SAND2011-3814 C

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A Finite-Element Method for Modeling Fracture in Disordered Media using Randomly Close-Packed Voronoi Tessellations with Applications to Fragmentation, CO2 sequestration, and HydroFracking

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Albuquerque, NM

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Computational Modeling of Fracture and Failure of Materials and Structures

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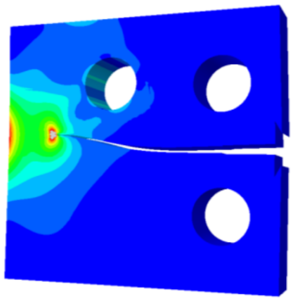
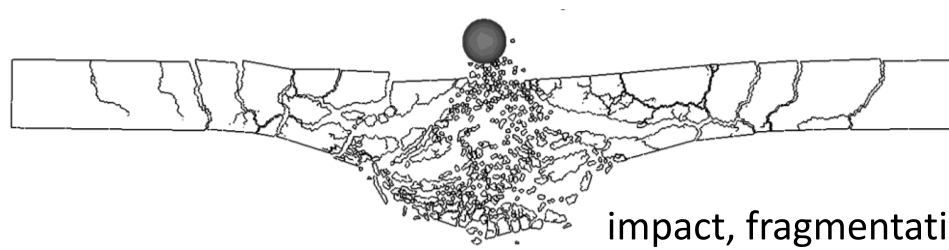
Outline

1. Disordered media, pervasive fracture
2. Modeling approach
3. Application to geosystems: hydro-mechanical coupling
4. 3D formulation and verification
5. Summary

Spectrum of Fracture Problems





impact, fragmentation

spectrum of fracture problems

single crack ⟷ pervasive fracture

- well defined deterministic propagation path
- analytical solutions
- enrichment methods (GFEM, XFEM, . . .)

- crack branching
- crack coalescence
- tortuous crack paths (sensitive to material heterogeneity)
- stochastic behavior

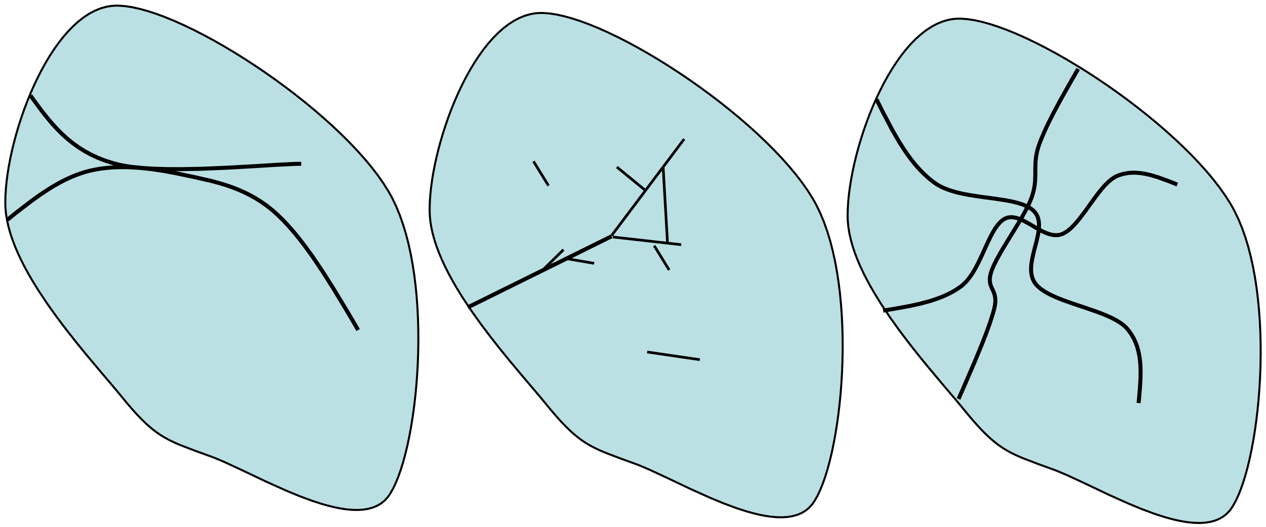
How far can we extend the computational tools used for one end of the spectrum to the other?

Typical Fracture Shapes

Note: no smooth cracks!

- Crack-front samples the subscale heterogeneity.
- Probability of seeing a straight crack propagate through a random field is zero.

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?

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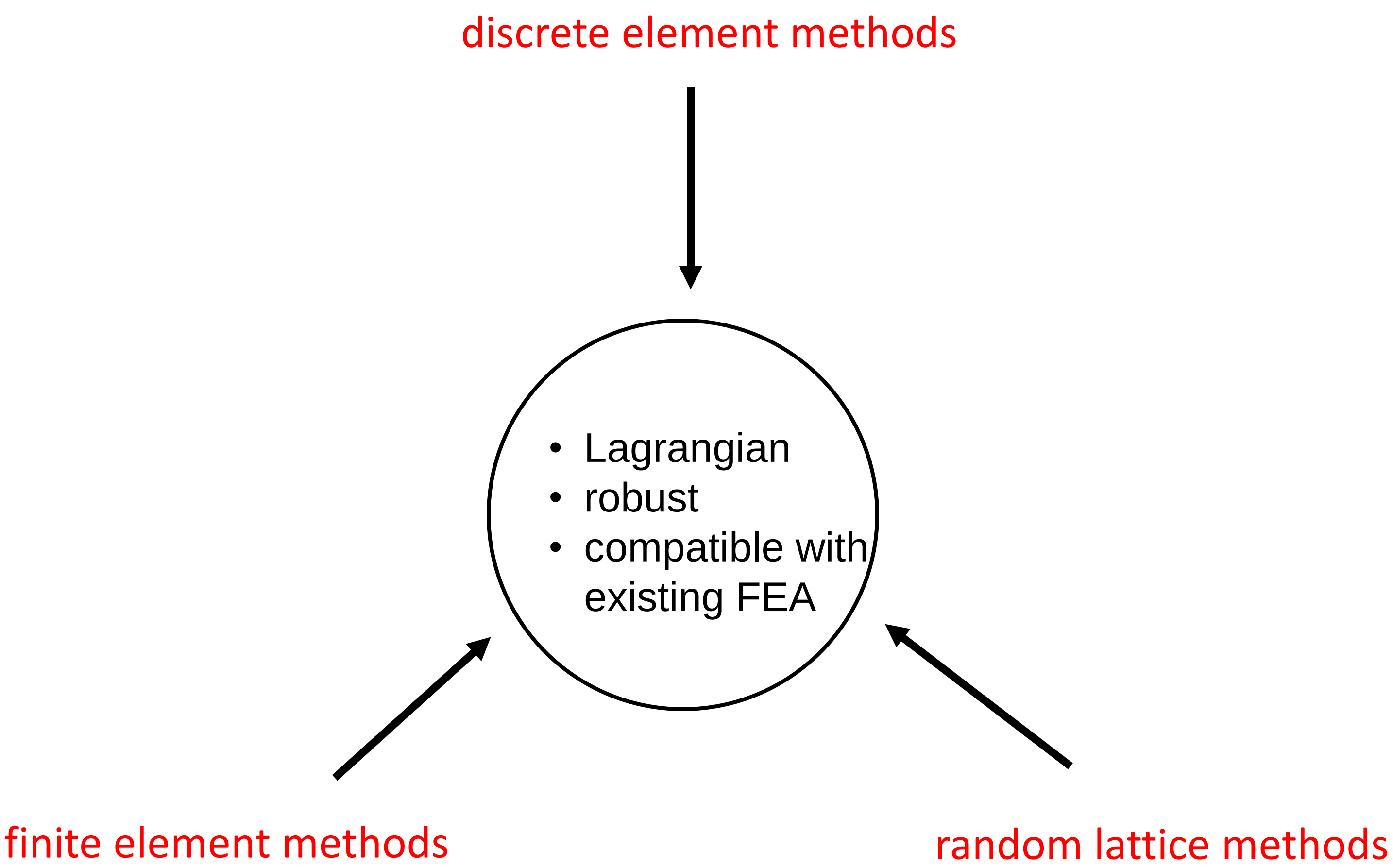
Computational Approach



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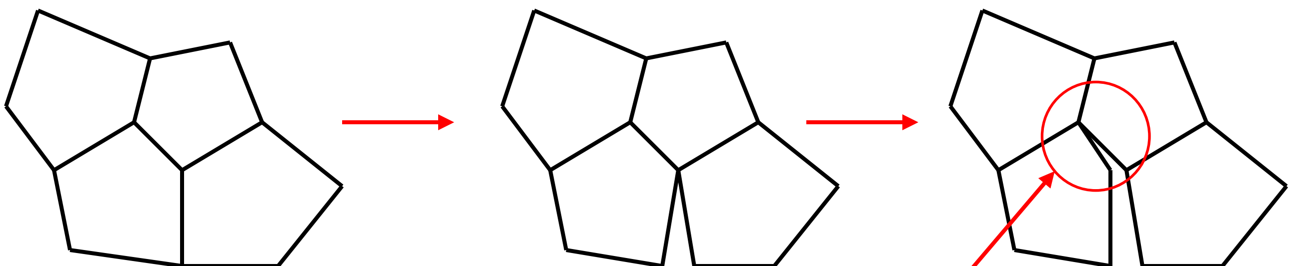
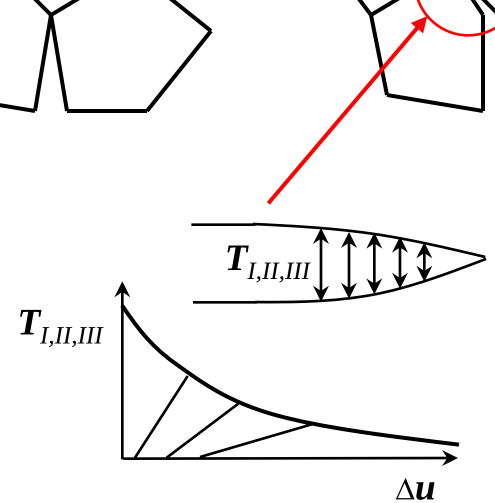
Computational Approach

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



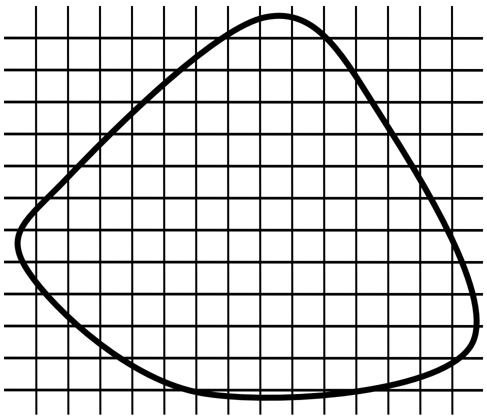
changing mesh connectivity

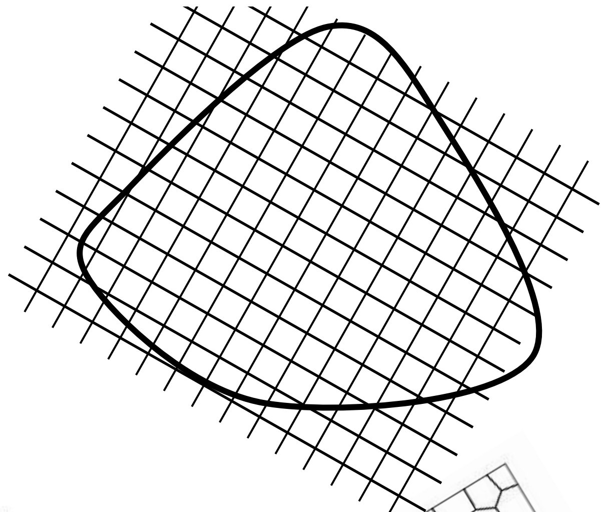


cohesive tractions
at crack tip

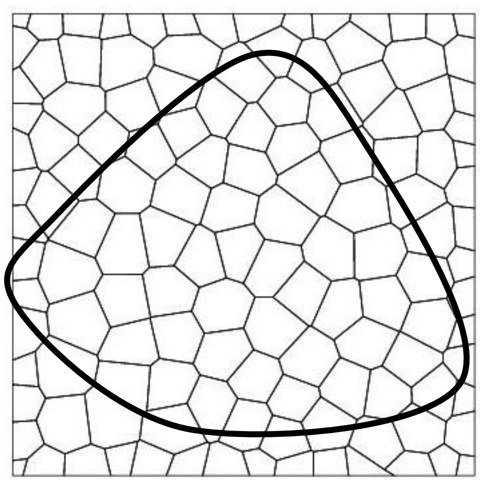
Why a Random Voronoi Mesh?

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

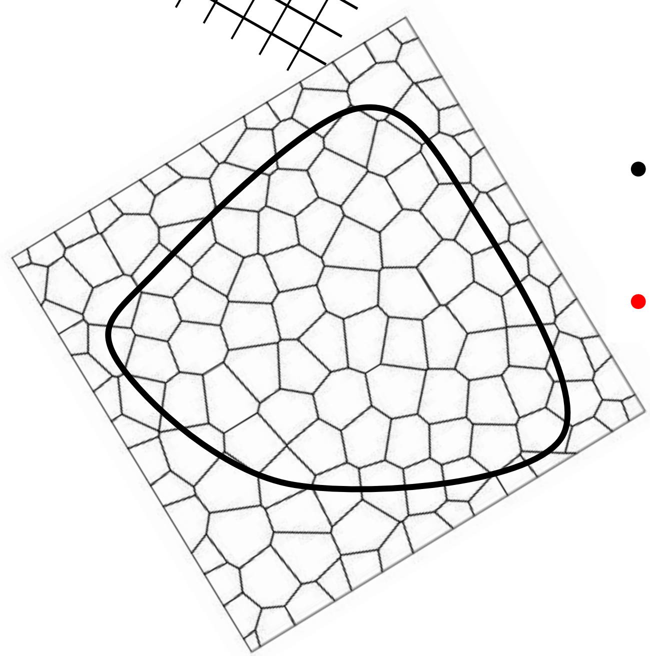




Structured grids can result in strong mesh induced bias (nonobjective).



Voronoi tesselation of
with random seeding



- need to use 'random' discretizations
- statistically isotropic

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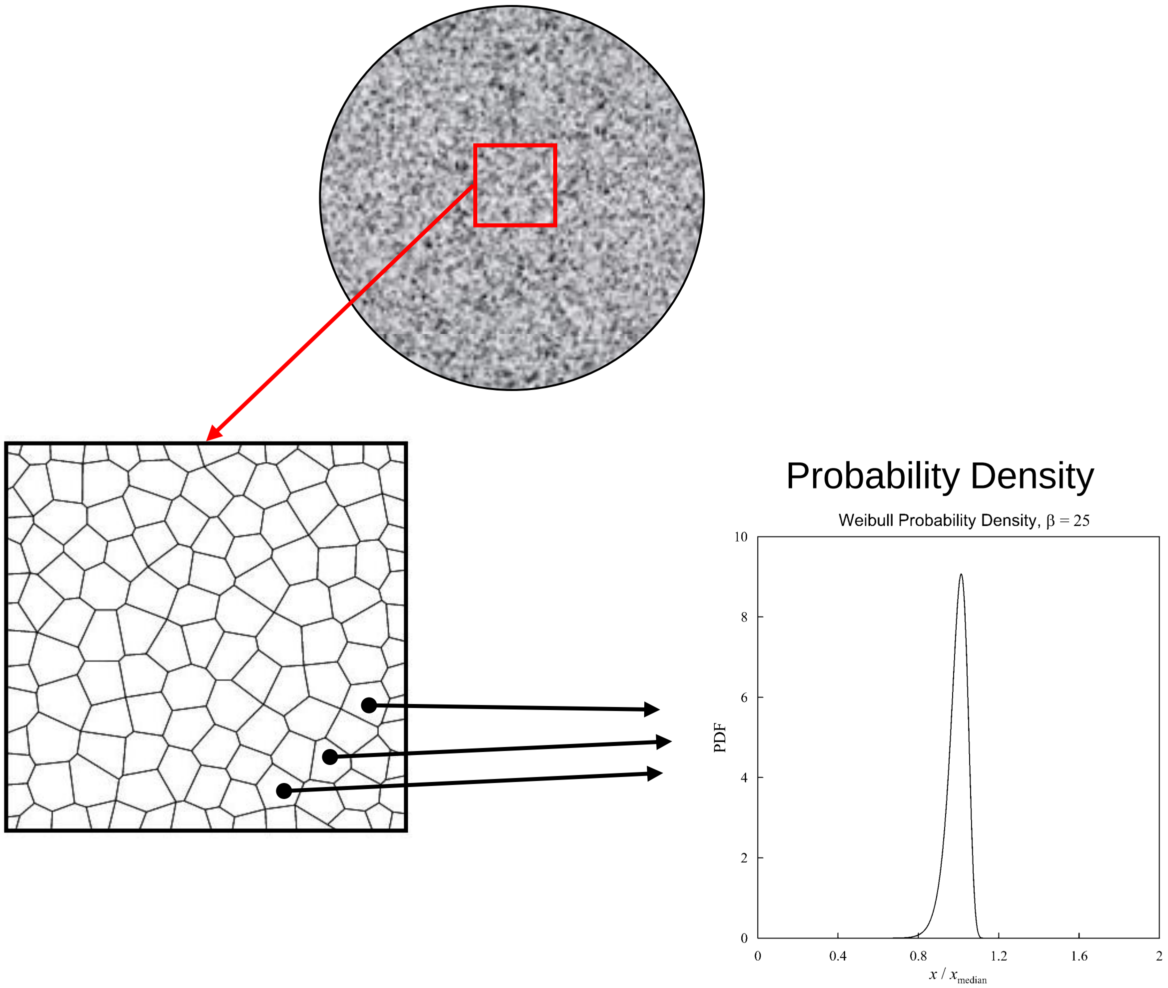
Voronoi Texture Augments Material Variability



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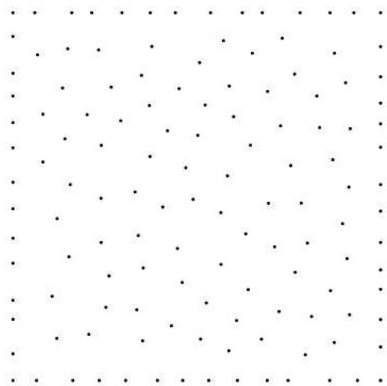
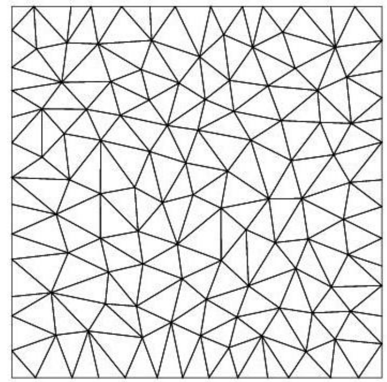
Voronoi Mesh Generation

Bolander, J., Saito, S., 1998, 'Fracture Analyses using Spring Networks with Random Geometry,' *Engineering Fracture Mechanics*, 61, 569-591

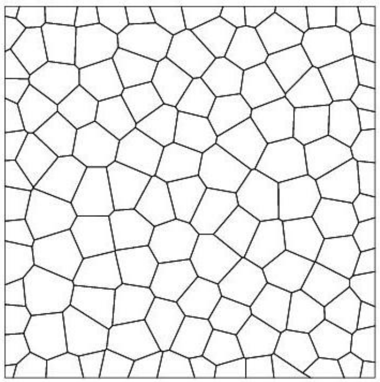


hard core Gibb's process

- constraint on min. dist.
- seed until 'max' packing

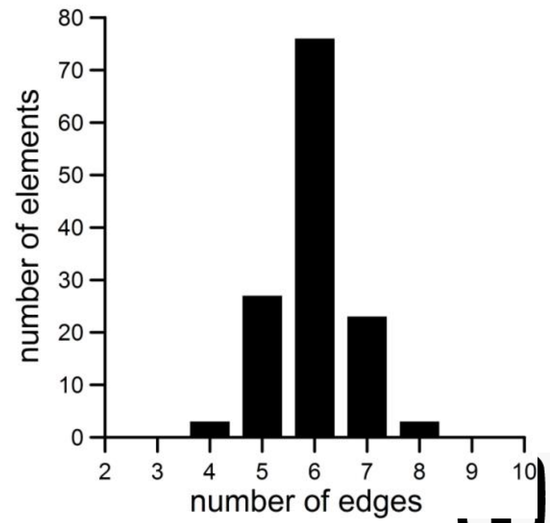


Delaunay triangulation



dual Voronoi

- Note that each Voronoi junction is randomly oriented.
- Most Voronoi junctions are triples.
- Average interior angles are 120°.



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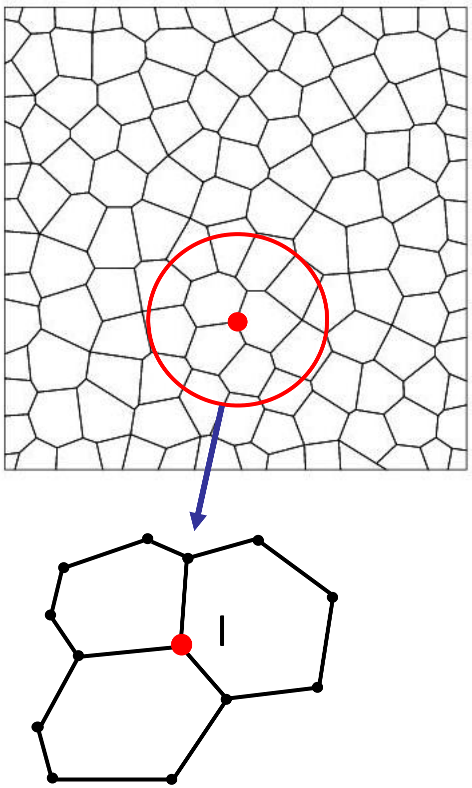
Polyhedral Element Formulation

Use EFG/RKPM methodology to generate shape functions.

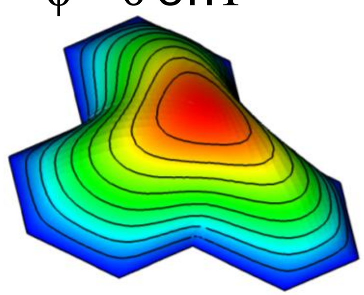
1. Generate nodal *weight* function ϕ by solving Poisson equation on compact support.
2. Generate nodal *shape* function ψ at each integration point using Reproducing Kernel Method.
3. Correct shape function derivatives to satisfy integration consistency (Gauss's theorem).



local support for node I

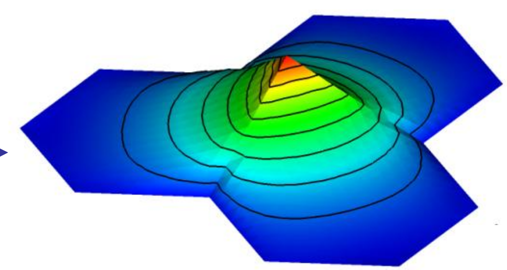
$$\nabla^2\phi + 1 = 0$$

$$\phi = 0 \text{ on } \Gamma$$



weight function ϕ

RKPM methodology →



shape function ψ

Shape Function Integration Consistency

Chen, J.S. et al (2001) ‘A stabalized conforming nodal integration for Galerkin mesh-free methods,’ *International Journal for Numerical Methods in Engineering,* 50, 435-466.

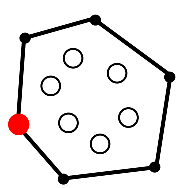
Gauss’s theorem

$$\int_{\Omega_e} \psi_{,i} = \int_{\Gamma_e} \psi\, n_i$$

$$\sum_j w_j \psi^j_{,i} = \sum_j w^\Gamma_j \psi^j n_i$$

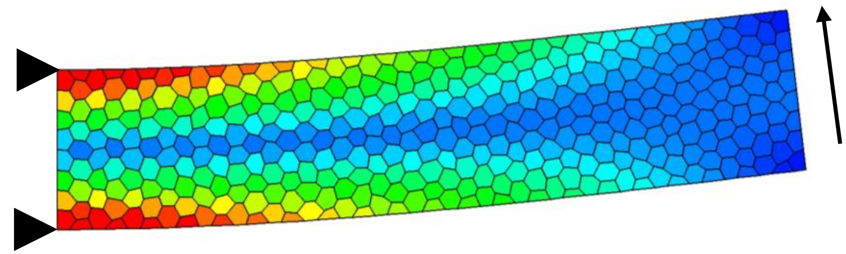
ψ = shape function

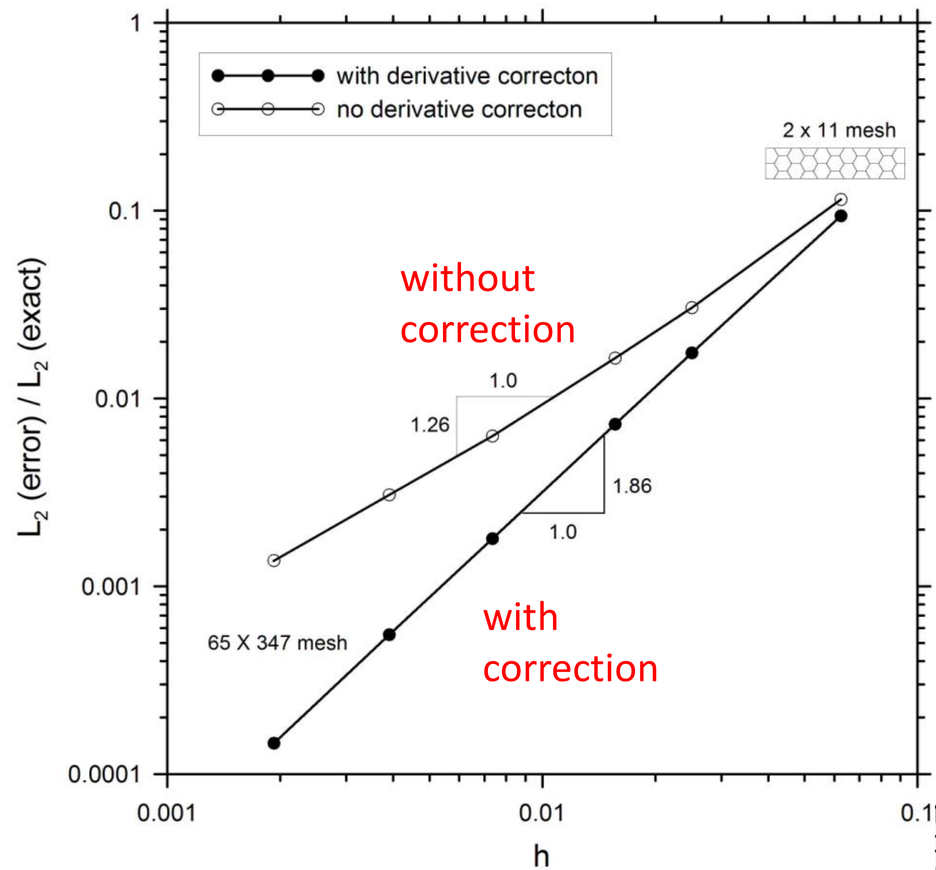
w_j = integration weight,



○ integration point

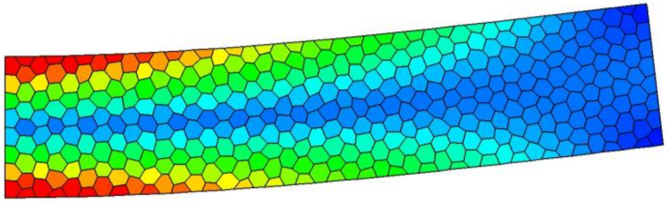
‘Tweak’ $\psi_{,i}$ to satisfy this constraint while maintaining previous properties.





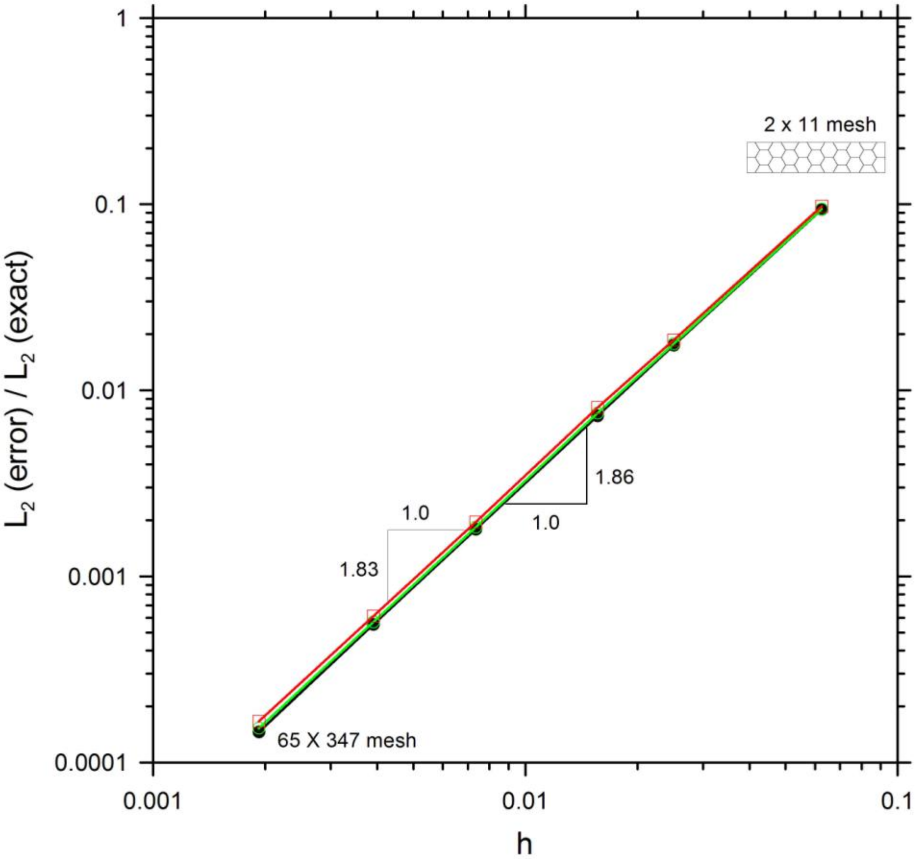
Verification of Convergence

beam with end load



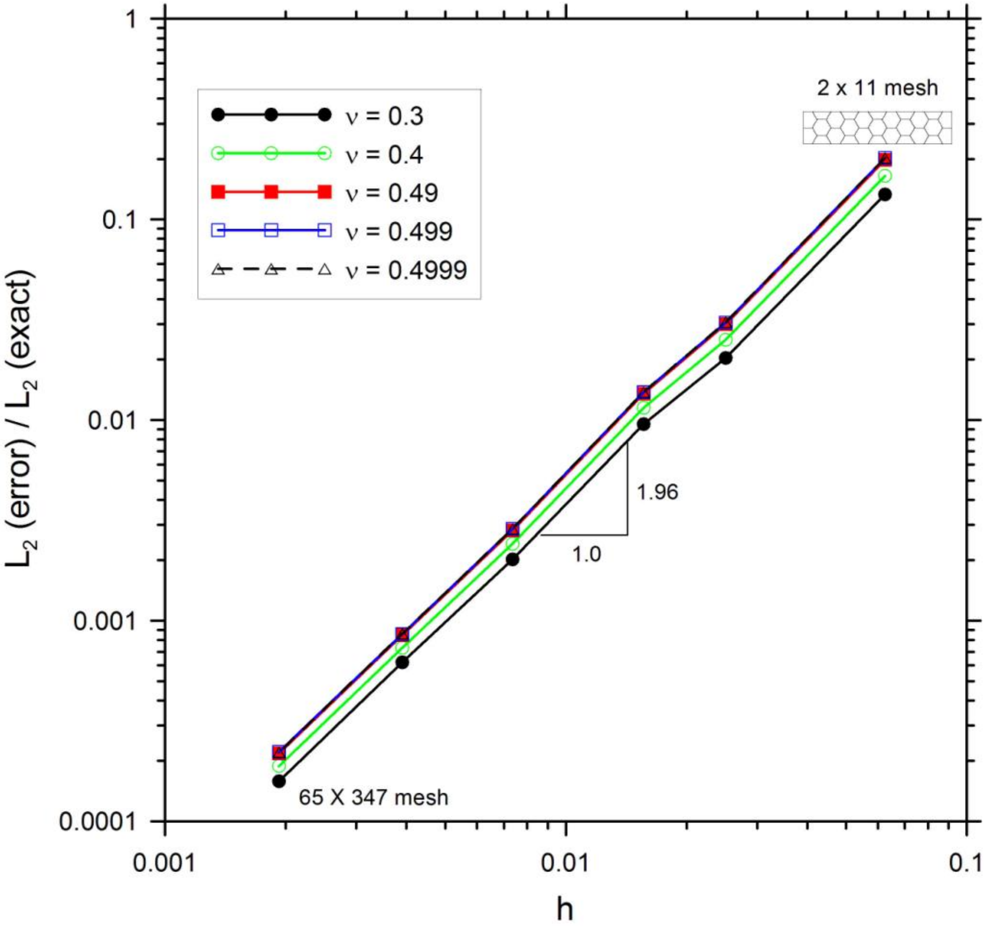
Mises stress field

Error norm vs. mesh size



Mean Dilation Formulation

same as conventional FEM



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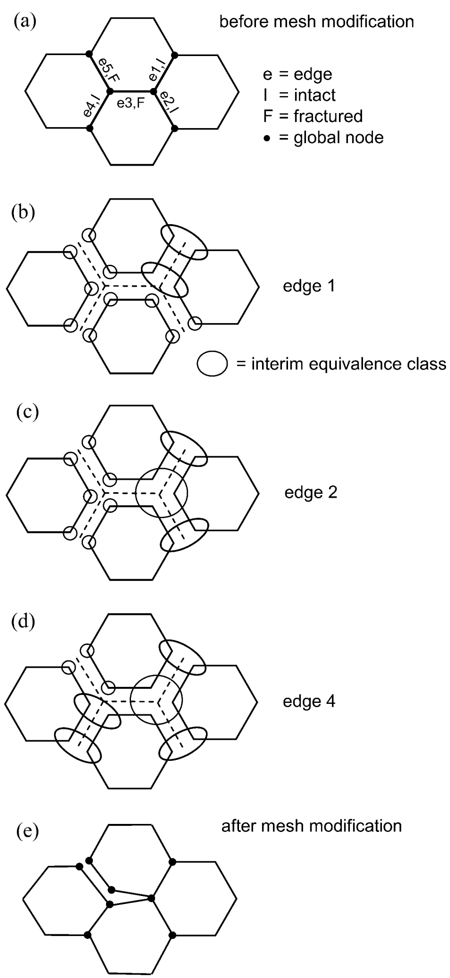
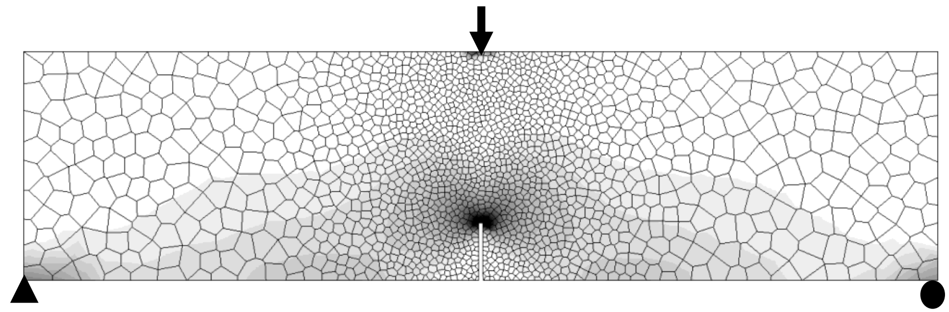
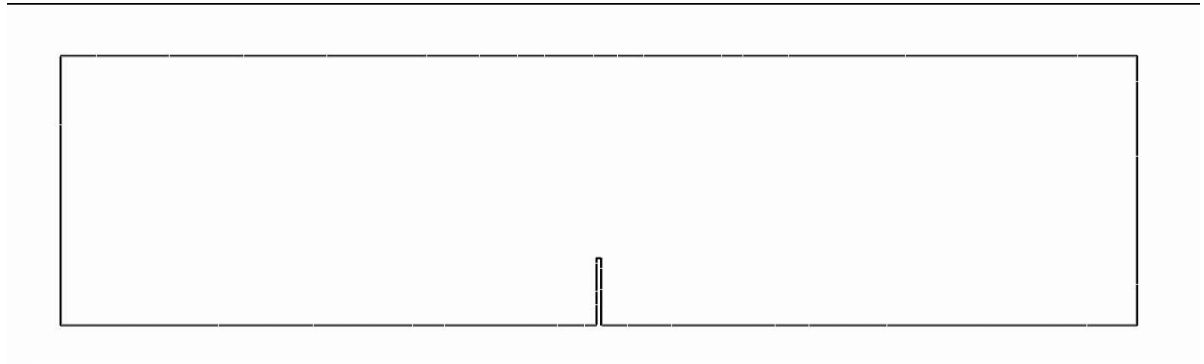
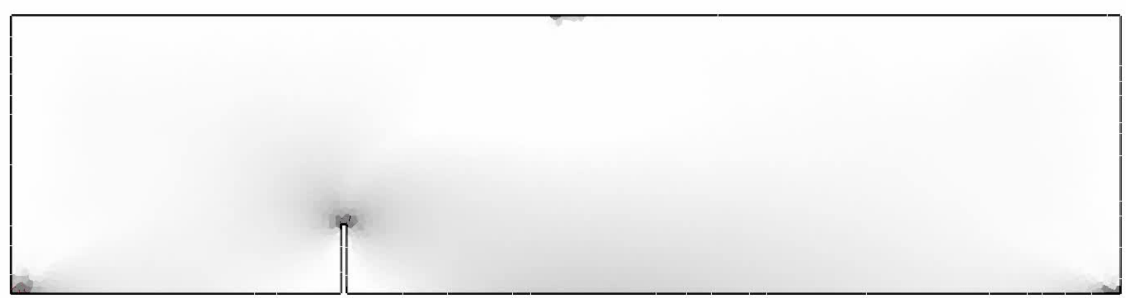
Dynamic Mesh Connectivity

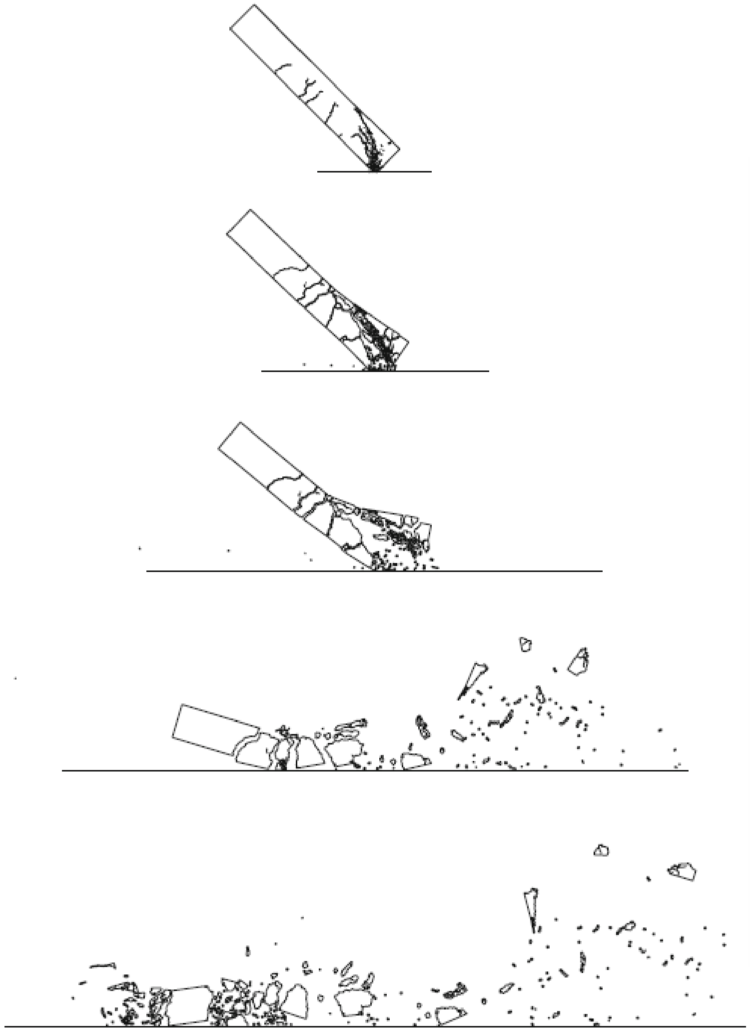


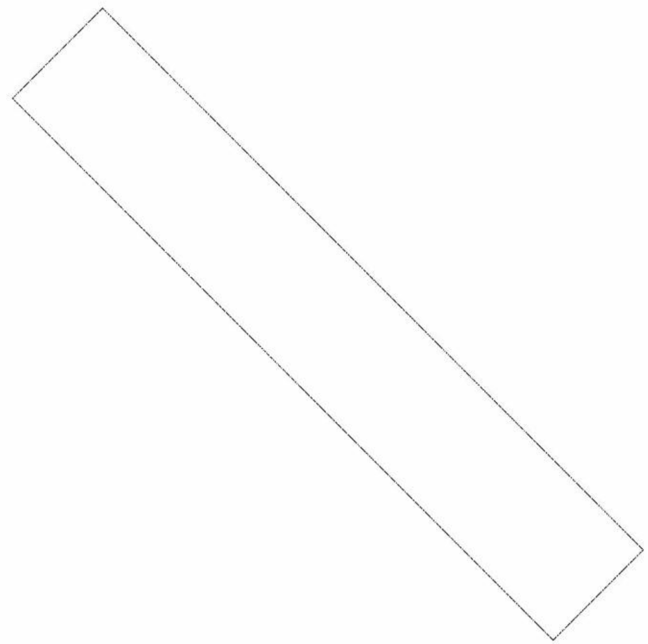




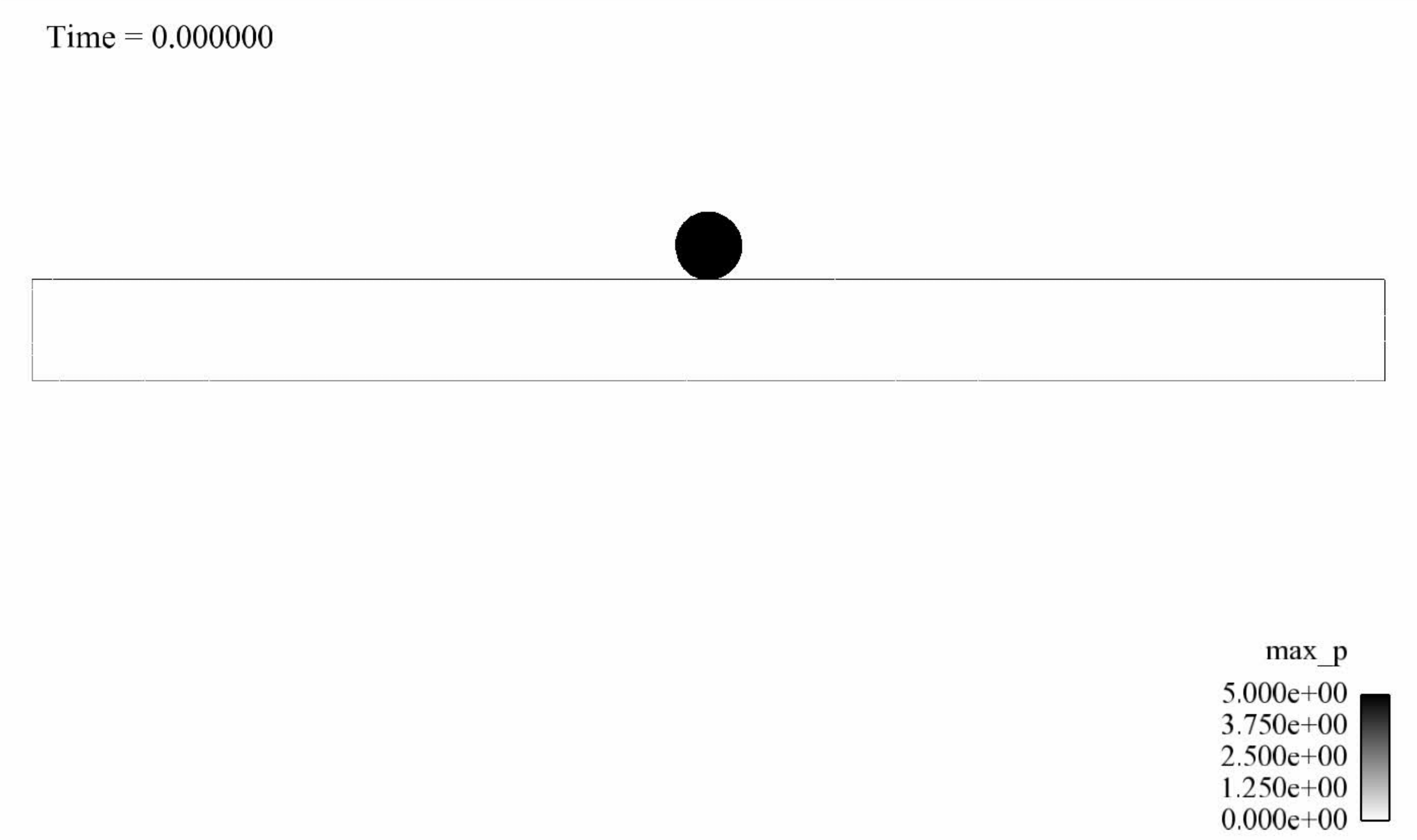


Quasi-Brittle Material Impact





Impact Example



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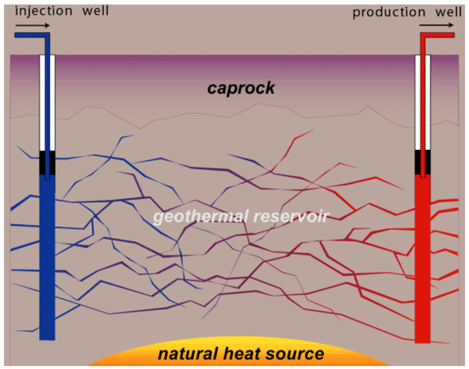
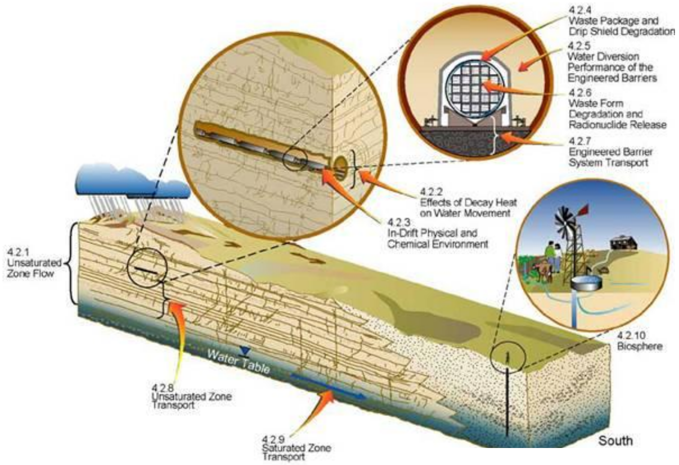
Geo Applications

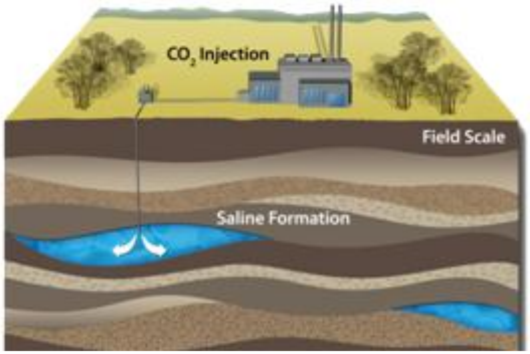
Engineered Geothermal



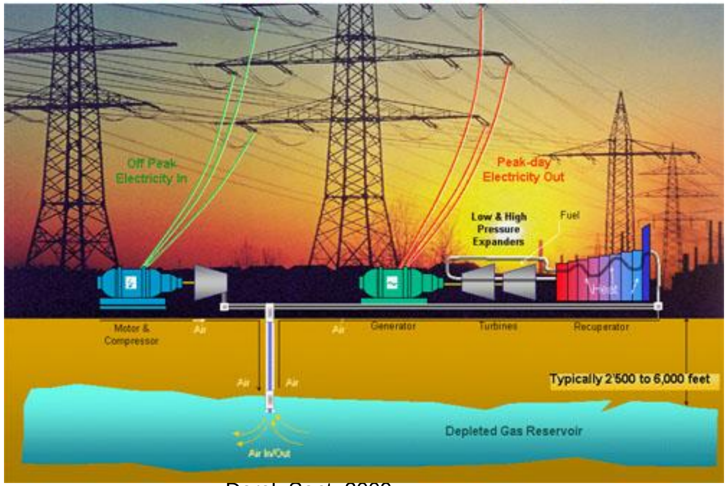
Nuclear Waste Isolation



CO_2 Sequestration

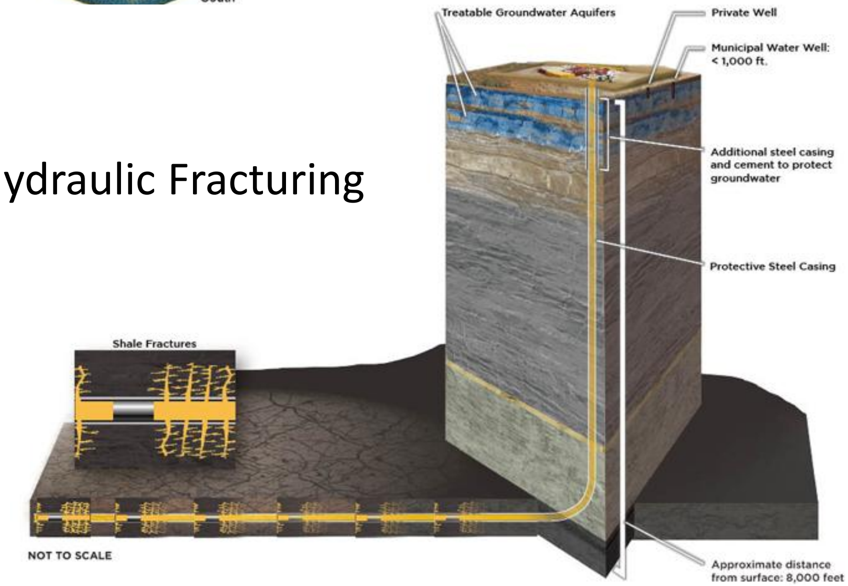


Compressed Air Energy Storage



Derek Sept. 2009

Hydraulic Fracturing



http://www.hydraulicfracturing.com

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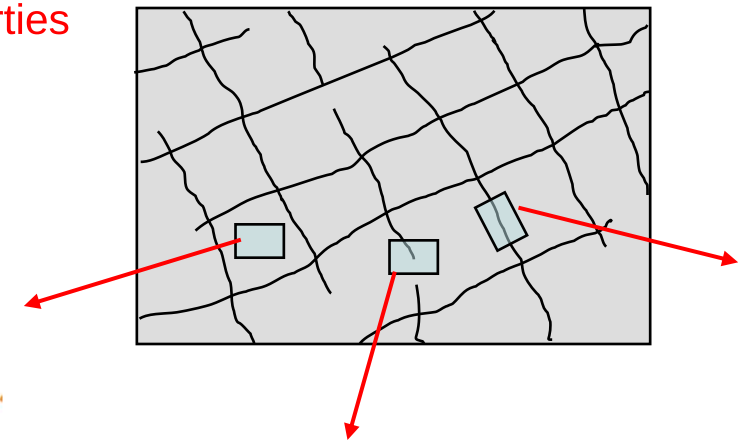
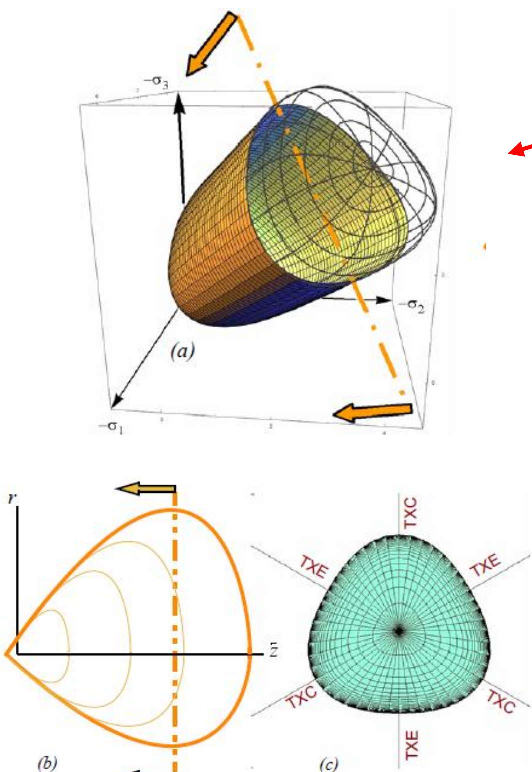
Hydromechanical Coupling in Fractured Rock

Fractured Porous Rock



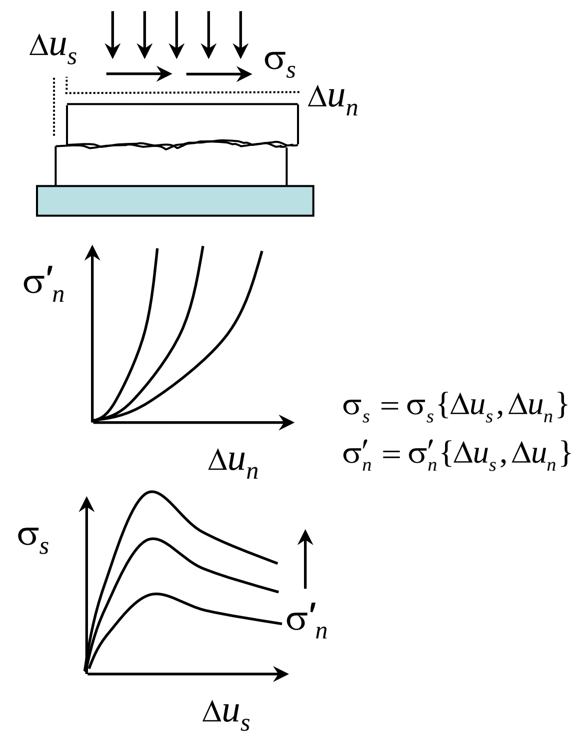
bulk constitutive properties

(Sandia GeoModel
Fossum & Brannon, 2004)

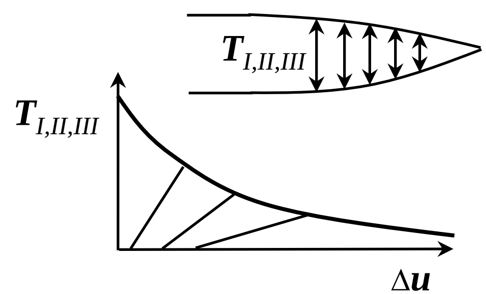


fracture contact properties

$\sigma'_n = \sigma_n - p$



crack-tip cohesive properties



additional challenges

- scale dependence
- history dependence
- precipitation
- dissolution

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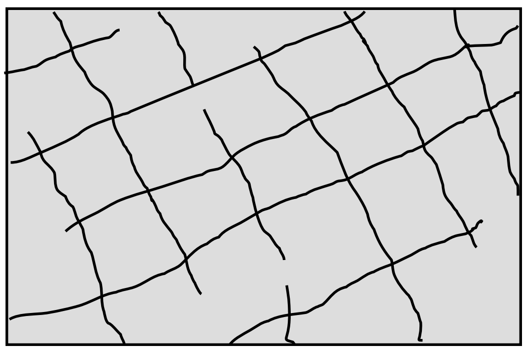
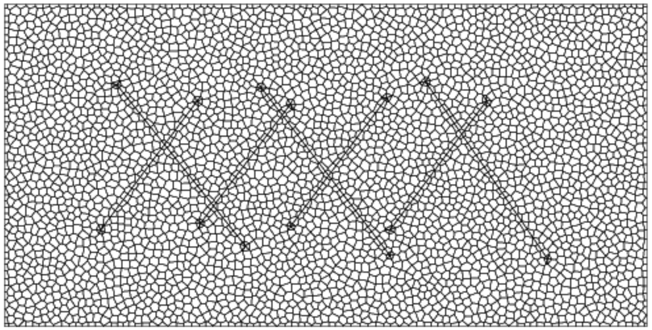
MeshingGenie (Trilinos)

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

Fractured Rock





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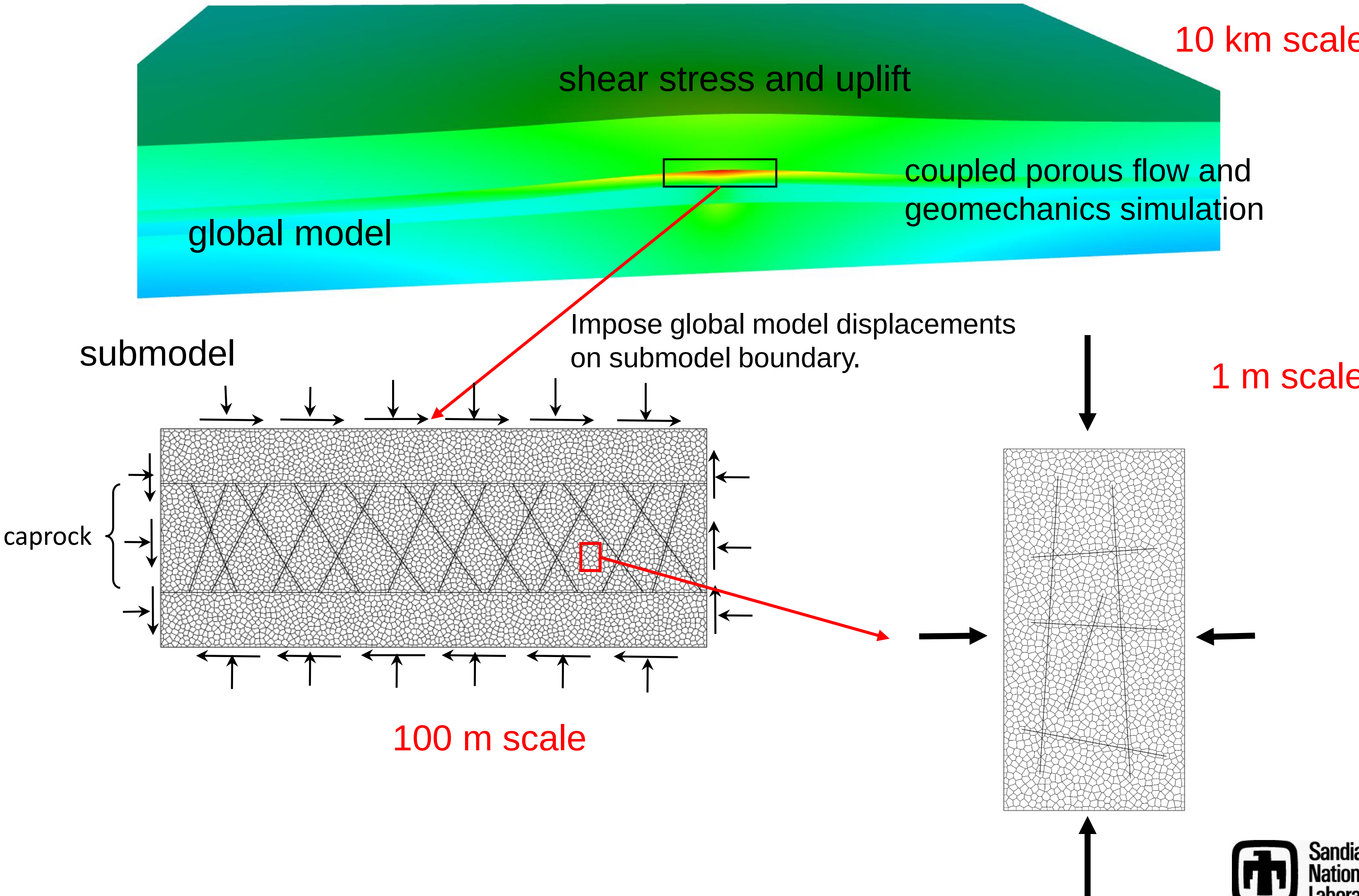
Multiscale analysis of caprock integrity during CO2 injection



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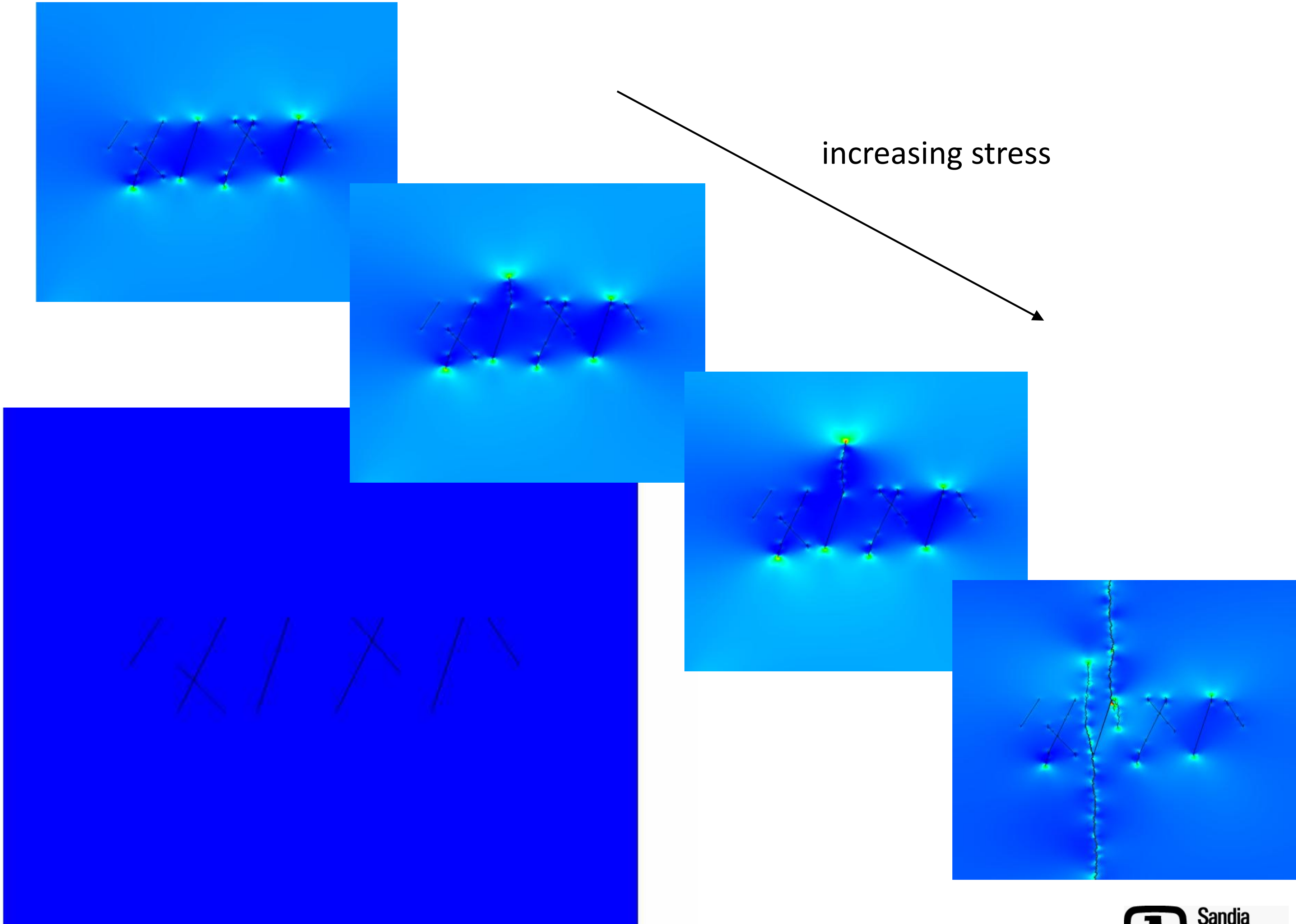

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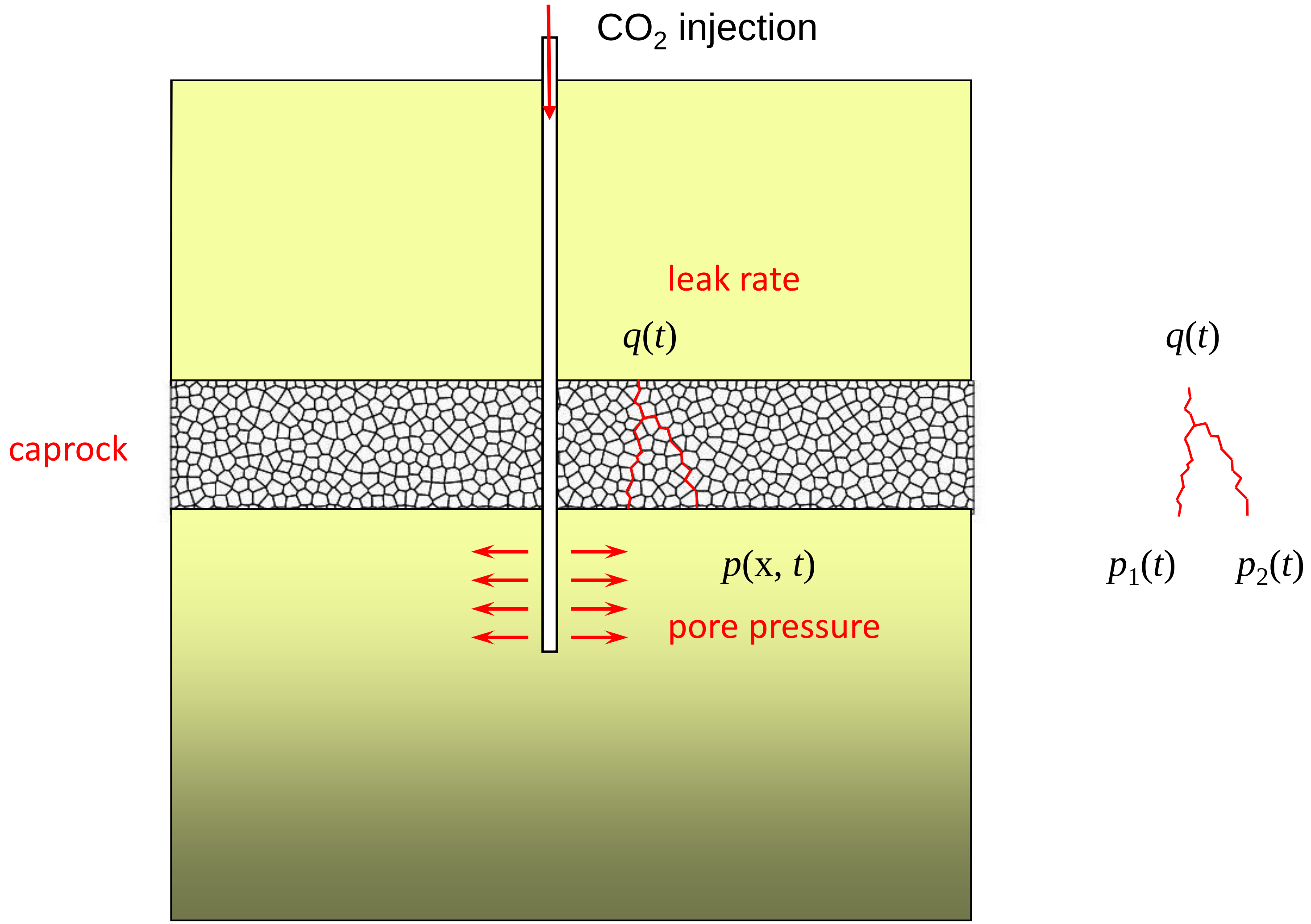
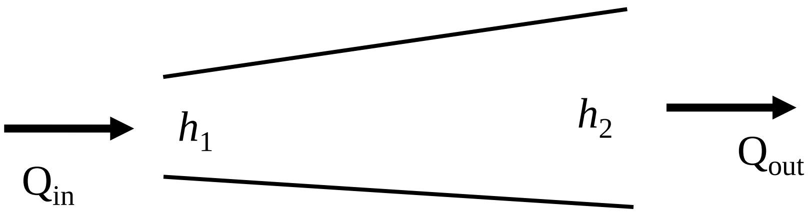
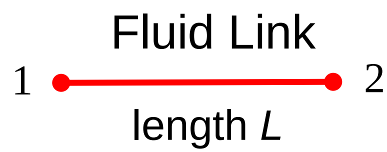
Fluid Flow in 2D Discrete Fracture Networks



Fluid Flow in 2D Discrete Fracture Networks

Solve fluid network to get nodal pressures and flow rates.





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

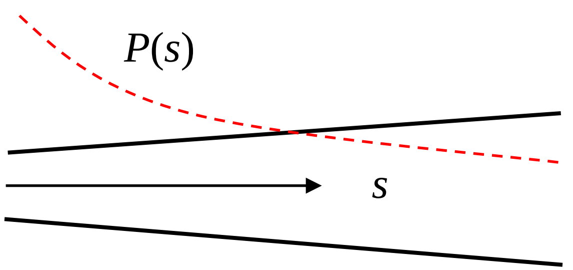
$$T = \frac{h_1^2 h_2^2}{6L} \frac{1}{h_1 + h_2}$$

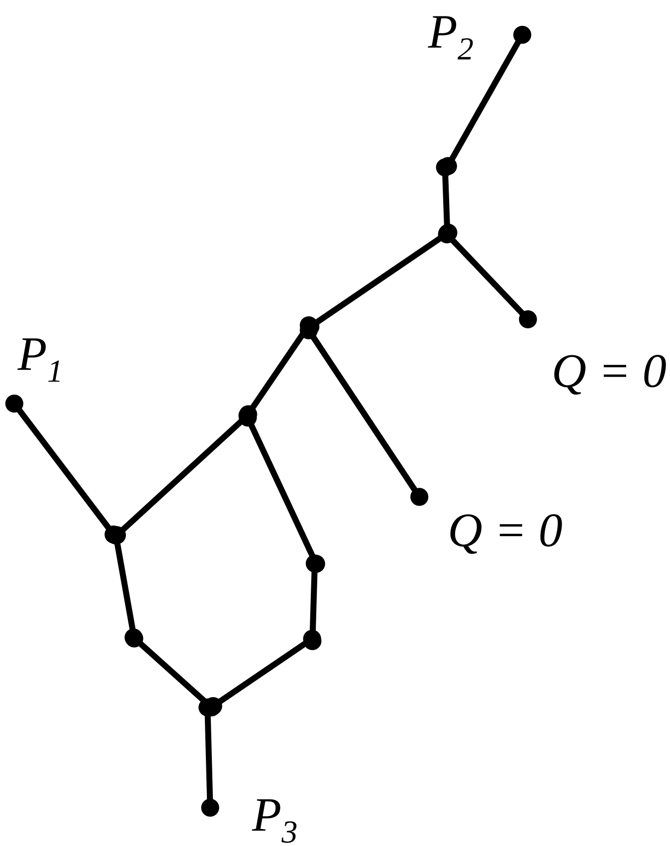
Q = flow rate
P = pressure
μ = viscosity
T = transmissibility

Reynold's lubrication equation

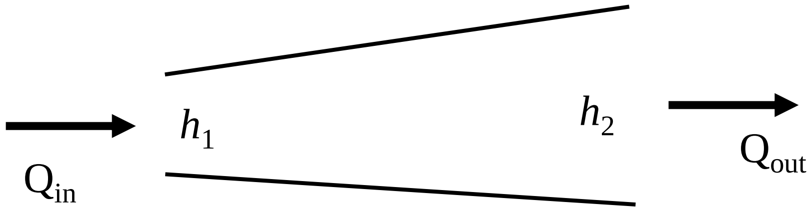
$$\nabla(\rho \mathbf{Q}) = 0$$

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





Fluid Flow in Discrete Fracture Networks



Reynold's lubrication equation

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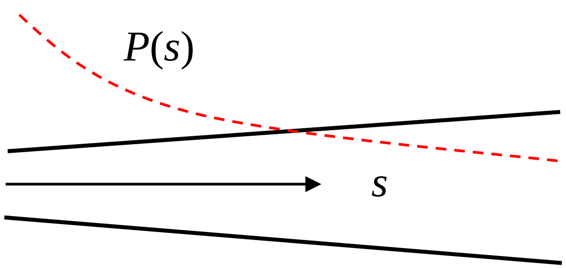
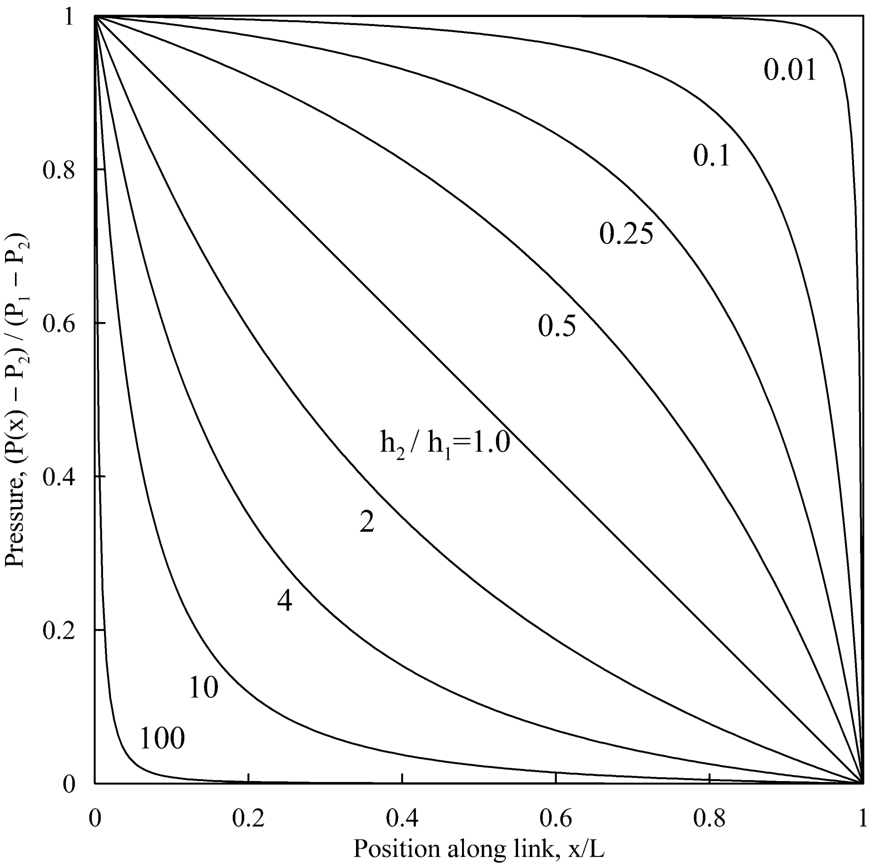
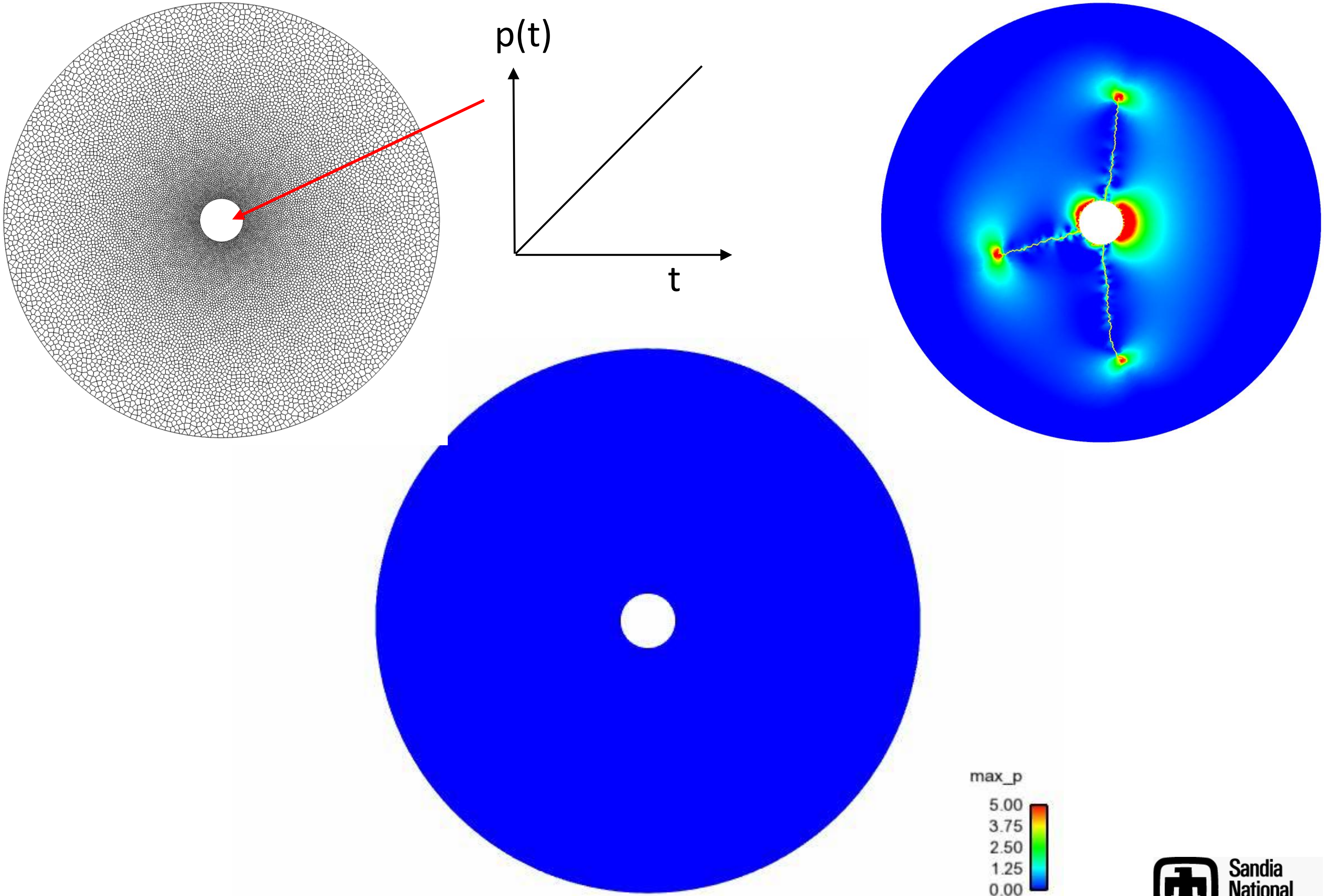
$$\mathbf{Q} = -\frac{h^3}{12\mu}(\nabla p - \rho g h)$$





Hydraulic Fracture Simulation



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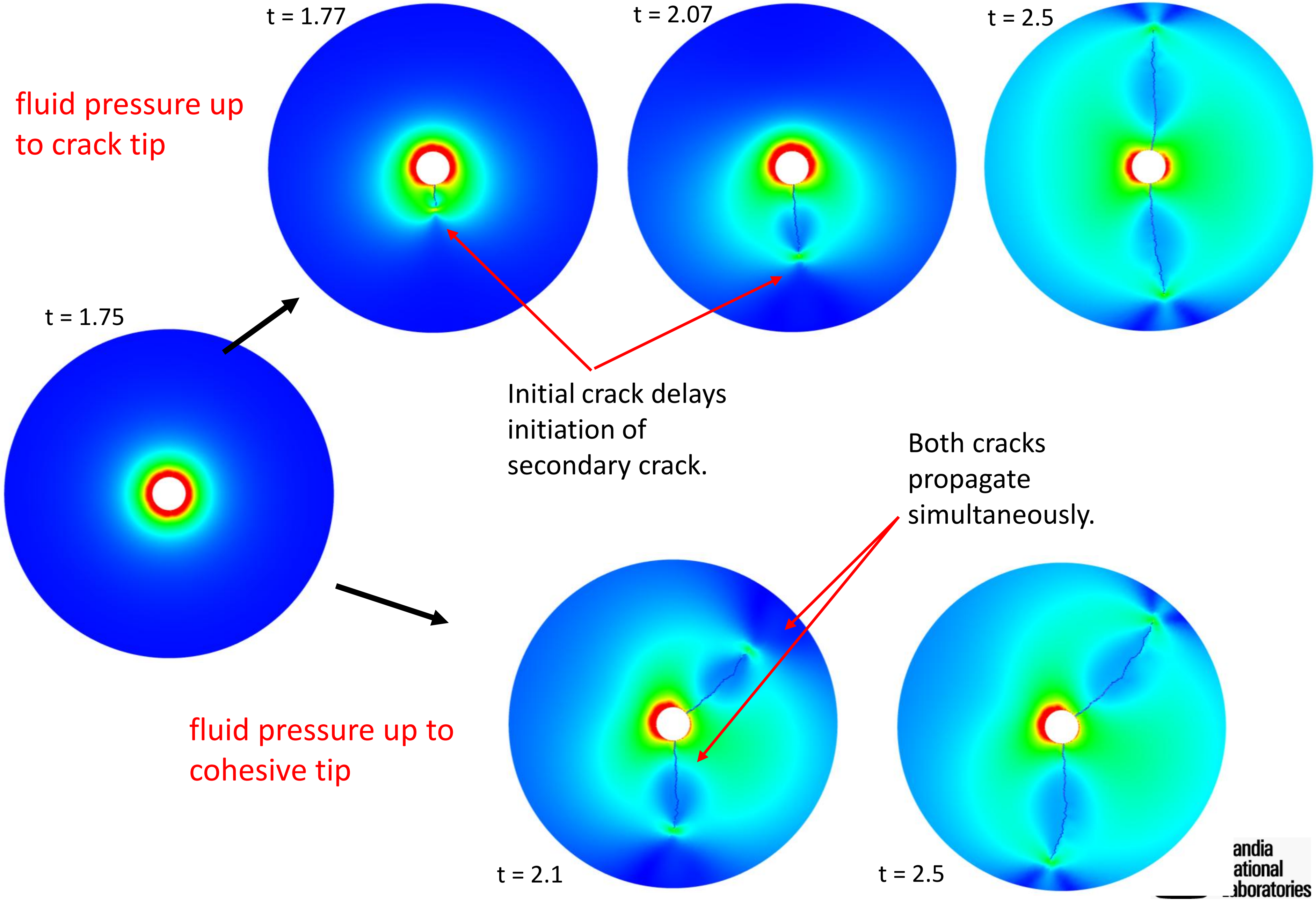
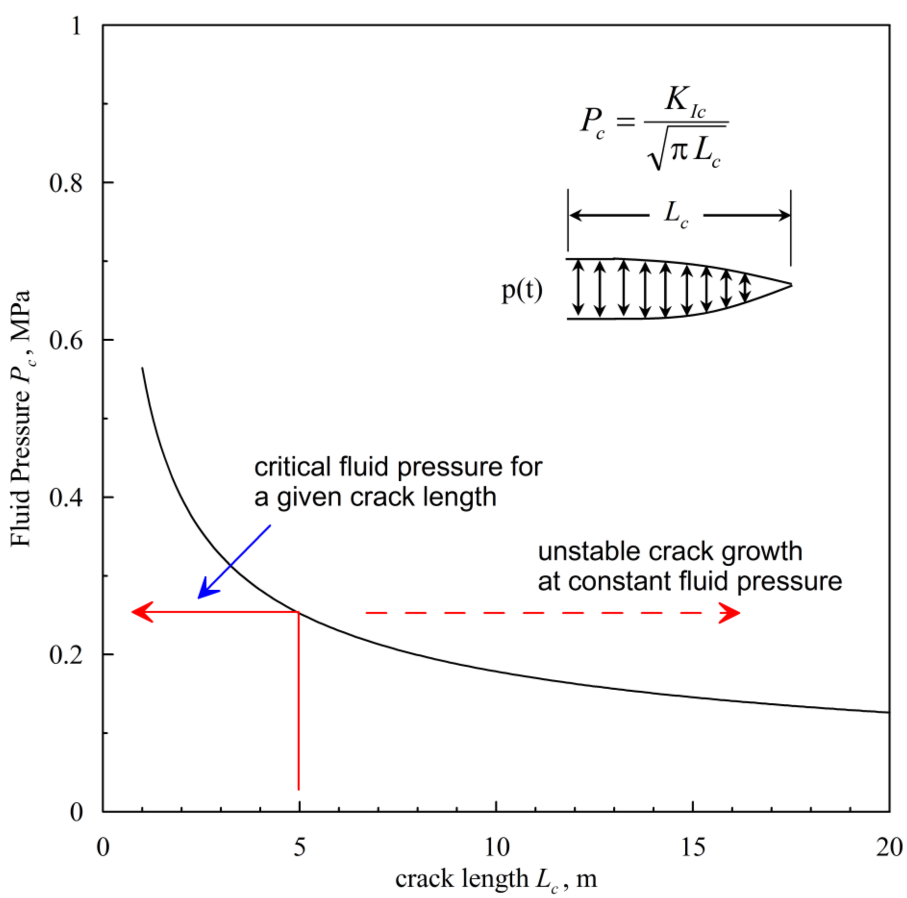
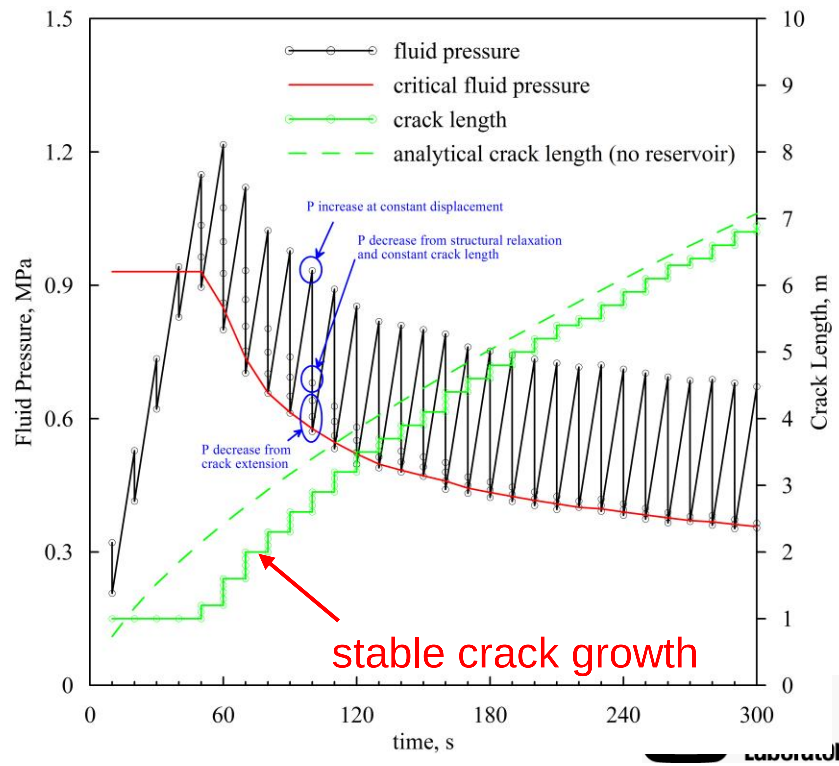


Hydraulic Fracture Simulation

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



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



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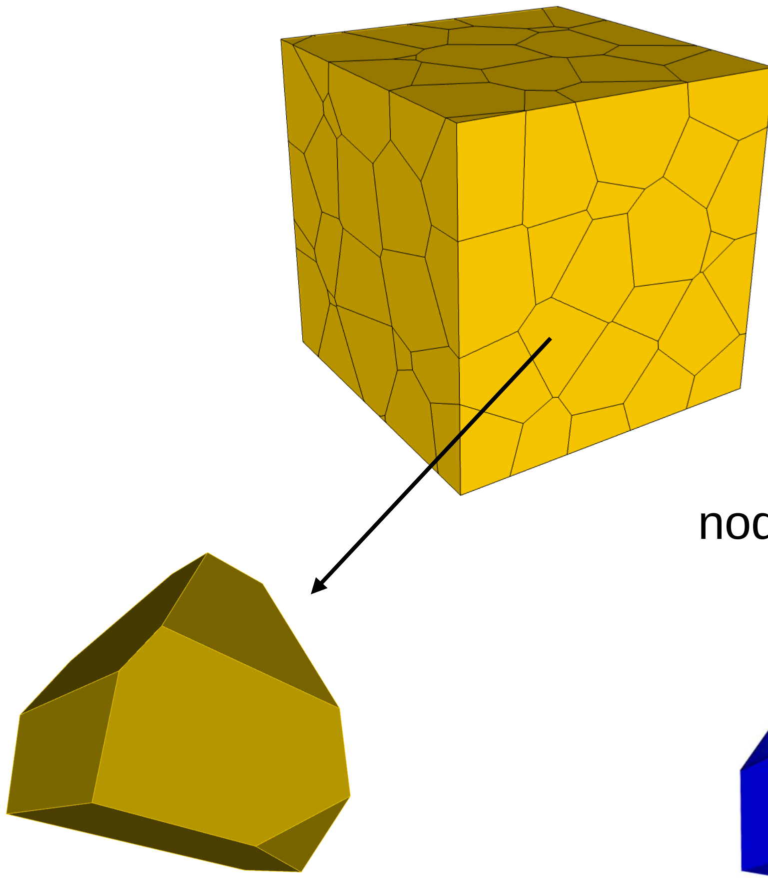
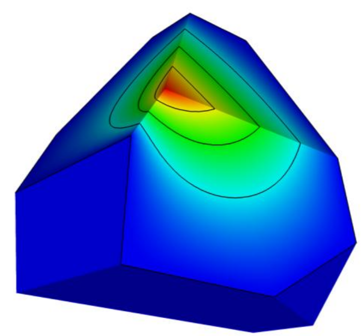
3D Element Formulation



nodal shape function



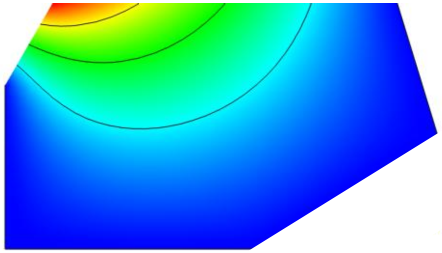
Harmonic Functions

A harmonic function is a solution of Laplace's equation.

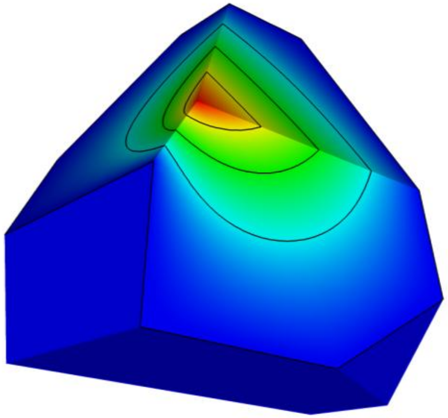
$$\nabla^2 \varphi = 0 \quad \text{or} \quad \frac{\partial^2 \varphi}{\partial x^2} + \frac{\partial^2 \varphi}{\partial y^2} + \frac{\partial^2 \varphi}{\partial z^2} = 0$$

Can solve efficiently using BEM, or can just use FEM.

example in 2D



example in 3D



A subset of a broader notion of "energy minimizing" functions.

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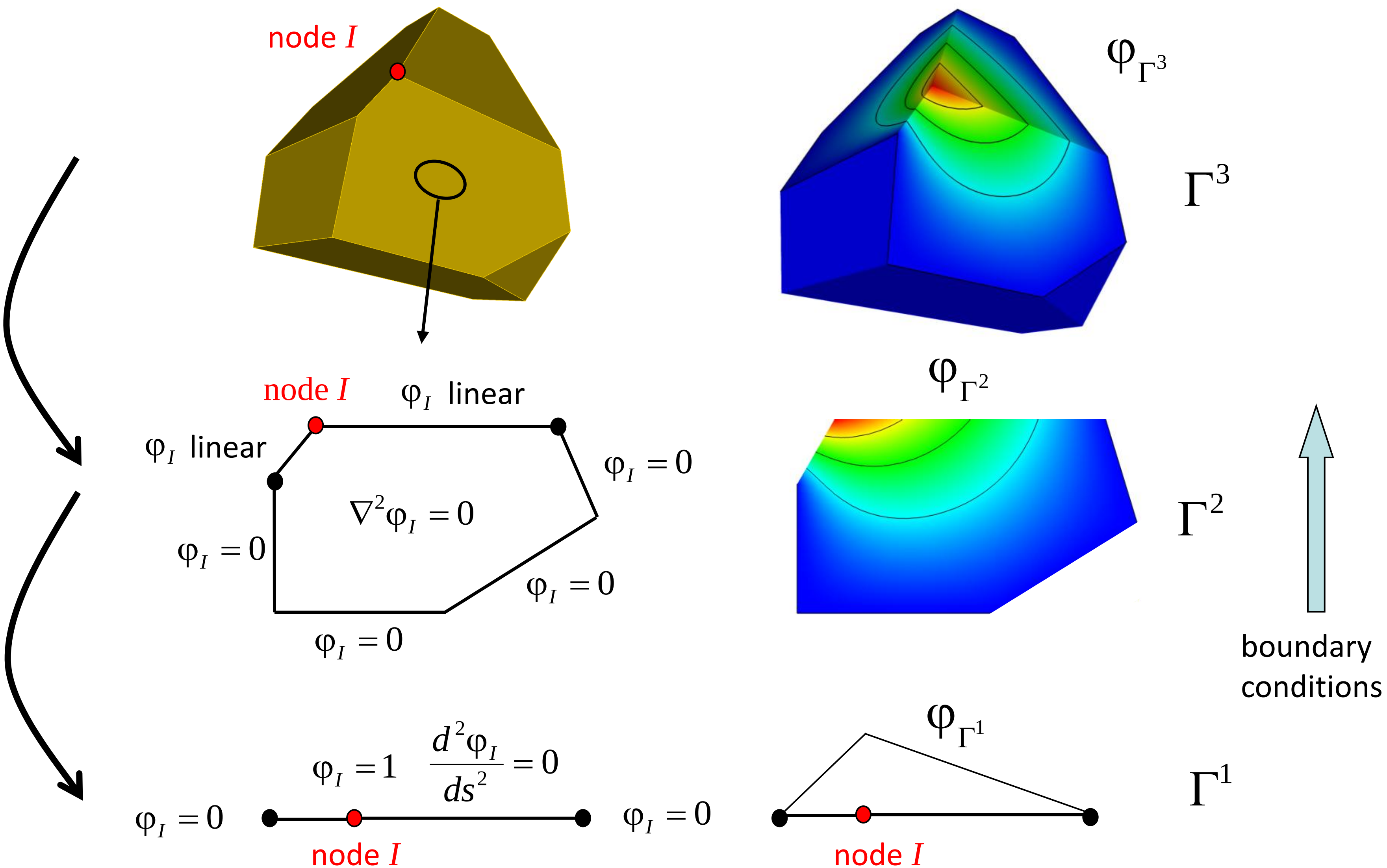
Construction of Harmonic Shape Functions in 3D

(Joshi, 2007, “Harmonic coordinates for character articulation”)



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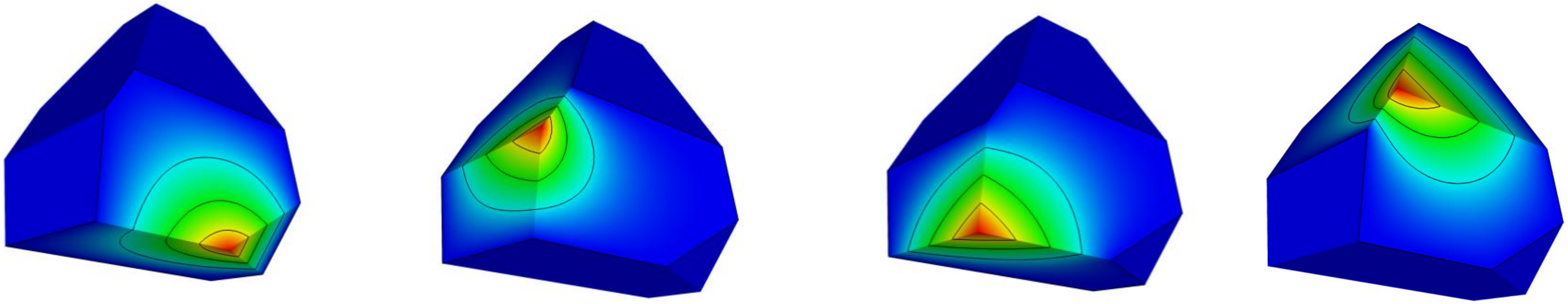
Harmonic Shape Function Properties

- partition of unity and reproduce space $\sum_I \psi_I(\mathbf{x}) = 1, \quad \sum_I \psi_I(\mathbf{x})\ \mathbf{x}_I = \mathbf{x}$

  even for the discrete harmonic solution $\sum_I \psi_I^h(\mathbf{x}) = 1, \quad \sum_I \psi_I^h(\mathbf{x})\ \mathbf{x}_I = \mathbf{x}$

- Kronecker delta property at nodes $\psi_I(\mathbf{x}_J) = \delta_{IJ}$
- linear on edges (low order)
- shape functions defined on original configuration (no mapping to 'parent' shape)



shape functions

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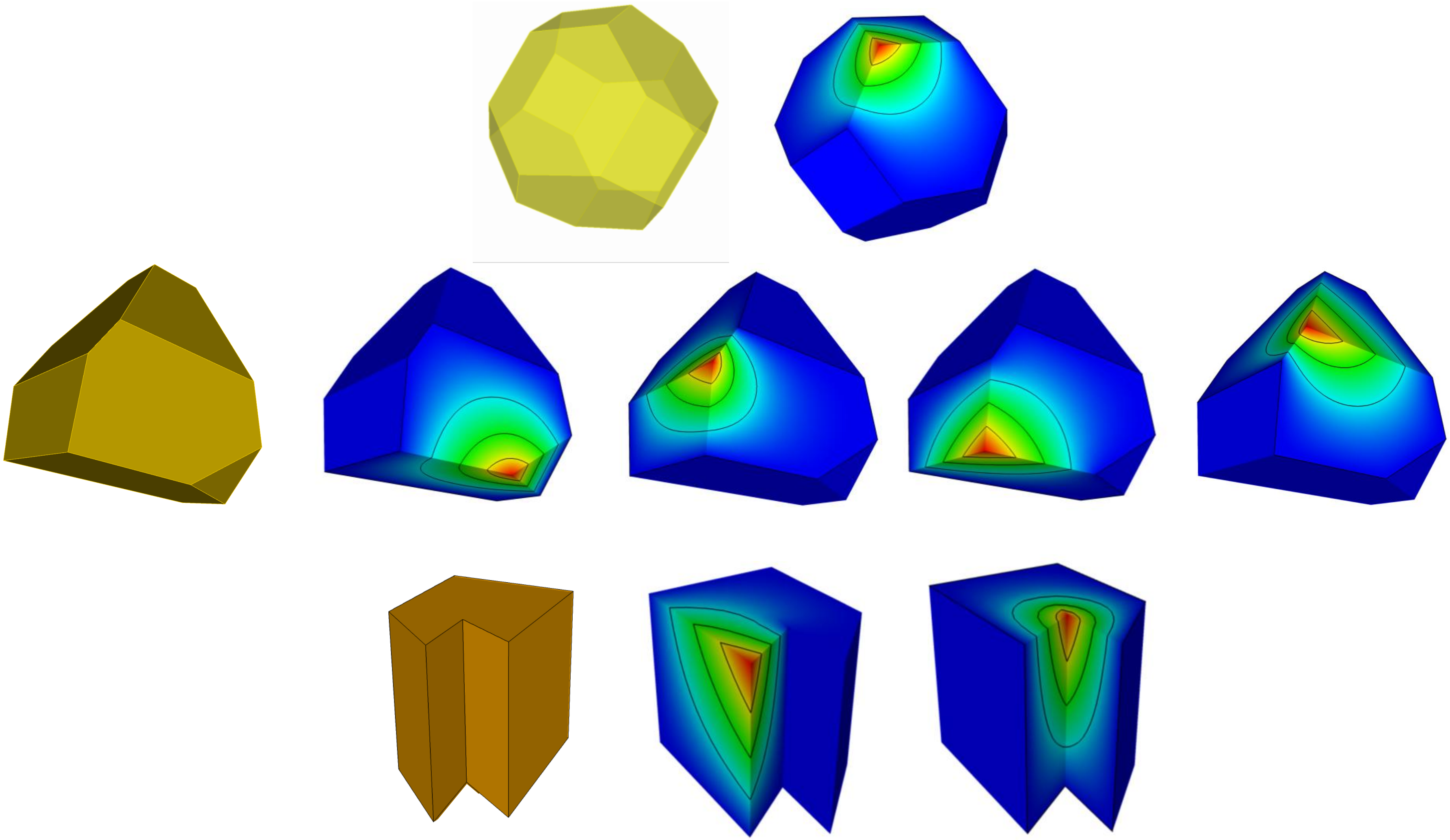
Harmonic Shape Function Examples



Only need to store shape functions and derivatives at integration points.
Discard everything else.

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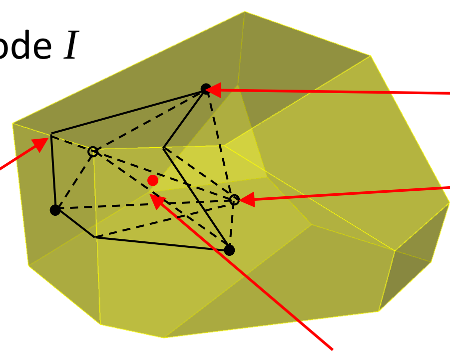
Element Integration

- Due to computational expense of plasticity models, want to minimize the number of integration points.
- Follow approach of Rashid and Selimotec, 2006.
- Each node is associated with a “tributary” volume, connected to the centroid. (more general approaches for non “star-haped” elements.
- Number of integration points is equal to the number of vertices.



$$\int_{\Omega^e} f \, d\Omega^e \approx \sum_{k=1}^{M} w_k \, f(\mathbf{x}_k)$$

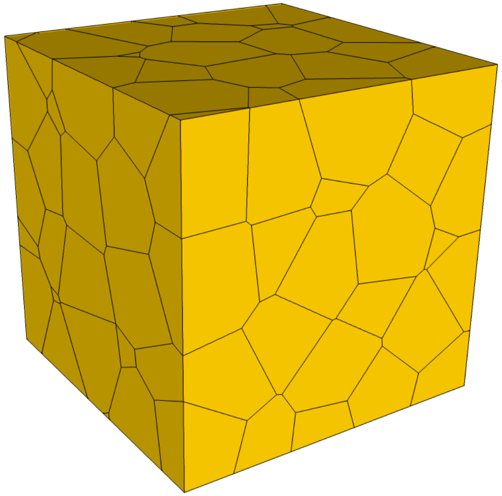
integration point $\mathbf{x}_k$ = centroid of tributary volume

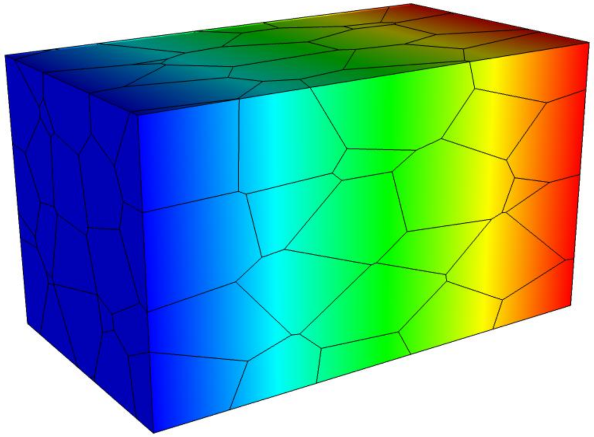
integration point weight w_k = tributary volume

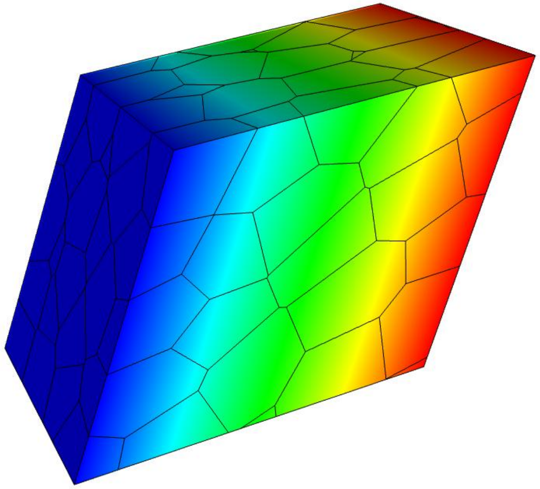
- Integration is only first order accurate.
- Sufficient to eliminate any zero energy modes.

However, can’t pass the patch test with this low-order integration.

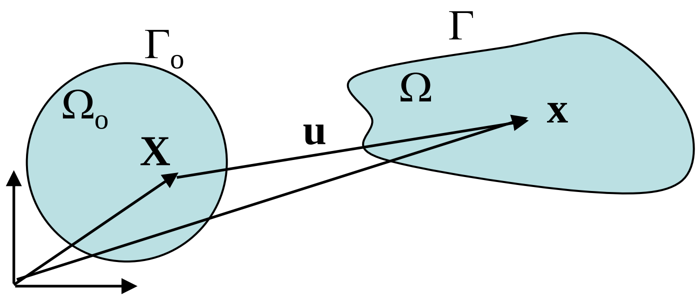
3D Verification: Engineering Patch Test







What About Large Deformations?



- Shape functions, their derivatives, and the integration points were defined in the initial configuration (Ω_o, Γ_o).
- All integrations of the weak form are from the original configuration (total-Lagrangian formulation).

momentum strong form

$$\frac{\partial \mathbf{P}}{\partial \mathbf{X}} : \mathbf{I} + \rho_o \mathbf{f} = \rho_o \ddot{\mathbf{u}}$$

$\mathbf{P}$ is the first Piola-Kirchhoff stress tensor.
$\mathbf{X}$ is the position vector of a material point.
$\mathbf{x}$ is the spatial vector.
$\mathbf{u} = \mathbf{x} - \mathbf{X}$, is the displacement vector
$\mathbf{f}$ is the body force vector per unit mass.

momentum weak form

$$\int_{\Omega_o} \rho_o \ddot{\mathbf{u}} \cdot \delta \mathbf{u} \, d\Omega_o = \int_{\Gamma_o} \mathbf{t}_o \cdot \delta \mathbf{u} \, d\Gamma_o + \int_{\Omega_o} \rho_o \mathbf{f} \cdot \delta \mathbf{u} \, d\Omega_o - \int_{\Omega_o} \rho_o \mathbf{P} : (\partial(\delta \mathbf{u})/\partial \mathbf{X}) \, d\Omega_o$$

However, most material models are hypoelastic.

deformation gradient

$$F = \frac{\partial \mathbf{x}}{\partial \mathbf{X}} \quad (3\times3)$$

rate of deformation

$$\frac{\partial \mathbf{v}}{\partial \mathbf{x}} = \frac{\partial \mathbf{v}}{\partial \mathbf{X}} F^{-1}$$

PK1 stress

$$P = J \, \sigma \, F^{-T}$$
$$J = \det(F)$$

Cauchy stress

$$\sigma = J^{-1} P \, F^{T}$$

Lots of multiplications by F and F^{-1}

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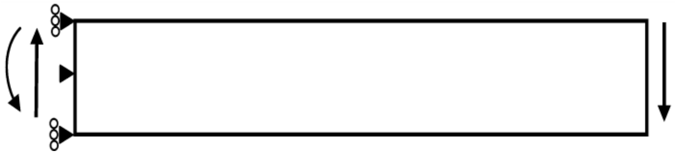
Verification Test: Beam with a Transverse End-Load



3D exact linear elasticity solution, (Barber, 2010)

$$\sigma_{xx} = \sigma_{yy} = \sigma_{xy} = 0$$

$$\sigma_{zz} = \frac{F_y}{I_x} yz$$

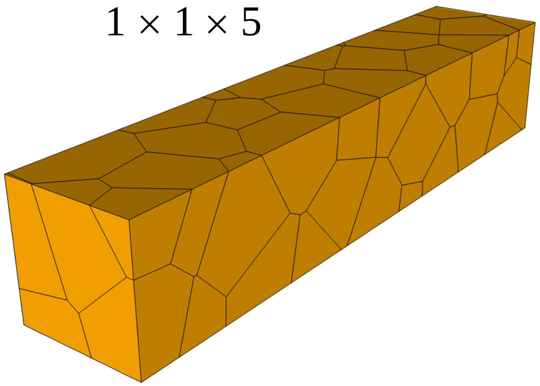
$$\sigma_{xz} = \frac{2F_y a^2}{\pi^2 I_x} \frac{\nu}{1+\nu} \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \sin\left(\frac{n\pi x}{a}\right) \frac{\sinh\left(\frac{n\pi y}{a}\right)}{\cosh\left(\frac{n\pi b}{a}\right)}$$

$$\sigma_{yz} = \frac{F_y}{I_x} \left\{ \frac{1}{2}(b^2 - y^2) + \frac{1}{6}(3x^2 - a^2) \frac{\nu}{1+\nu} - \frac{2a^2}{\pi^2} \frac{\nu}{1+\nu} \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \sin\left(\frac{n\pi x}{a}\right) \frac{\sinh\left(\frac{n\pi y}{a}\right)}{\cosh\left(\frac{n\pi b}{a}\right)} \right\}$$

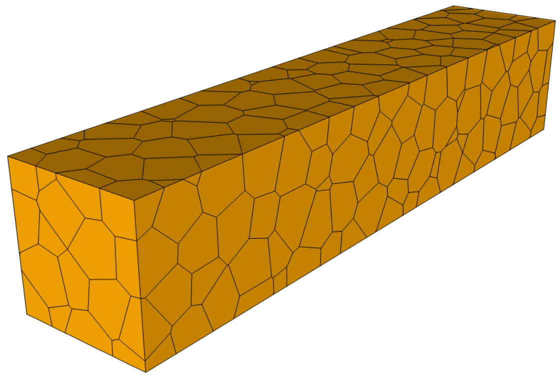
From this stress field → strain field → integrate to get displacement field using compatibility equations.

Randomly Close-Packed Voronoi Meshes

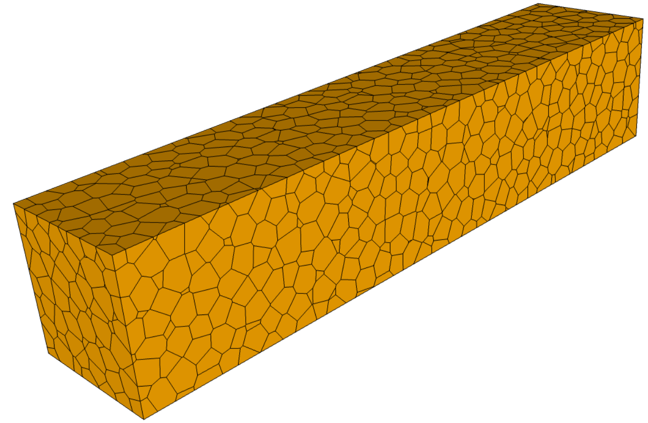
beam dimension = $1 \times 1 \times 5$



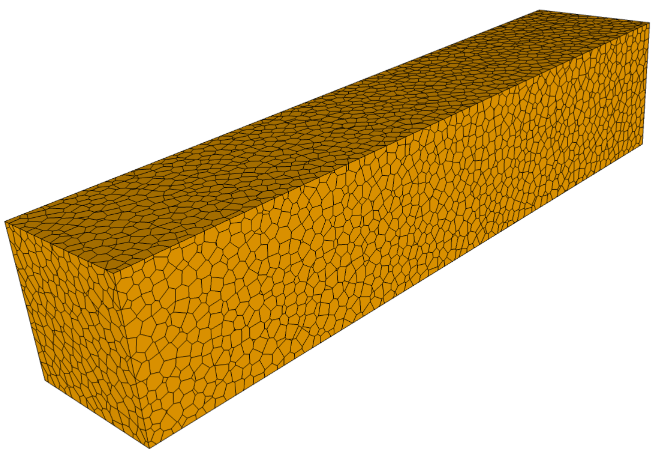
point spacing = 0.5



point spacing = 0.25

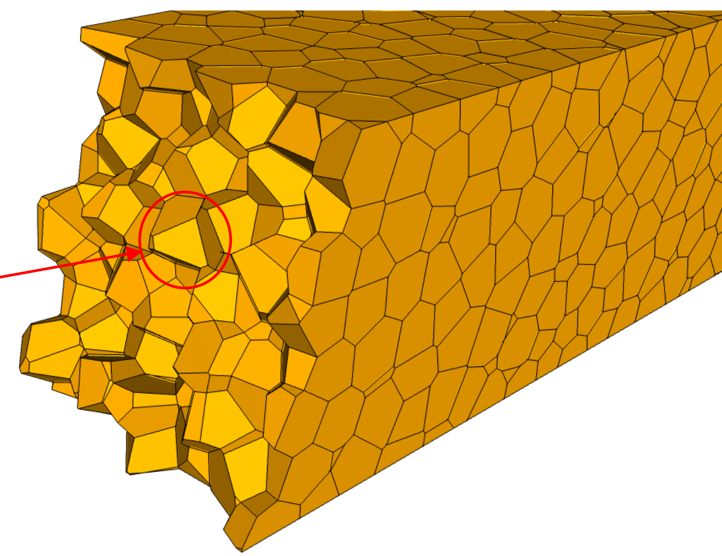


point spacing = 0.125

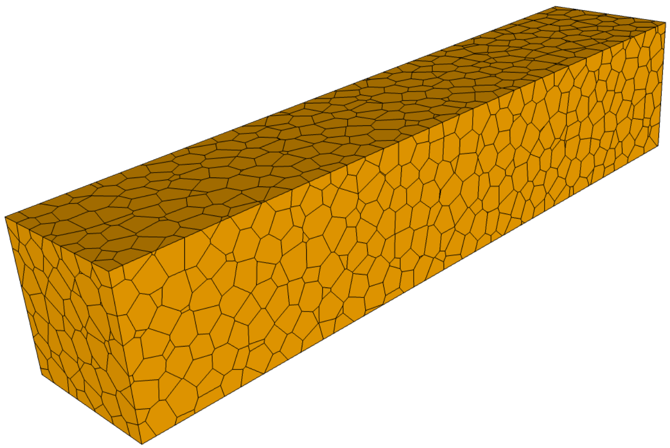


point spacing = 0.0625

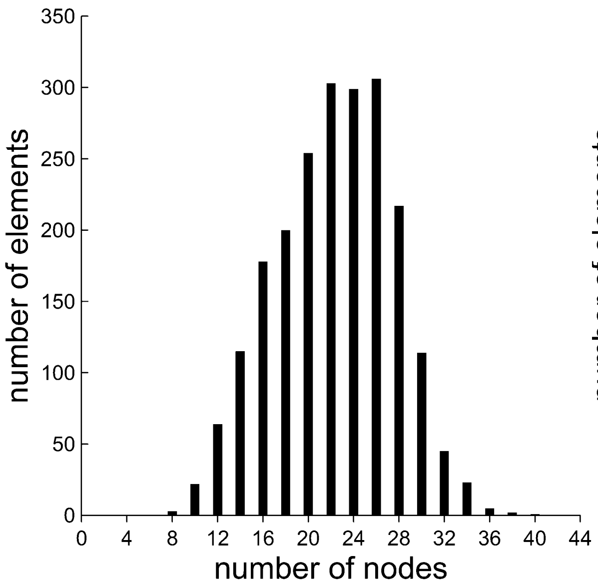
minimum edge to diameter ratio = 10^{-4}

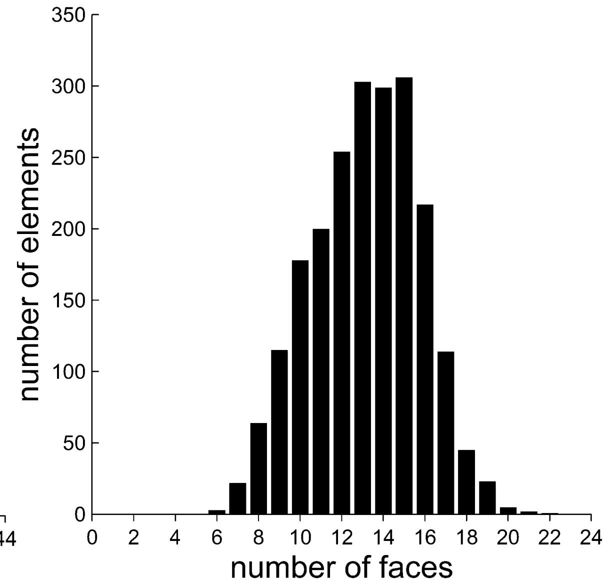


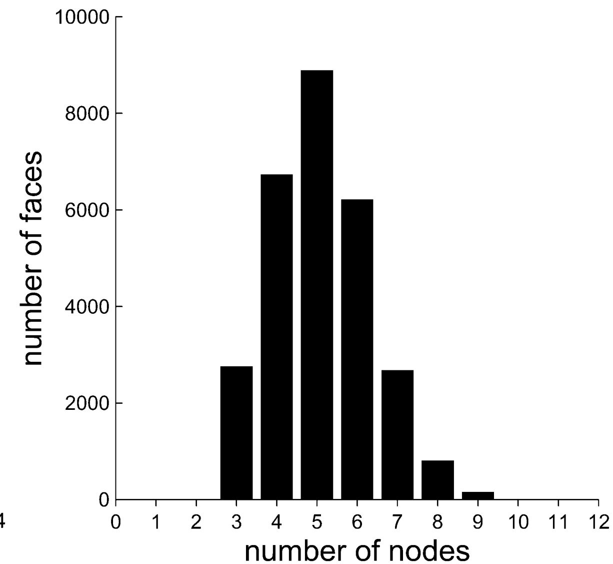
Randomly Close-Packed Voronoi Meshes



mesh statistics







median 24 nodes per element

median 14 faces per element

median 5 nodes per face

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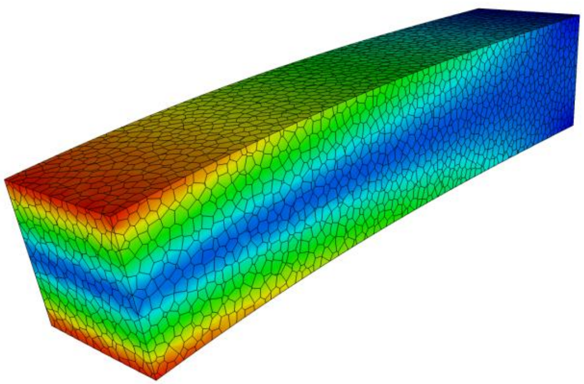
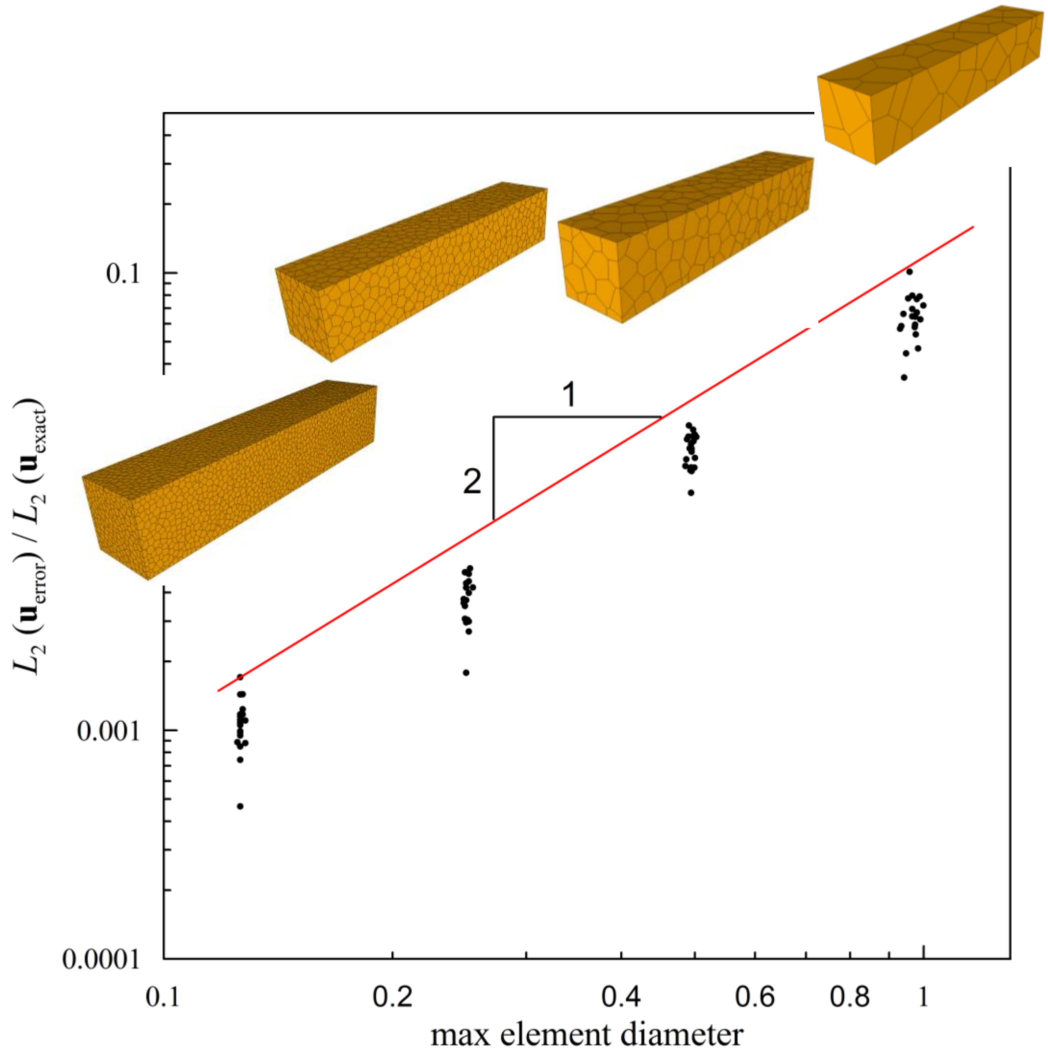
Verification Test: Bending+Shear of a Prismatic Bar

deformed shape, Von Mises stress



exact linear elasticity solution

$$
\begin{aligned}
\sigma_{xx} &= \sigma_{yy} = \sigma_{xy} = 0 \\
\sigma_{zz} &= \frac{F_y}{I_x} yz \\
\sigma_{xz} &= \frac{2F_y a^2}{\pi^2 I_x} \frac{\nu}{1+\nu} \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \sin(\frac{n\pi x}{a}) \frac{\sinh(\frac{n\pi y}{a})}{\cosh(\frac{n\pi b}{a})} \\
\sigma_{yz} &= \frac{F_y}{I_x} \left\{ \frac{1}{2}(b^2 - y^2) + \frac{1}{6}(3x^2 - a^2)\frac{\nu}{1+\nu} - \frac{2a^2}{\pi^2}\frac{\nu}{1+\nu} \sum_{n=1}^{\infty} \frac{(-1)^n}{n^2} \sin(\frac{n\pi x}{a}) \frac{\sinh(\frac{n\pi y}{a})}{\cosh(\frac{n\pi b}{a})} \right\}
\end{aligned}
$$



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Summary and Future Work

1. Researching the use of randomly close-packed Voronoi meshes for modeling pervasive fracture processes.
2. Finite-element formulations of 2D polygons and 3D polyhedra
3. Developed statistical methods for verifying mesh convergence in nonlinear dynamical systems displaying extreme sensitivity to initial conditions.
4. Applications to geomechanics, hydraulic fracturing, CO_2 sequestration.
5. Implementation into Sandia's massively-parallel multiphysics codes in progress:
    1. Aria – porous flow, flow in discrete fracture networks
    2. Adagio – solid mechanics

    } coupled