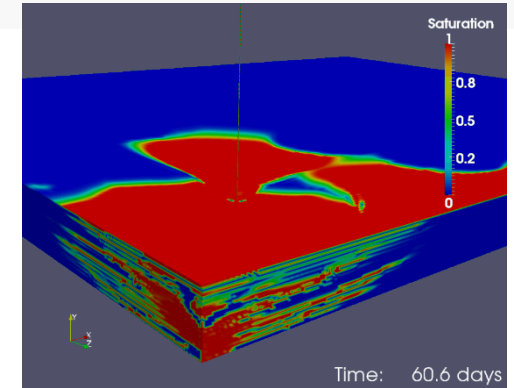
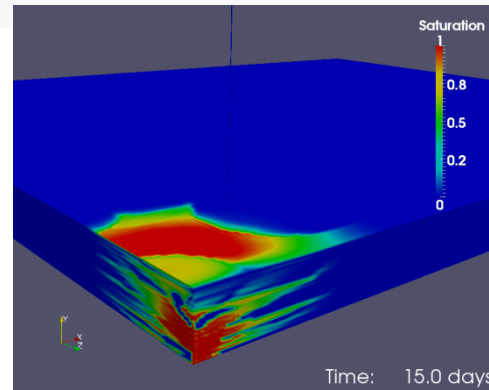
$$S_w = 1 - S_n$$

$$\phi = \phi_0 (1 + C_r (p - p_0))$$

# CO<sub>2</sub> Leakage Through an Abandoned Well Heterogeneous Layered Media

## Some Results (10 realizations)

- Correlation between fast paths and permeability distribution is evident
- Leakage, arrival time are heavily dependent on permeability distribution
- Heterogeneous layer media results in similar leakage rates.





# Contact Algorithm

 A node-face contact capability is implemented with a two-part strategy:

1. A search algorithm to define contact constraints which
  - operates on the current configuration
  - produces a list of interactions
2. An enforcement algorithm to enforce the contact constraints
  - Includes the physics, i.e. friction model

The enforcement algorithm satisfies equilibrium across the contact interface and also enforces frictional sliding based on the following slip condition:

$$\Phi := \|t_T\| - \mu t_N \leq 0 \quad \text{no slip due to shear}$$

$$\Phi := \|t_T\| - \mu t_N \succ 0 \quad \text{slip will occur due to shear}$$

3D disposal room closure behavior in salt at different locations along drift