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SAND2018-3304C

Subsurface Applications for Peridynamics

6th European Congress on Computational Mechanics

MS62 - Nonlocal Models and Methods for Material Failure and Damage Simulation

June 12, 2018

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Outline

- Peridynamics Review
- Seismic Inversion and Wellbore Stimulation Review
- Inverse Problems in Heterogeneous Fractured Media with Peridynamics
- Borehole Stimulation with Peridynamics
- Conclusions

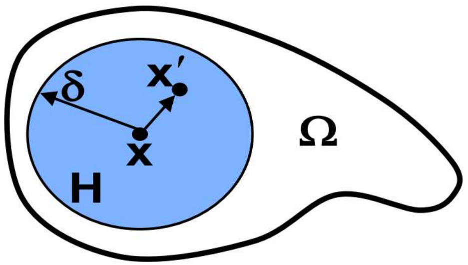
What is Peridynamics?

- **Peridynamics is a nonlocal extension of classical solid mechanics**

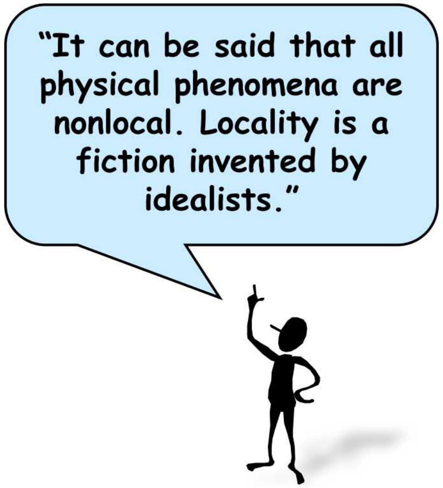
- Peridynamic equation of motion **(integral, nonlocal)**

$$\rho \ddot{u}(x,t) = \int_{H_x} f(u(x') - u(x), x'-x)\,dV' + b(x,t)$$

  - Replace PDEs with integral equations
  - **Utilize same equation everywhere; nothing "special" about cracks**
  - No assumption of differentiable fields (admits fracture)
  - No obstacle to integrating nonsmooth functions
  - $f(\cdot,\cdot)$ is "force" function; contains constitutive model
  - $f = 0$ for points x,x' more than δ apart (like cutoff radius in MD!)
  - Peridynamics is "continuum form of molecular dynamics"
- **Impact**
  - Nonlocality
  - Larger solution space (fracture)
  - Account for material behavior at small & large length scales **(multiscale material model)**
- **Ancestors**
  - Kröner, Eringen, Edelen, Kunin, Rogula, etc.

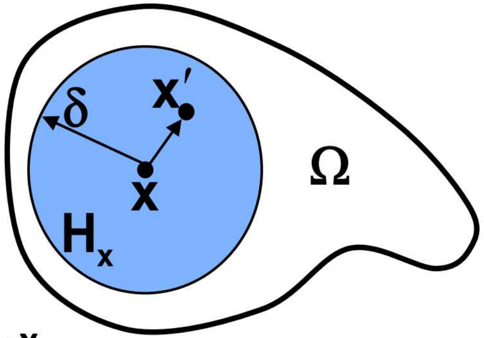


Point x interacts directly with all points x' within H



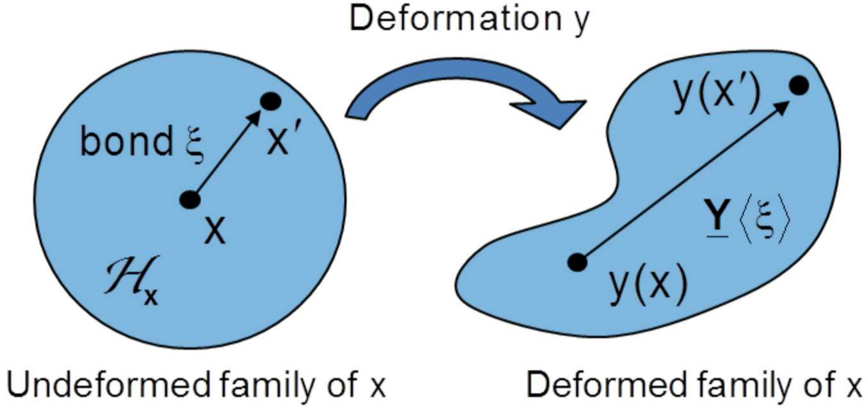
A. Cemal Eringen

Peridynamics: The Basics



- **Horizon and family**
  - Point **x** interacts directly with all points with distance δ (***horizon***)
  - Material within distance δ of **x** is denoted H_x (***family of x***)
- **Bonds and bond forces**
  - Vector between **x** and any point in its family is called a ***bond:*** **ξ = x' – x**
  - Each bond has ***pairwise force density vector*** applied at both points: **f(x', x, t)**
  - This vector is determined jointly by collective deformation of $\mathbf{H_x}$ and collective deformation of $\mathbf{H_{x'}}$
  - Bond forces are antisymmetric: **f(x', x, t) = - f(x, x', t)**
  - Bond degrade and fail, admitting damage, failure, and fracture.
- **Deformation state**
  - Deformation state operator <u>Y</u> maps each bond ξ into its deformed image

$$\underline{\mathbf{Y}}\langle \xi \rangle = \mathbf{y}(\mathbf{x}') - \mathbf{y}(\mathbf{x})$$



Peridynamics: The Basics

- **Bonds and states**
  - **f(x', x)** has contributions from material models at both **x** and **x'**

$$\mathbf{f}(\mathbf{x}',\mathbf{x}) = \underline{\mathbf{T}}[\mathbf{x},t]\langle \mathbf{x}'-\mathbf{x}\rangle - \underline{\mathbf{T}}[\mathbf{x}',t]\langle \mathbf{x}-\mathbf{x}'\rangle$$

  - $\underline{\mathbf{T}}[\mathbf{x}]$ is the ***force state*** – it maps bonds onto bond force densities
  - $\underline{\mathbf{T}}[\mathbf{x}]$ is determined by the constitutive model $\underline{\mathbf{T}} = \hat{\underline{\mathbf{T}}}(\underline{\mathbf{Y}})$, where $\hat{\underline{\mathbf{T}}}$ maps deformation state to force state
- **Peridynamics vs. standard equations**
  - Peridynamic operators and relationships are nonlocal analogues of standard theory

Relation	Peridynamic theory	Standard theory
Kinematics	$\underline{\mathbf{Y}}\langle \mathbf{x}'-\mathbf{x}\rangle = \mathbf{y}(\mathbf{x}') - \mathbf{y}(\mathbf{x})$	$\mathbf{F}(\mathbf{x}) = \frac{\partial \mathbf{y}}{\partial \mathbf{x}}(\mathbf{x})$
Linear momentum balance	$\rho\ddot{\mathbf{u}}(\mathbf{x}) = \int_{H_x} \left(\underline{\mathbf{T}}[\mathbf{x}]\langle \mathbf{x}'-\mathbf{x}\rangle - \underline{\mathbf{T}}[\mathbf{x}']\langle \mathbf{x}-\mathbf{x}'\rangle\right) dV_{x'} + \mathbf{b}(\mathbf{x})$	$\rho\ddot{\mathbf{y}}(\mathbf{x},t) = \nabla\cdot\sigma(\mathbf{x}) + \mathbf{b}(\mathbf{x})$
Constitutive model	$\underline{\mathbf{T}} = \hat{\underline{\mathbf{T}}}(\underline{\mathbf{Y}})$	$\sigma = \hat{\sigma}(\mathbf{F})$
Angular momentum balance	$\int_{H_x} \underline{\mathbf{Y}}\langle \mathbf{x}'-\mathbf{x}\rangle \times \underline{\mathbf{T}}\langle \mathbf{x}'-\mathbf{x}\rangle dV_{x'} = 0$	$\sigma = \sigma^T$
Elasticity	$\underline{\mathbf{T}} = W_{\underline{Y}}$ (Frechet derivative)	$\sigma = W_F$ (tensor gradient)
First law of thermodynamics	$\dot{\varepsilon} = \underline{\mathbf{T}} \bullet \dot{\underline{\mathbf{Y}}} + h + r$	$\dot{\varepsilon} = \sigma\cdot\dot{\mathbf{F}} + h + r$

Peridynamic Material Models

- **Linear Peridynamic Solid (LPS)***
- Nonlocal analog to linear isotropic elastic solid
- k is bulk modulus, μ is shear modulus

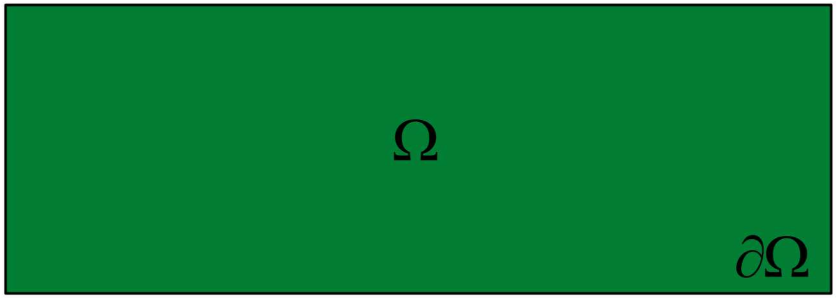
$$\rho \ddot{\mathbf{u}}(\mathbf{x},t) = \int_H \left(\mathbf{T}[\mathbf{x},t]\langle \mathbf{x}' - \mathbf{x} \rangle - \mathbf{T}[\mathbf{x}',t]\langle \mathbf{x} - \mathbf{x}' \rangle \right) dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t)$$

$$\mathbf{T}[\mathbf{x},t]\langle \mathbf{x}' - \mathbf{x} \rangle = \left(\frac{3k\theta}{m} \underline{\omega}\,\underline{\mathbf{x}} + \frac{15\mu}{m} \underline{\omega}\,\mathbf{e}^d \right) \frac{\mathbf{x}' - \mathbf{x}}{\left\| \mathbf{x}' - \mathbf{x} \right\|}$$

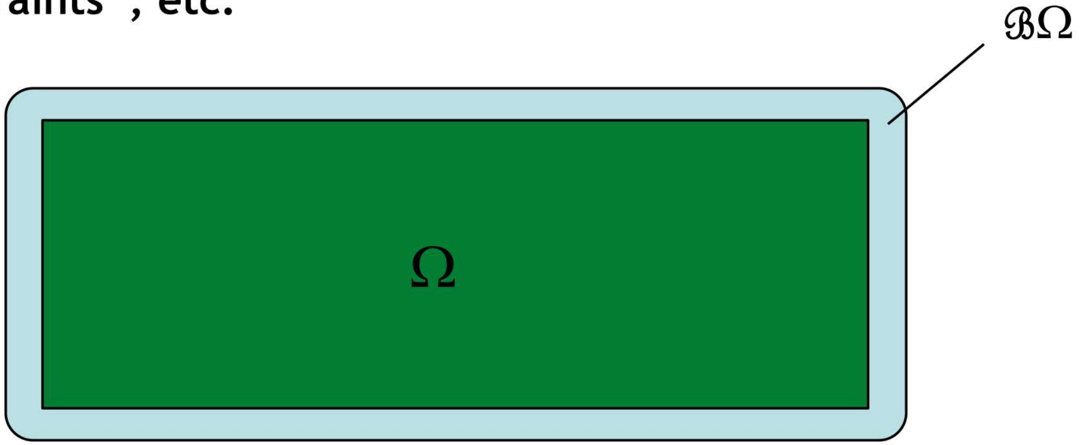
*S.A. Silling, M. Epton, O. Weckner, J. Xu, & E. Askari, Peridynamic States and Constitutive Modeling, J. Elasticity, 88, pp. 151-184, 2007.

Nonlocal Boundary Conditions

- For local models (for example, PDE-based models), we apply boundary conditions on the boundary of the domain (hence the name).



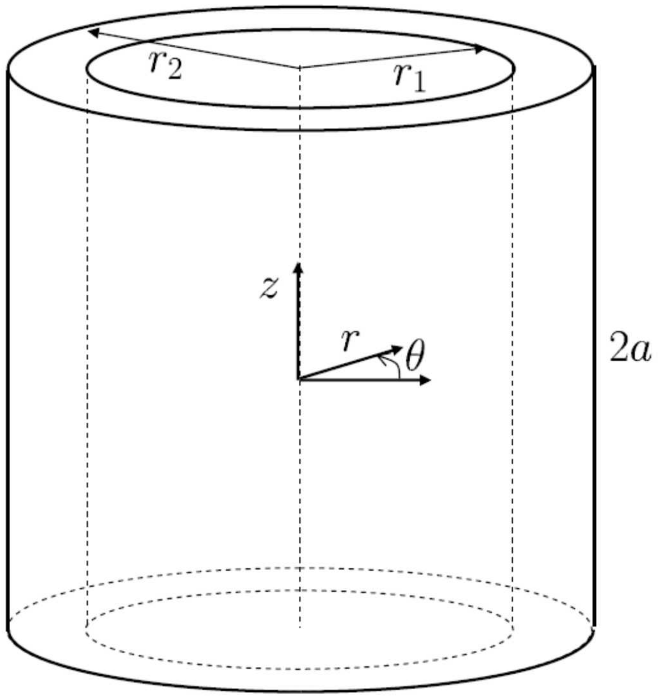
- A Peridynamic "boundary" becomes a volumetric region, sometimes called a "nonlocal boundary", "collar", etc.
- Boundary conditions for these models are called "nonlocal boundary conditions", "volume constraints", etc.



Fragmenting Cylinder

- **Fragmenting Cylinder**
  - Motivated by tube fragmentation experiments of Winter (1979), Vogler (2003)*

- **Material properties**
  - Inner radius r1 = 0.020 m
  - Outer radius r2 = 0.025 m
  - Length 2a = 0.1 m
  - Density ρ = 7800 kg/m^3
  - Bulk modulus k = 130 GPa
  - Shear modulus μ = 78 GPa
  - Yield stress Y = 500 GPa
  - Ultimate stress σ = 700 GPa
  - Elongation at failure ε = 0.02



- **Initial Velocity**
  - $\mathbf{v(r) = V_{r0} - V_{r1}(a/z)^2}$
  - $\mathbf{v(z) = V_{z0}(a/z)}$
  - $\mathbf{v(\theta) = 0}$

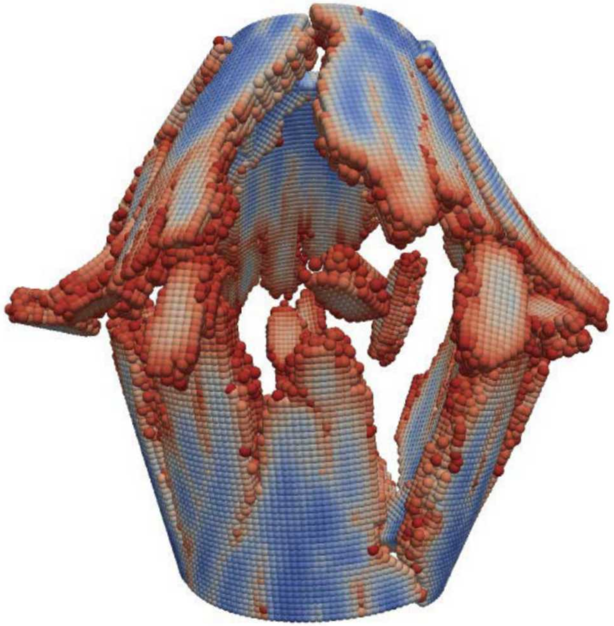
where $\mathbf{V_{r0}}$ **= 200 m/s,** $\mathbf{V_{r1}}$ **= 50 m/s,** $\mathbf{V_{z0}}$ **= 100 m/s**

* D. Grady, Fragmentation of Rings And Shells: The Legacy of N.F. Mott, Springer, 2006.

Fragmenting Cylinder

Simulation performed with Peridigm

Before



After
(brittle failure)

Fracture in Glass Plate

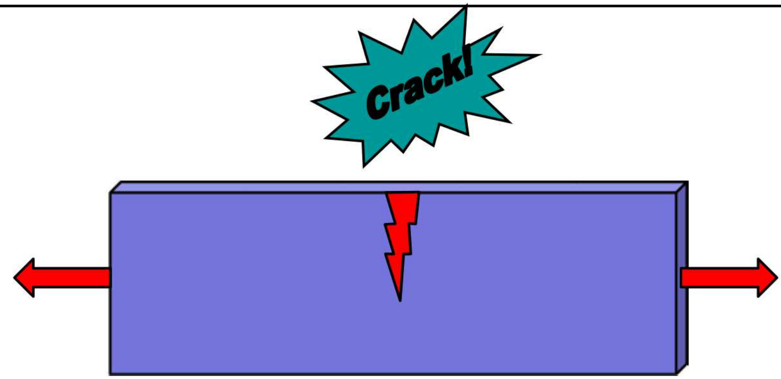
- With Florin Bobaru (Nebraska), Youn-Doh Ha, & Stewart Silling (Sandia)

- Soda-lime glass plate (microscope slide)
  - Dimensions: 3" x 1" x 0.05"
  - Density: 2.44 g/cm3
  - Elastic Modulus: 79.0 Gpa

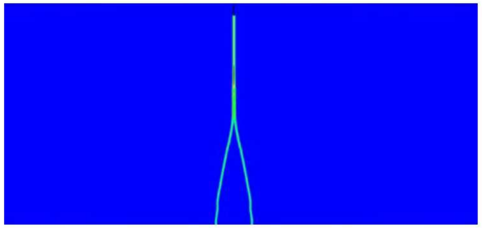
- Dawn (LLNL): IBM BG/P (500 TF; 147,456 cores)
  - Mesh spacing: 35 microns
  - Approx. 82 million particles
  - Time: 50 microseconds (20k timesteps)
  - 6 hours on 65k cores

Setup

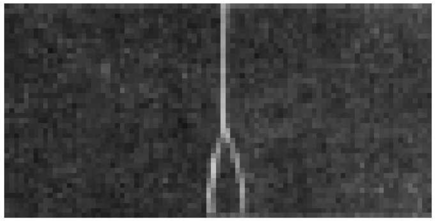
- Glass microscope slide
- Dimensions: 3" x 1" x 0.05"
- Notch at top, pull on ends



Results



Peridynamics



Physical Experiment*

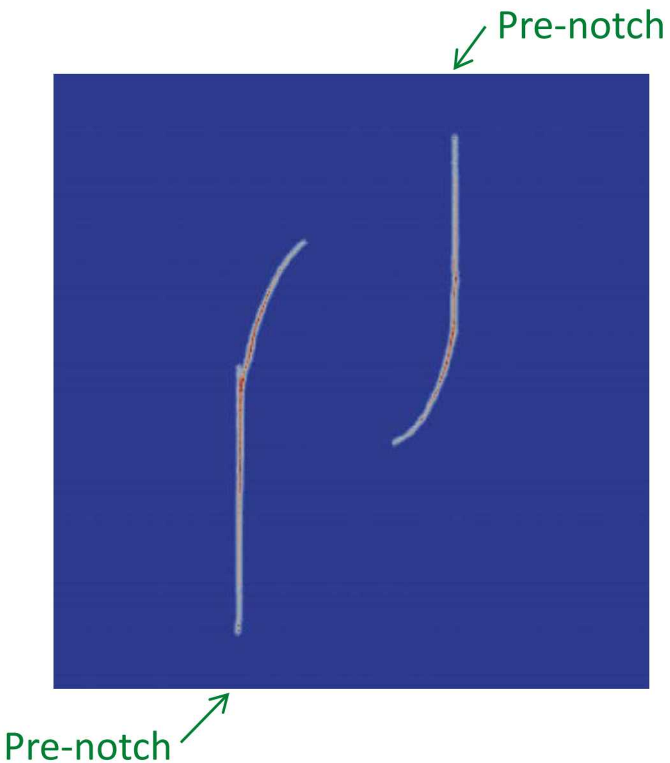
Strain Energy Density

*S F. Bowden, J. Brunton, J. Field, and A. Heyes, *Controlled fracture of brittle solids and interruption of electrical current*, Nature, 216, 42, pp.38-42, 1967.

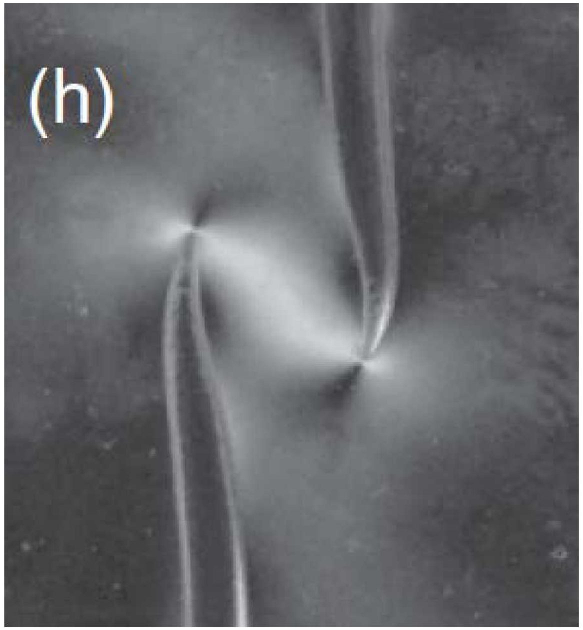
Two Interacting Cracks

- ❑ Offset notches thin rectangular elastic plate
- ❑ Uniaxial strain applied from sides
- ❑ Approaching cracks produce “en passant” crack pattern

Simulation performed with PDLAMMPS



Peridynamics



Physical Experiment*

* M. Fender, F. Lechenault, and K. Daniels, Universal Shapes Formed by Two Interacting Cracks, Phys. Rev. Lett. 105, 125505 (2010) .

Codes

- **PDLAMMPS (Peridynamics-in-LAMMPS)** (**Open source**, C++)
  - Developers: Parks, Seleson, Plimpton, Silling, Lehoucq
  - Particular discretization of PD has computational structure of molecular dynamics (MD)
  - LAMMPS: Sandia's open-source massively parallel MD code (**lammps.sandia.gov**)
  - More info & user guide: **www.sandia.gov/~mlparks**

- **Peridigm** (**Open Source**, C++)
  - **peridigm.sandia.gov; github.com/peridigm/peridigm**
  - Developers: Parks, Littlewood, Mitchell, Silling
  - Intended as Sandia's primary open-source PD code
  - Built upon Sandia's Trilinos Project **(trilinos.sandia.gov)**
  - Massively parallel
  - Explicit, implicit time integration
  - State-based linear elastic, elastic-plasticity, viscoelastic models
  - DAKOTA interface for UQ/optimization/calibration, etc. **(dakota.sandia.gov)**

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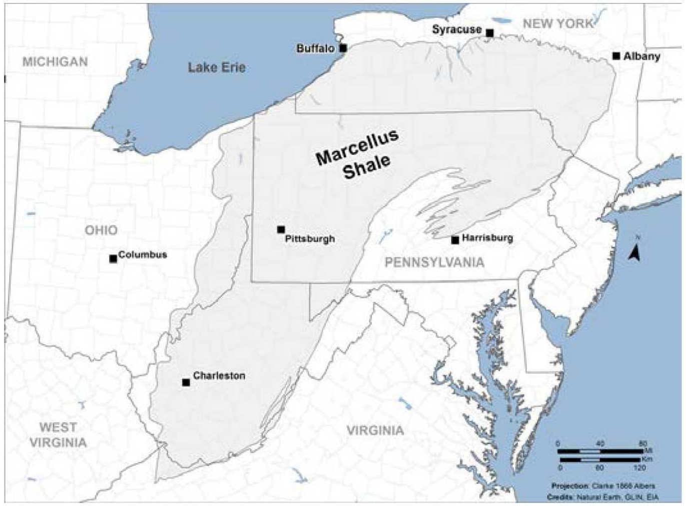
- ❑ Conclusions

Hydrocarbon Exploration

- Search for oil and gas (hydrocarbon) deposits in the subsurface
- Expensive, high-risk operation generally undertaken by large companies or national governments.
- Deep water wells can cost $100M+.
- Marcellus shale may hold 50 trillion cubic feet (TCF) and 500 TCF of natural gas.

Deepwater Offshore Drilling Rig



Marcellus Shale

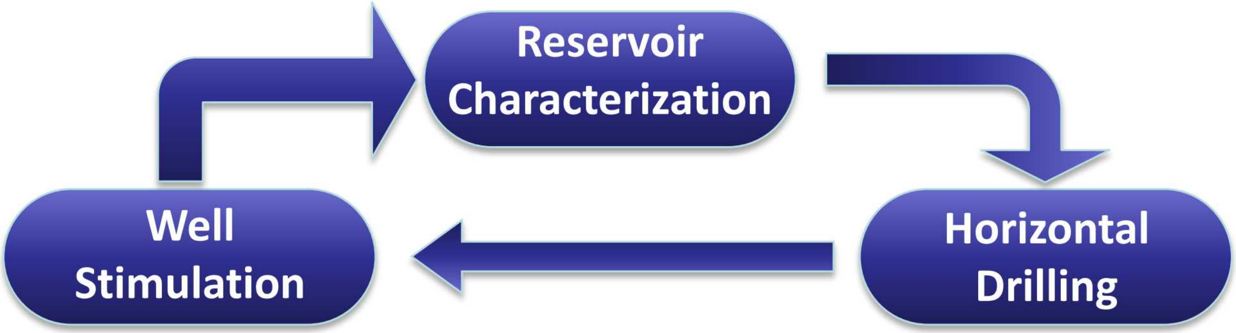
Natural Gas Derrick, Pennsylvania

Hydrocarbon Exploration

- Computational modeling can play numerous roles. I'll discuss two aspects today, where nonlocal (peridynamics) models have been applied to both.

- **Reservoir Characterization via Seismic Inversion**
  - Transform seismic reflection data into quantitative rock properties that are descriptive of the reservoir.

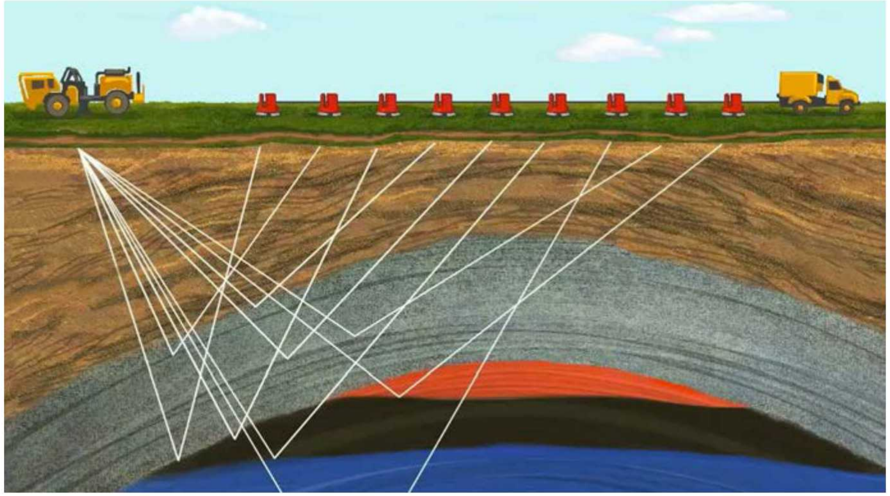
- **Well Stimulation**
  - Well intervention technique performed on an oil or gas well to increase production by improving the flow of hydrocarbons from the drainage area into the well bore.
  - This is especially important for so-called unconventional resources (shale gas, tight gas, tight oil plays) with low revivor permeability

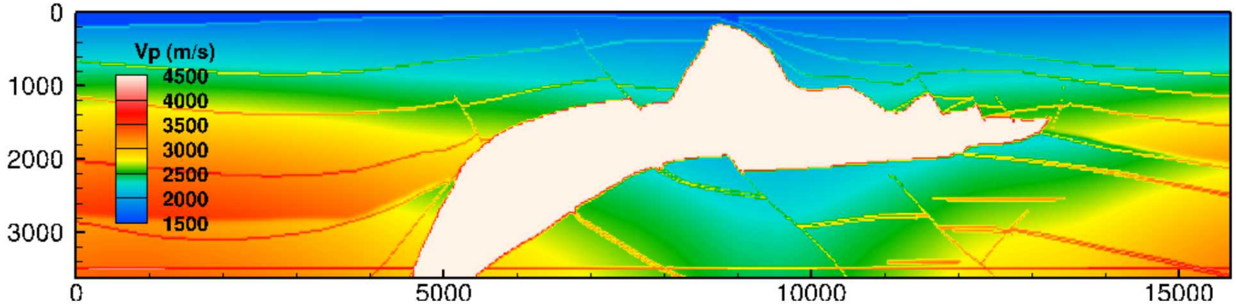


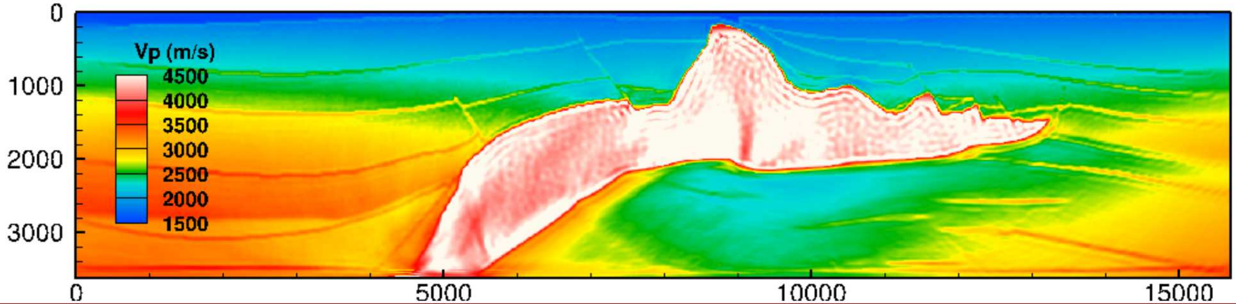
Reservoir Characterization via Seismic Inversion

- Accurate subsurface models to reduce risk of drilling poorly producing wells and maximize production of reservoirs with fewest number of wells.

- Seismic inversion transforms seismic reflection data into quantitative rock-property description of reservoir.







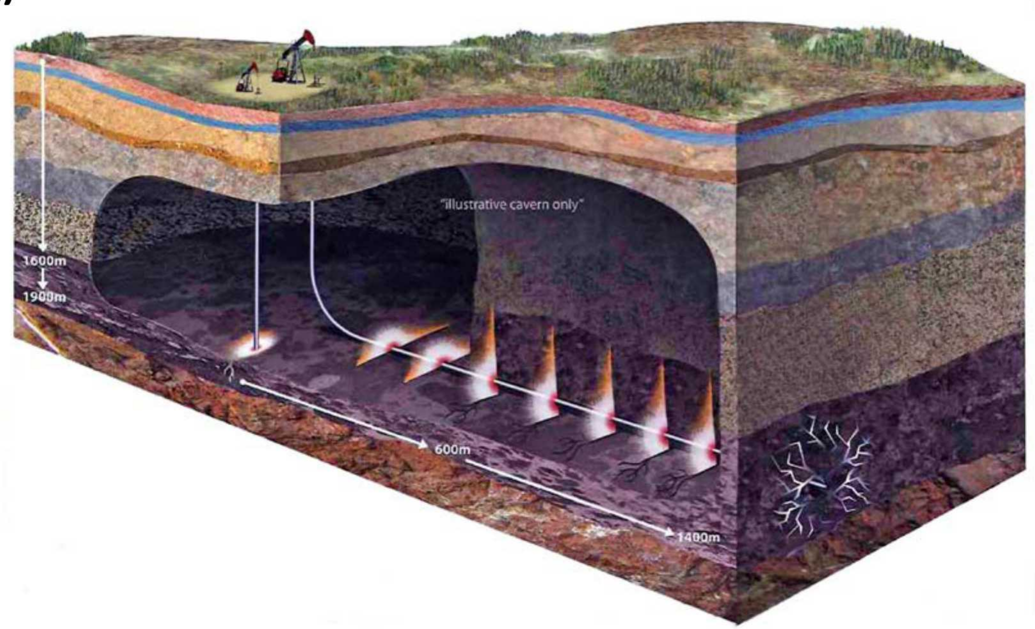
Top: The true compressional wave speed for the SEG Salt Model*.

Bottom: Inverted results. Salt structure well defined. Steep faults under the salt not captured due to the lack of illumination from the source & receiver locations.

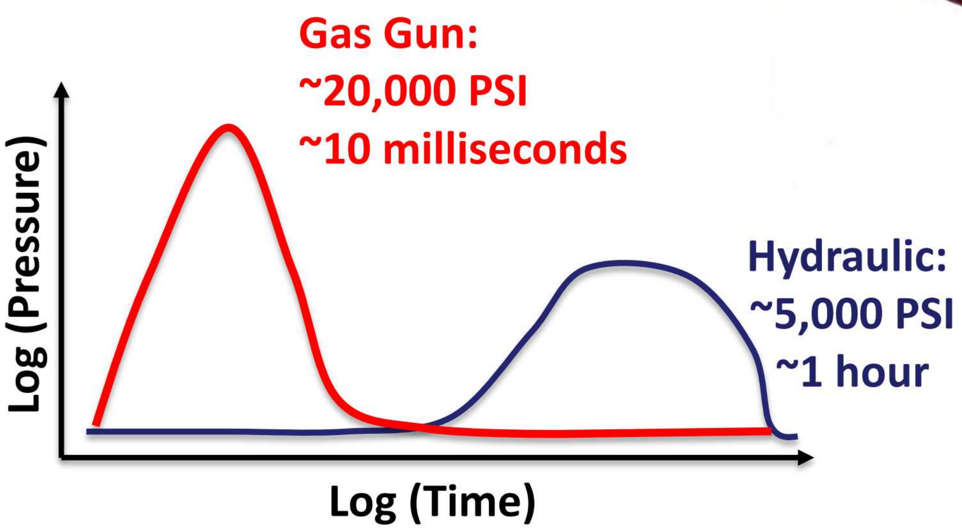
*C. Ober et al., Large-Scale Full-Waveform Inversion for Complex Media and Structure, Center for Computing Research Glossy, Sandia National Laboratories, 2017.

Wellbore Stimulation

- Restore or enhance well production by improving the connection of the wellbore with the reservoir.
- This can be done in multiple ways; Two prominent methods are
  - Hydraulic fracturing (fracking)
  - Gas guns
- These have different pressure profiles and different effects on surrounding rock.



Stimulation of Horizontally Drilled Well



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Peridynamic Inverse Problem

- Given the demonstrated ability of peridynamics to model fractures, we seek to demonstrate if it can be used in the context of inversion.
- Specifically,
  - Can we invert for material properties (k(x) μ(x)) with peridynamics?
  - Can we invert in the presence of fractures?
- Formulate nonlinear constrained least-squares optimization problem (IDE-constrained optimization):

$$\min_{\mathbf{u},k,\mu} \mathbf{g}(\mathbf{u},k,\mu) \quad \text{subject to} \quad \begin{cases} \mathbf{c}(\mathbf{u},k,\mu) = \mathbf{0} & \text{in } \Omega \\ \mathbf{u} = \mathbf{u}_0 & \text{in } \Omega^u \quad \text{(nonlocal Dirichlet bc)} \\ \mathbf{b} = \mathbf{q} & \text{in } \Omega^q \quad \text{(nonlocal Neumann bc)} \end{cases}$$

where

$$\mathbf{g}(\mathbf{u},k,\mu) = \sum_{j=1}^{N_{obs}} \int_{\Omega} \left\| \mathbf{u} - \mathbf{u}^* \right\| \delta\left(\mathbf{x} - \mathbf{x}_j\right) \, d\Omega + \frac{\alpha_k}{2} \int_{\Omega} k^2 \, d\Omega + \frac{\alpha_\mu}{2} \int_{\Omega} \mu^2 \, d\Omega$$

$$\mathbf{c}(\mathbf{u},k,\mu) = \int_{\mathbf{H}_\mathbf{x}} \mathbf{T}[\mathbf{x}]\langle \mathbf{x}' - \mathbf{x} \rangle - \mathbf{T}[\mathbf{x}']\langle \mathbf{x} - \mathbf{x}' \rangle \, d\Omega$$

Optimality Condition

- Introduce Lagrange multiplier field (adjoint variable) to give

$$\mathbf{L}(\mathbf{u},\boldsymbol{\lambda},\mathbf{d}) = \mathbf{g}(\mathbf{u},\mathbf{d}) + \int_{\Omega} \left(\mathbf{c}^{T}\boldsymbol{\lambda} - \mathbf{d}^{T}\boldsymbol{\lambda} \right) d\Omega$$

- where d contains the material parameters k and μ.

- Linearizing and taking variations with respect to u, d, λ gives

$$\begin{aligned} \mathbf{c} &= \mathbf{0} \quad \text{in}\,\Omega \ \text{(state)} \\ \mathbf{J}_{u}^{T}\boldsymbol{\lambda} + \mathbf{g}_{u} &= \mathbf{0} \quad \text{in}\,\Omega \ \text{(adjoint)} \\ \mathbf{J}_{u}^{T}\boldsymbol{\lambda} + \mathbf{g}_{u} &= \mathbf{0} \quad \text{in}\,\Omega \ \text{(decision)} \end{aligned}$$

- After discretization:

$$\mathbf{u},\boldsymbol{\lambda} \in \mathbb{R}^{M} \qquad \mathbf{J}_{u} = \partial\mathbf{c}/\partial\mathbf{u} \in \mathbb{R}^{M\times M} \qquad \mathbf{g}_{u} = \partial g/\partial\mathbf{u} \in \mathbb{R}^{M}$$

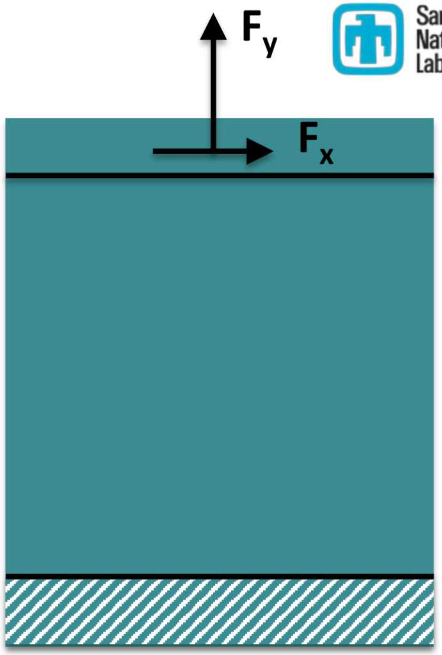
$$\mathbf{d} \in \mathbb{R}^{P} \qquad \mathbf{J}_{d} = \partial\mathbf{c}/\partial\mathbf{d} \in \mathbb{R}^{M\times P} \qquad \mathbf{g}_{d} = \partial g/\partial\mathbf{d} \in \mathbb{R}^{P}$$

- Solve using trust-region algorithm with conjugate gradient solver.

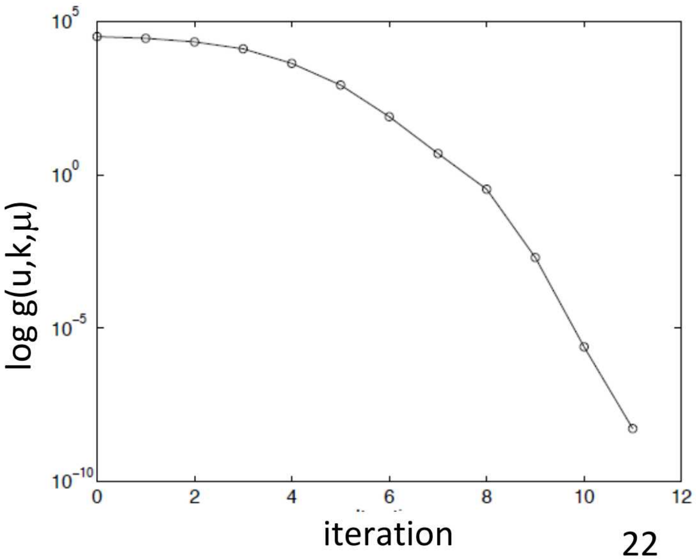
Numerical Example #1

- Verification for constant material parameters (P=2)
- Consider a 2D, square domain L × L domain with bottom held fixed and force applied to top.
  - L = 1000,
  - $F_x = F_y = 1000$
  - h = 100, piecewise constants
- Observed displacement u* manufactured by solving forward problem with k = 666.67 and μ = 400.0.
- Solve for k, μ, given loading and least squares misfit of computed displacement field, u, to observed displacement field u*. $k_{init} = \mu_{init} = 100$.
- No regularization used ($\alpha_k = \alpha_\mu = 0$).

Parameter	Exact	Computed	Error (%)
k	666.67	666.6700	0.0000644
μ	400.00	399.9984	0.0003950



$u_x = u_y = 0$



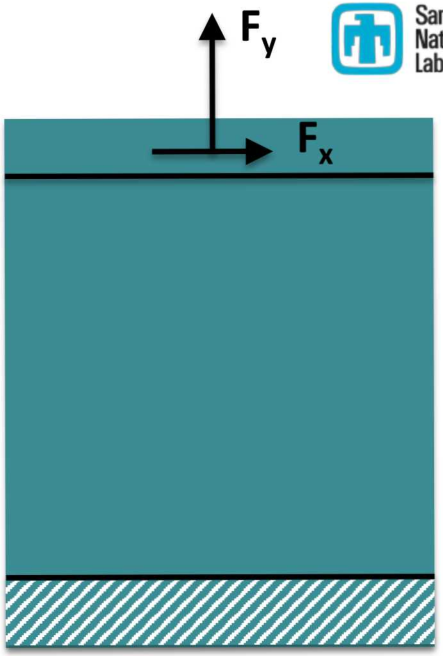
Numerical Example #2

- Verification for heterogeneous material parameters (P=121)
- Observed displacement u* manufactured by solving forward problem with

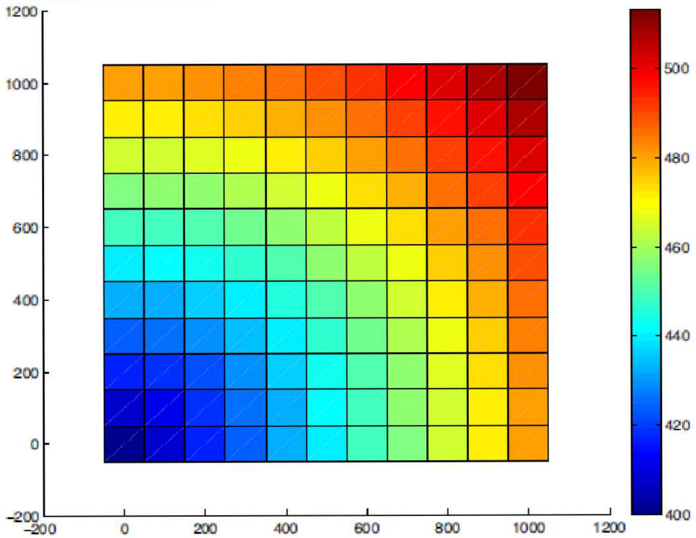
  $k(x) = -\gamma_k\, r\, k_0 + k_0$

  $\mu(x) = -\gamma_\mu\, r\, \mu_0 + \mu_0$

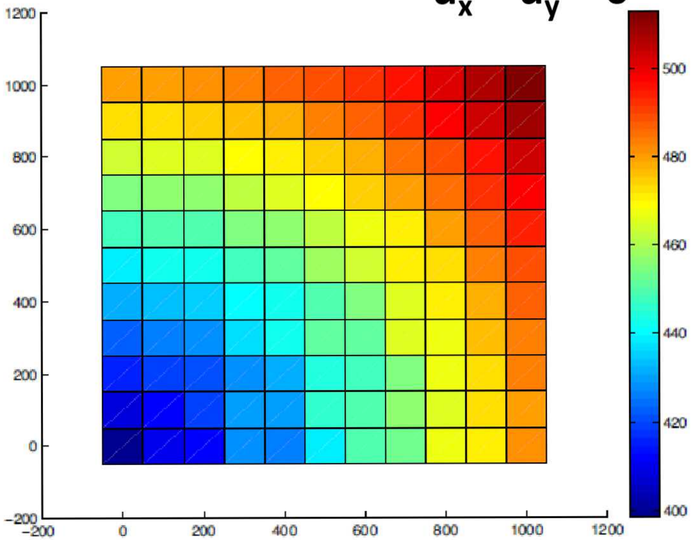
  - $\gamma_k = 0.00025$
  - $\gamma_\mu = 0.00020$
  - $k_0 = 666.67$, $\mu_0 = 400.0$
- Invert for μ. $\mu_{init} = \mu_0$.



$u_x = u_y = 0$



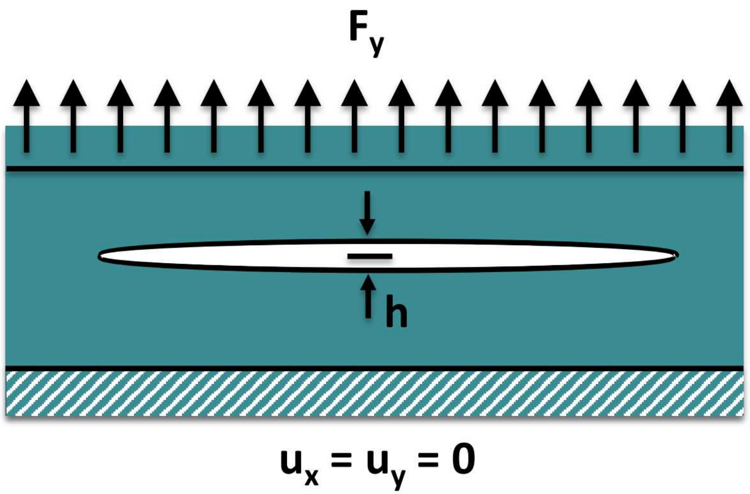
True $\mu(x)$



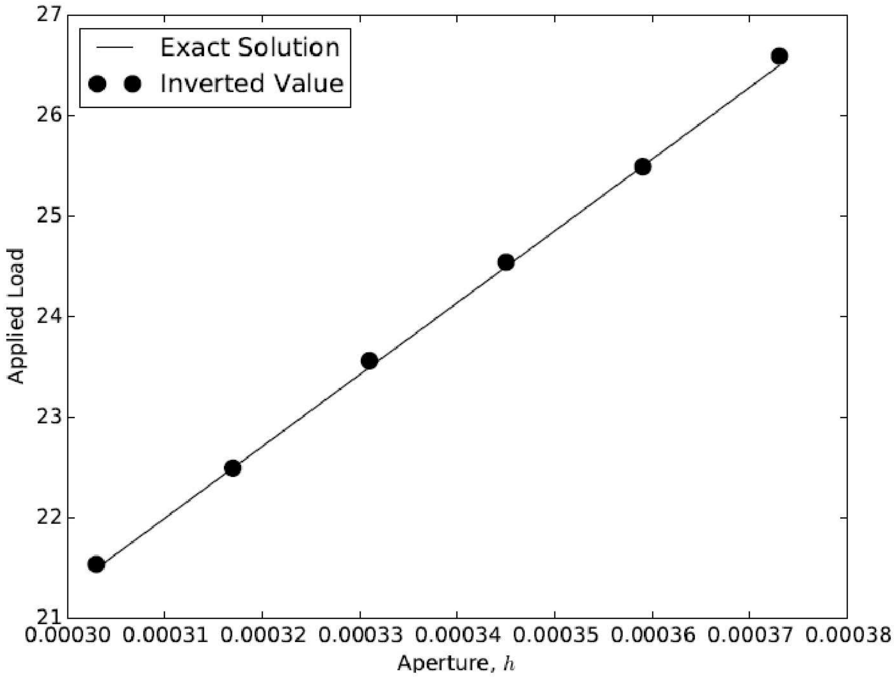
Inverted $\mu(x)$ (1.2% error)

Numerical Example #3

- Inversion for load state with fracture
- Consider 2D domain with bottom held fixed and force applied to top.
- Pre-crack applied in center
  - μ = 40 GPa
  - k = 66.6 GPa
- Observed crack aperture h* manufactured by solving forward problem with applied load F_y
- Invert for crack aperture h



$$\mathbf{g}(h) = \frac{1}{2}\sum_{j=1}^{N_{obs}} \int_{\Omega} \left(h - h^*\right)^2 \, \delta\left(\mathbf{x} - \mathbf{x}_j\right) \, d\Omega$$



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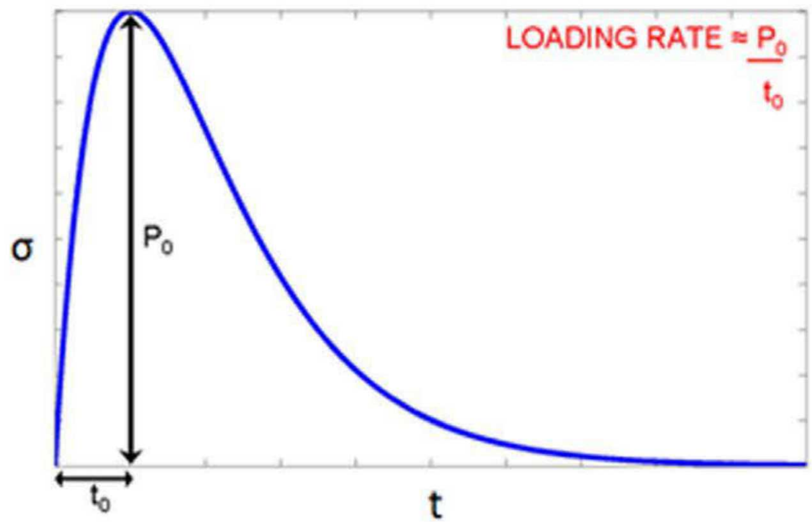
Well Stimulation

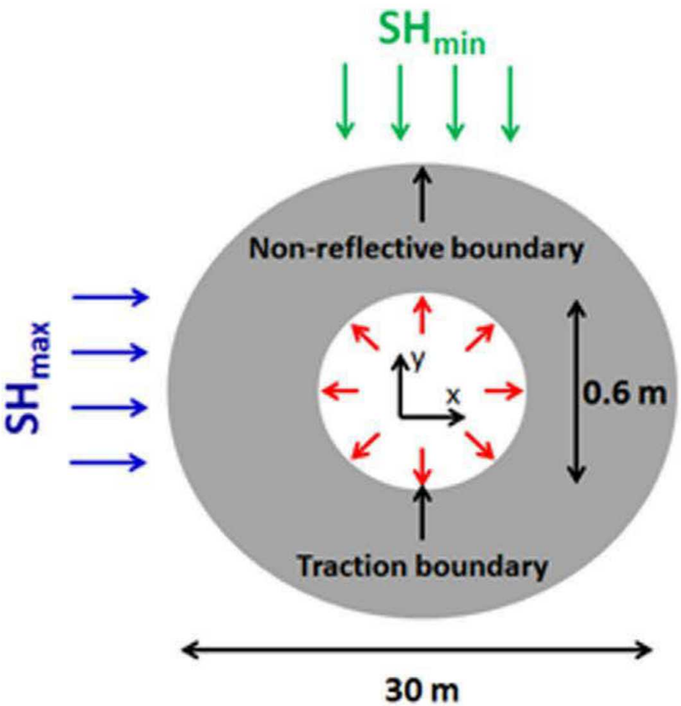
- Fracture patterns dependent on
  - in-situ stress
  - pressure profile

- Investigate combination of both
- Study conducted with PMB model

Property	Value
Density (ρ)	2700.0 kg/m3
Bulk modulus (k)	37.0 GPa
Energy release rate (G0)	298 J/m2
Rock diameter (D)	30 m
Borehole diameter (db)	0.6 m

$$\mathrm{P_b}(t) = e^{-at}\mathrm{P}_0 \frac{e^{-\alpha t} - e^{-\beta t}}{e^{-\alpha t_0} - e^{-\beta t_0}}$$





Well Stimulation

$$P_b(t) = e^{-at} P_0 \frac{e^{-\alpha t} - e^{-\beta t}}{e^{-\alpha t_0} - e^{-\beta t_0}}$$

Loading Rates

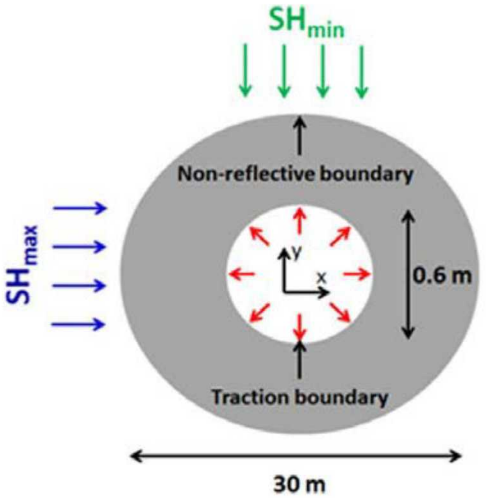
Case	P_0 (MPa)	t_0 (ms)	β/α
1	100.0	10.0	1.5
2	100.0	1.0	1.5
3	100.0	0.1	1.5
4	100.0	1.0	131.3
5	100.0	0.1	2120.0

Effect of loading rate (Cases 1–3)

Effect of decay rate (Cases 2–5)

In-situ Stress States

Case	SH_{max} (MPa)	SH_{min} (MPa)
A	0.0	0.0
B	10.0	10.0
C	12.5	7.5
D	15.0	5.0



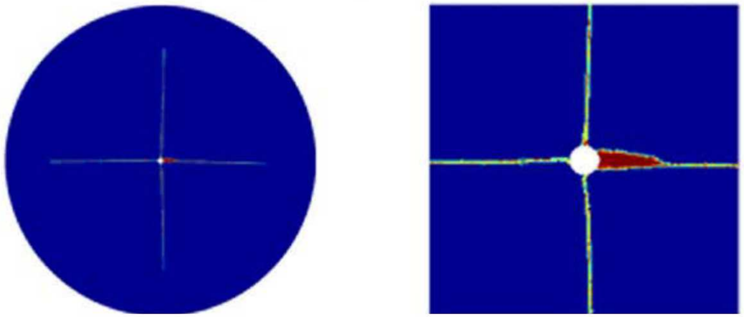
Influence of Loading Rate

- No in-situ stress
- Comparison of slow, fast, & fastest loading rates.

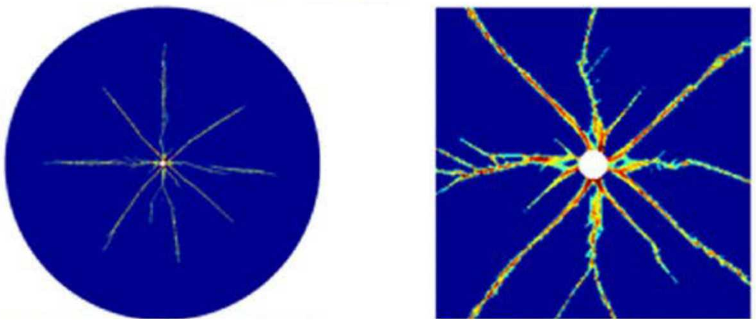
- Higher loading rate produces more radial fractures
- Slower loading rate produces fewer, longer radial fractures

- Close to borehole, higher loading rates produce ring of highly damaged material, consistent with region of crushed or pulverized material typically seen under explosive loading

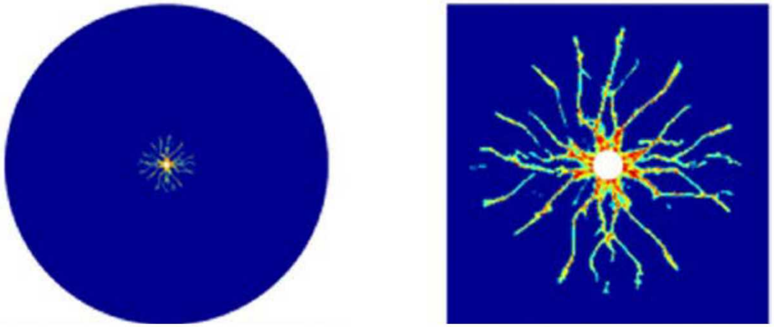
Case A-1 (slow)



Case A-2 (fast)



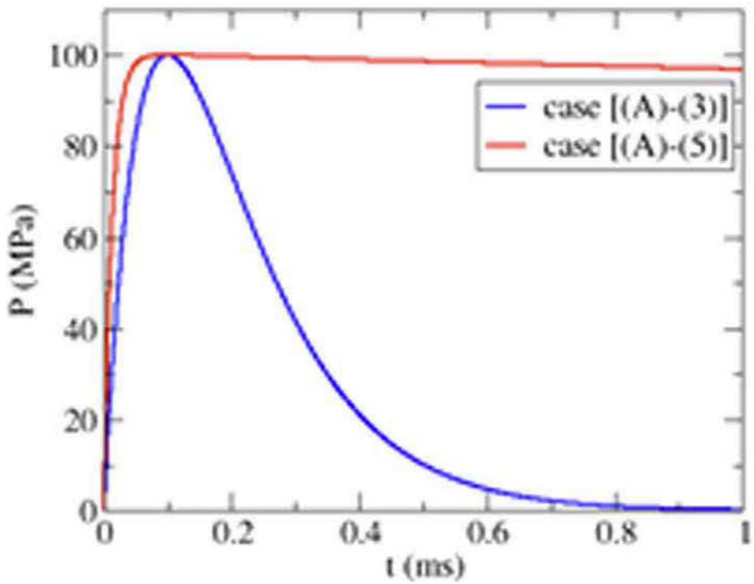
Case A-3 (fastest)



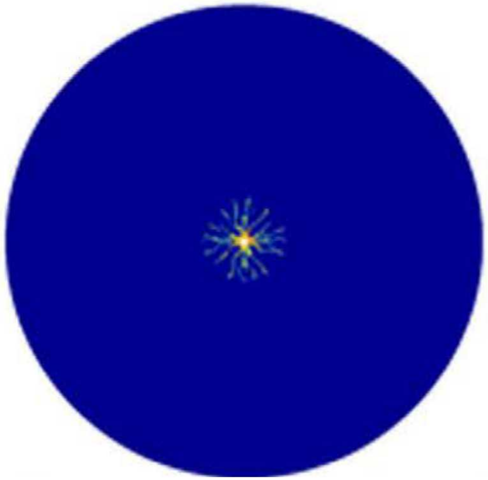
Influence of Decay Rate

- No in-situ stress
- Comparison of slow, fast, & fastest loading rates.

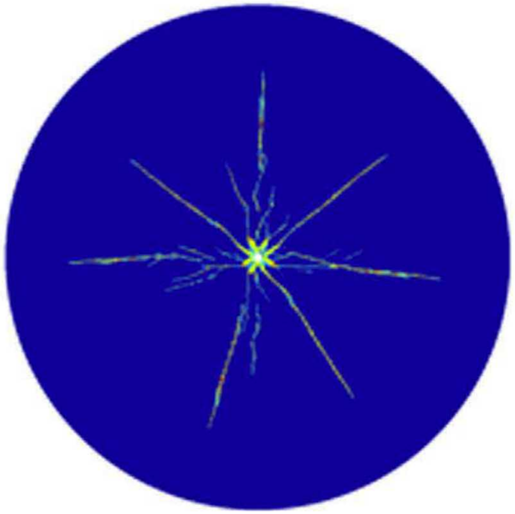
- Initiation nearly same for A-3, A-5.
- In A-5, pressure held nearly constant after initiation; fractures much longer before arrest.
- Number of fractures appears to depend on loading rate; length on decay rate.



Case A-3 (fastest loading; fast decay)



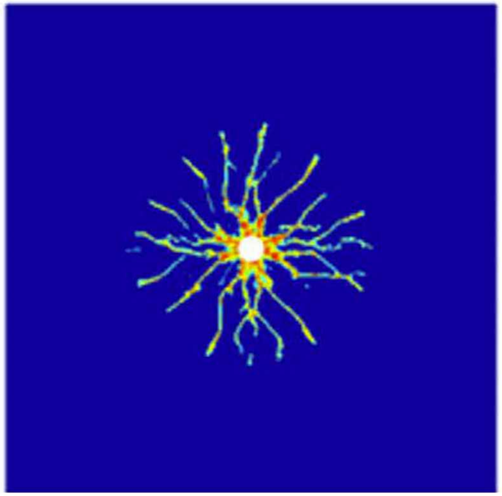
Case A-5 (fastest loading; long decay)



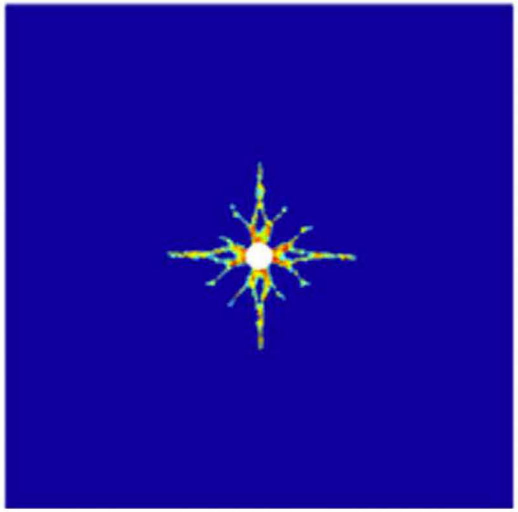
Influence of In-Situ Stress (1)

- Comparison of no in-situ stress vs. 10 MPa uniform in-situ stress for & fastest loading rate
- Maximum fracture length for B-3 about 50% that for A-3
- If the system is under compression, a larger amount of energy is required to generate a tensile state that initiates and propagates fractures.

Case A-3 (fastest loading; no stress)



Case B-3 (fastest loading; uniform stress)

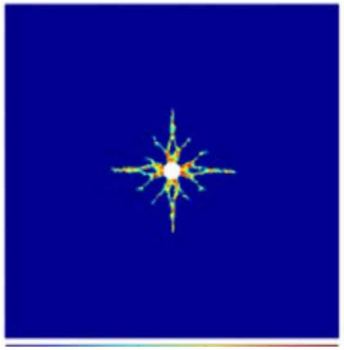


Influence of In-Situ Stress (2)

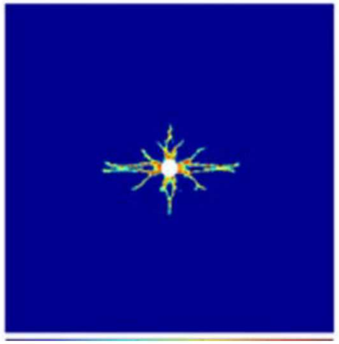
- Comparison of uniform in-situ stress vs. anisitropic in-situ stress

- For slower loading rates, stress anisotropy results in fractures oriented perpendicular to minimum confining stress direction, similar to what is expected in hydraulic fracturing

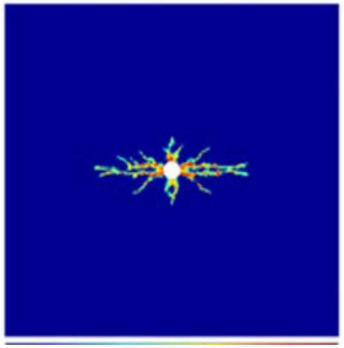
Case B-3
(fastest loading; no stress)



Case C-3
(fastest loading; anisotropic stress)



Case D-3
(fastest loading; very anisotropic stress)



Comparison with other models

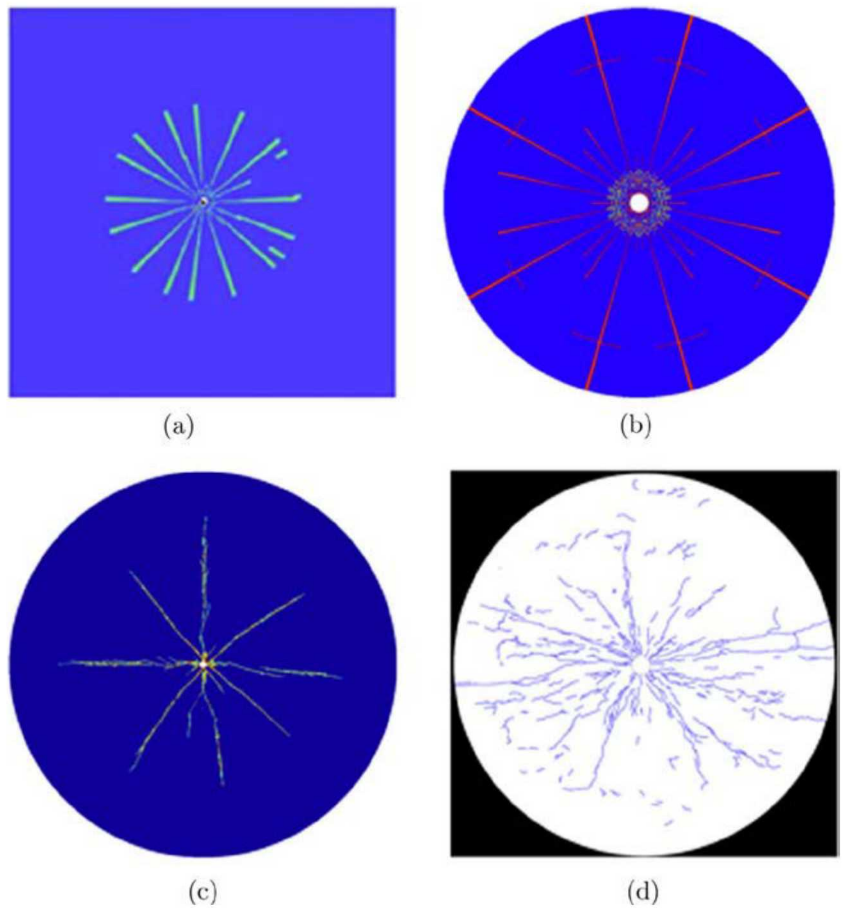
Sandia National Laboratories

- ***Qualitative*** **comparison to other models.**
- **LS-DYNA fracture patterns do not turn or branch. Current study show turning and branching fracture patterns, in qualitative agreement with experiment.**

Johnson-Holmquest Model (LS-DYNA)[a] (a), (b)

Peridynamics (current study) (c)

Physical Experiment[b] (d)



(a) Ma GW, An X. Numerical simulation of blasting-induced rock fractures. Int J Rock Mech Min Sci. 2008;45:966–975.
(b) Banadaki MMD, Mohanty B. Numerical simulation of stress wave induced fractures in rock. Int J Impact Eng. 2012;40:16–25.

Summary

- Demonstrated IDE-constrained optimization and borehole stimulation with peridynamics.

- Inversion with Peridynamics:
  - Daniel Turner, Bart van Bloemen Waanders and M.L.P, Inverse problems in heterogeneous and fractured media using peridynamics, Journal of Mechanics of Materials and Structures, 10(5), pp. 573-590, 2015.

- Borehole Stimulation with Peridynamics:
  - Rohan Panchadhara, Peter A. Gordon, and Michael L. Parks, Modeling propellant-based stimulation of a borehole with peridynamics, International Journal of Rock Mechanics and Mining Sciences, 93, pp. 330-343, 2017.

- Questions?