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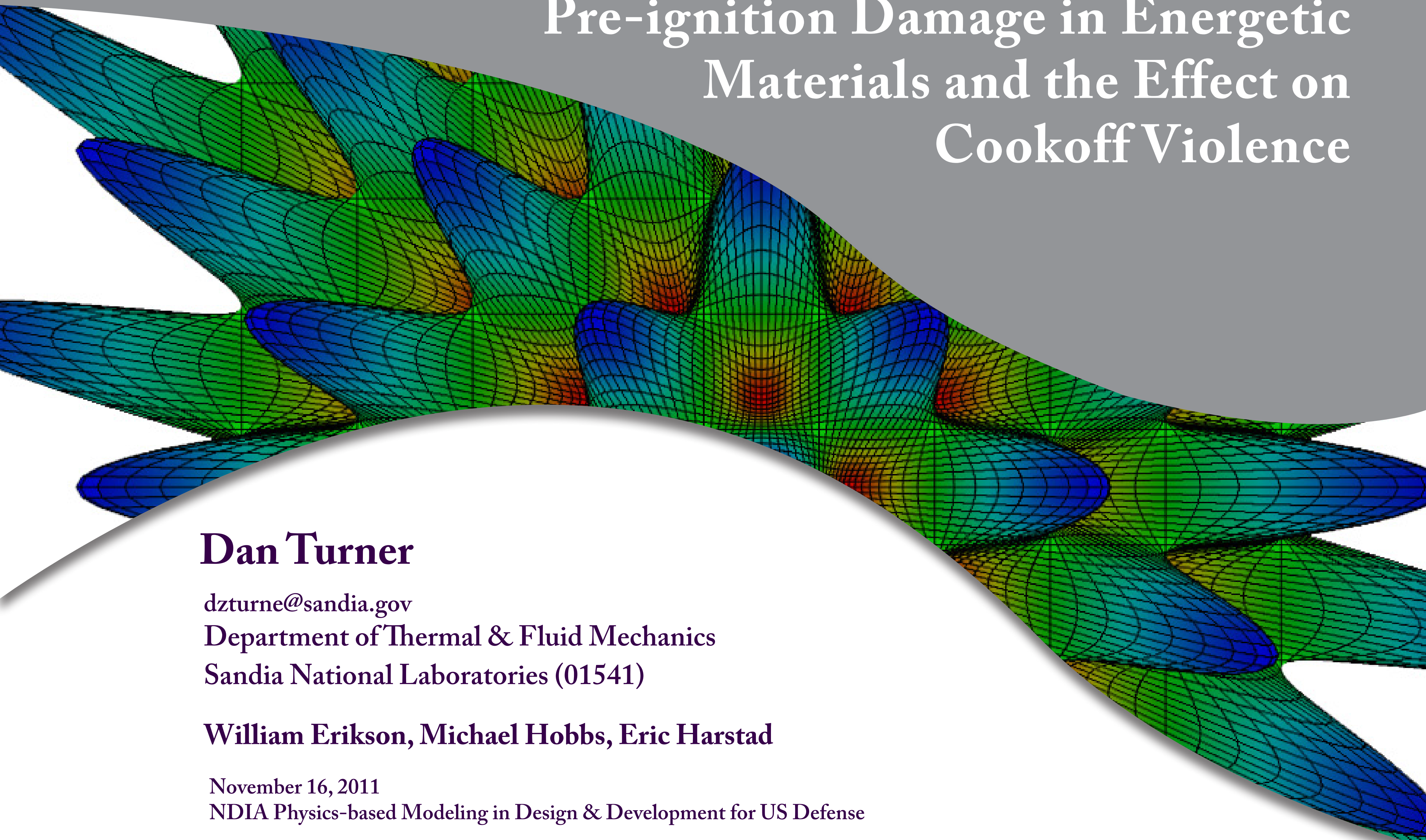
Multiphysics Modeling of Pre-ignition Damage in Energetic Materials and the Effect on Cookoff Violence



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November 16, 2011
NDIA Physics-based Modeling in Design & Development for US Defense

Outline

1. Motivation and context
2. Overview of coupling approach
3. Decomposition model description
4. Peridynamics
5. Examples
6. Future work and conclusions

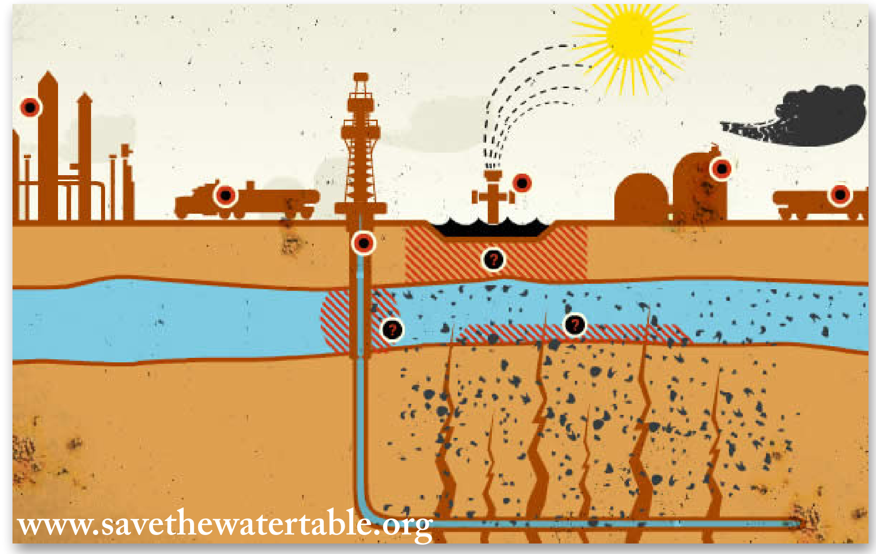
Motivation and Context

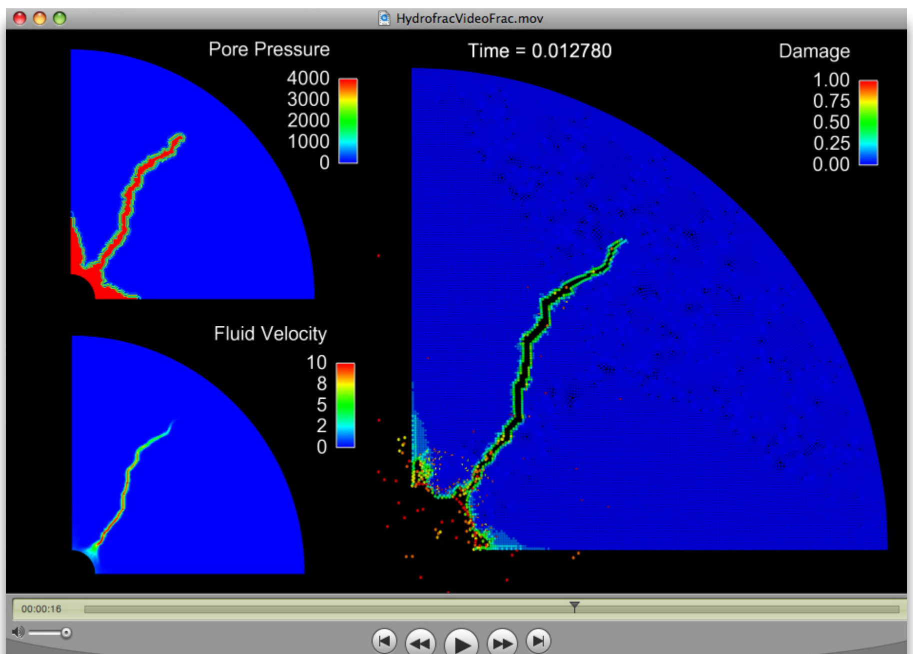
Carbon dioxide (CO_2) sequestration

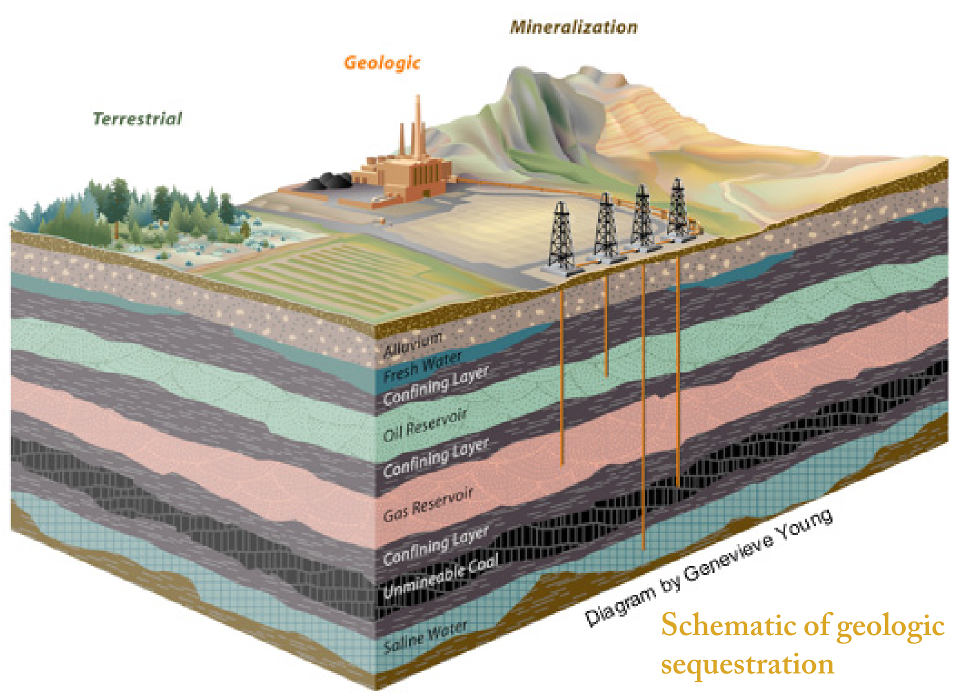
- Potential for caprock fracture leading to large-scale release back into the atmosphere

Hydraulic fracturing

- Extent of reservoir damage due to fracking and transport of chemicals







Schematic of geologic sequestration

Motivation and Context

Energetic materials

- Burn dynamics and reaction violence are strongly correlated with damage in explosive materials

Goals

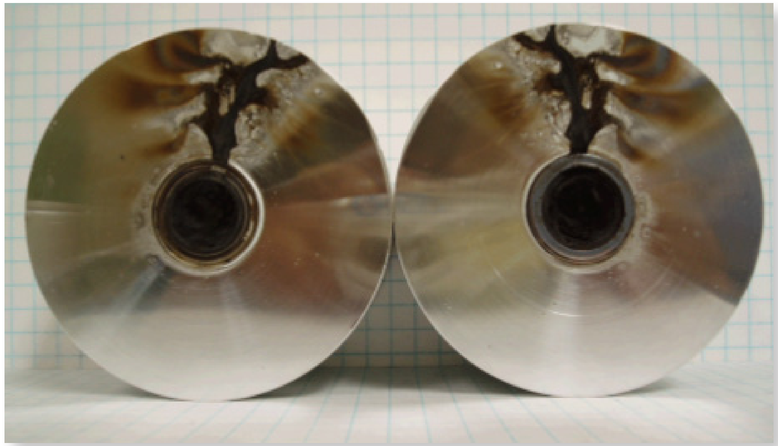
- Effect of pre-igintion damage on permeability of eneregetic materials
- Model enclosure breach and calculate gas production
- Determine fragmentation of confinement after ignition and relative energy of fragments

Hobbs, Kaneshige, and Wente. Correlating cookoff violence with pre-ignition damage. SAND2010-1183C

SITI experiements

Sealed confinement

Vented confinement



Koerner, Maienschein, Burnham, and Wemhoff, UCRL-CONF-232590

ODTX experiements: Evidence of breached confinement

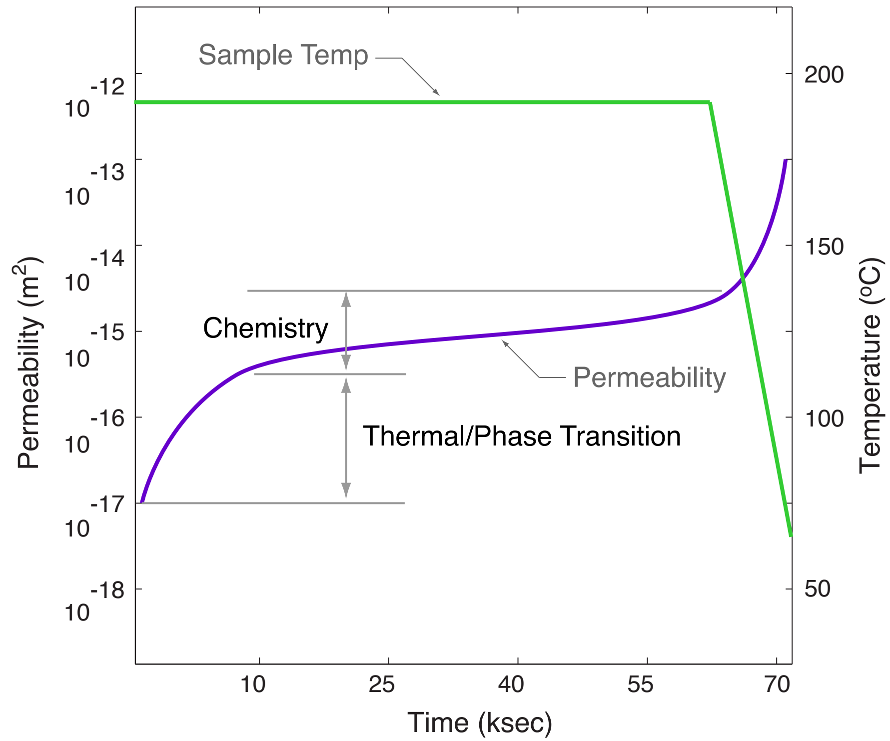
Theories for Damage Mechanisms

Primary drivers

- Phase change from condensed to gas phase leads to material weakening
- Thermal expansion of both the condensed and gas phases creates confinement pressurization that stresses the material
- Pore pressure pushes bonds in the material apart leading to weakening (inter-grain or intra-grain)
- Compounding effects like chemical reaction acceleration due to increased surface area from damage

Second order effects

- Dislocation movement and void coalescence
- Changes in crystal structure or packing



Stages of damage during heating

Diagram taken from Baine Asay lecture notes: Deflagration-to-Detonation Transition, Sept 2011

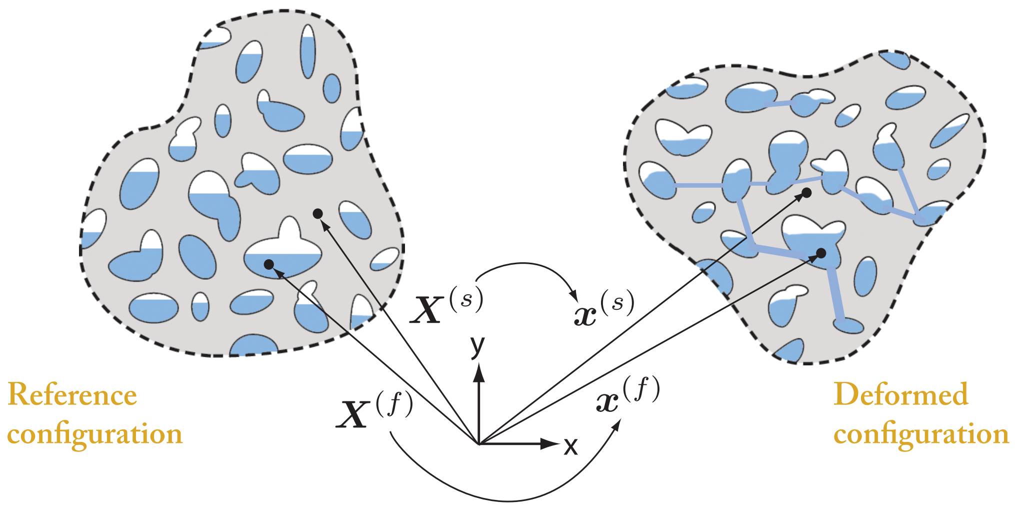
Coupling Approach Overview

Damage modified permeability

- Model race tracking and decreased resistance to flow (added permeability)
- Incorporate pore volume changes resulting from deformation of the solid media (added compressibility)

$$\bar{\alpha} = S_n \left(1.0 + \beta \frac{||\mathbf{T}^{(s)} - \mathbf{T}_0||}{||\mathbf{T}_0||} \right)$$

$$\phi = C_\phi (1 - (1 - \phi_0)/\det[\boldsymbol{F}])$$

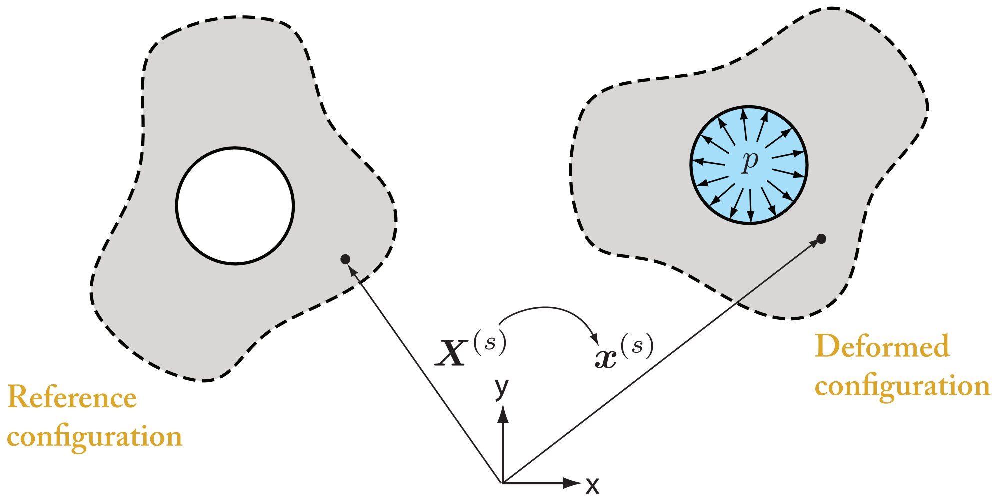


$$\alpha^{(f)} = \alpha^{(f)}(\text{damage, stress criterion})$$

$$\phi^{(s)} = \phi^{(s)}(\text{deformation gradient})$$

Effective stress

- Internal force on pores brought about by the fluid/gas pressure (added stress)



$$\boldsymbol{T}^{(s)} = \boldsymbol{T}_e^{(s)} + p^{(f)} \boldsymbol{I}$$

Decomposition Model

$$\rho C_p \frac{\partial T}{\partial t} - \mathrm{div}[\boldsymbol{q}] = \rho \dot{q} S$$

Energy equation for temperature, T

$$\boldsymbol{q} = k \ \mathrm{grad}[T]$$

Fickian diffusion

$$\frac{\mathrm{d}X}{\mathrm{dt}} = -S$$

Species equation for species, X

$$\frac{\partial \rho}{\partial t} + \rho \ \mathrm{div}[\boldsymbol{v}] = \rho S$$

Mass balance equation for pressure, p

$$\boldsymbol{v} = -\frac{\boldsymbol{K}}{\mu} \mathrm{grad}[p]$$

Darcy's law (momentum balance) for velocity, v

$$S = \underbrace{A\mathrm{exp}\left(-\frac{E}{RT}\right)}_{\text{Arrhenius}} \underbrace{\left(\frac{p}{p_0}\right)^r}_{\text{Pressure dependent}} \underbrace{X^n (1 - wX)^m}_{\text{Autocatalytic}}$$

Reaction rate model for source, S

Arrhenius

Pressure dependent

Autocatalytic

$$\boldsymbol{K} = f(\mathrm{damage})$$

Damage modified permeability

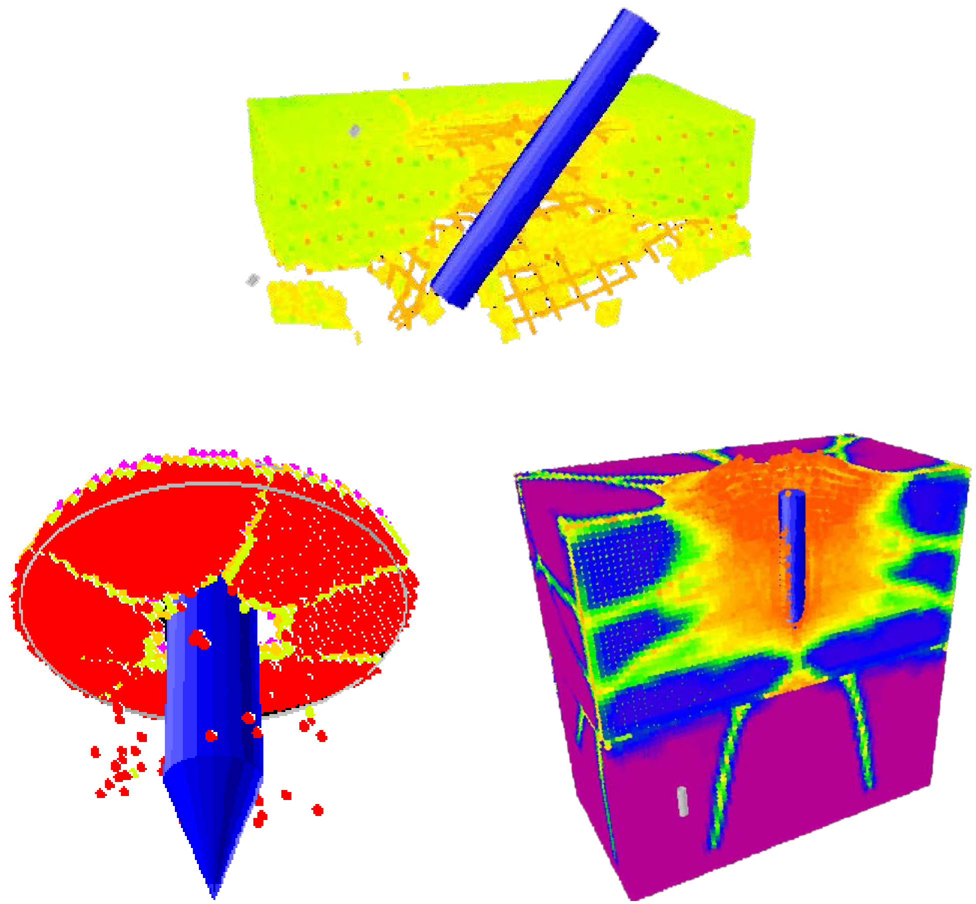
$$\int \mathrm{w} \cdot \mathcal{L}(\cdot) \ \mathrm{d}\Omega = 0$$

Standard Galerkin single field weak form

Deformation and Damage Evolution

Peridynamics

- Integral based formulation rather than differential equations
- Nice features regarding crack propegation paths
- Scalable for massively parallel
- Similarities with molecular dynamics
- Efficient for large scale damage evolution
- Can be used effectively in an explicit or implicit context
- Traditional elasticity theory can be recov-ered under the right circumstances

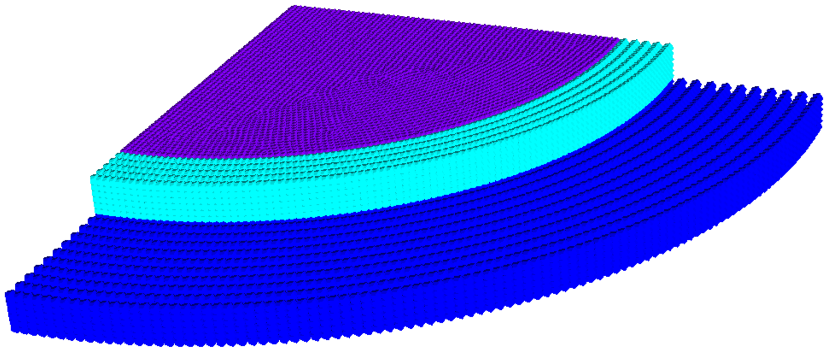


Various peridynamics simulations of projectile impact

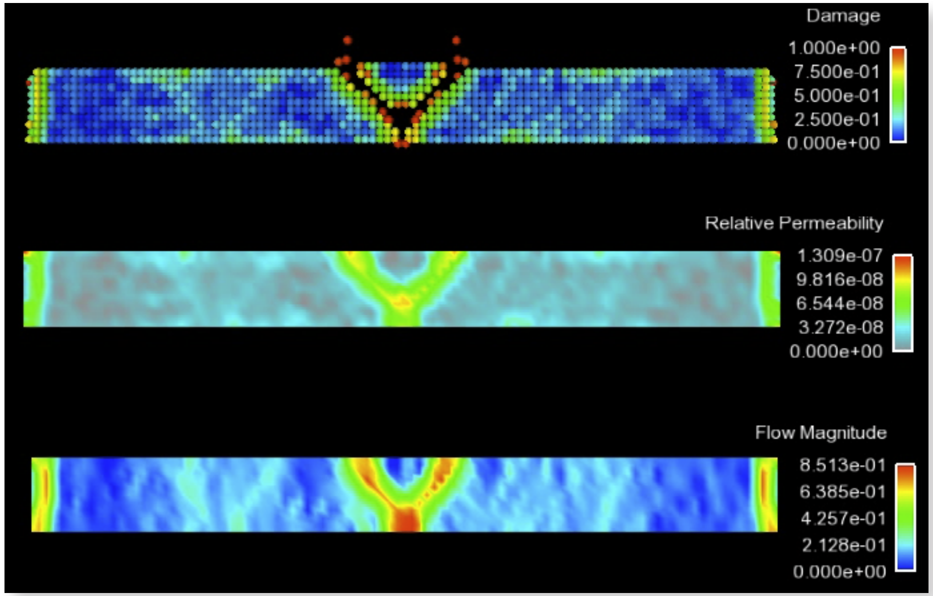
Images taken from EMU web page. Simulations done by Stewart Silling and co-workers

Various uses of peridynamics for modeling damage

- Mechanical deformation and fracture in the confinement
- Model for computing permeability due to damage caused by fluid-structure interaction (mixture theory)
- Cracking and void formation in the energetic material
- Combinations of the above



Model of energetic material, seal, and portion of the anvil



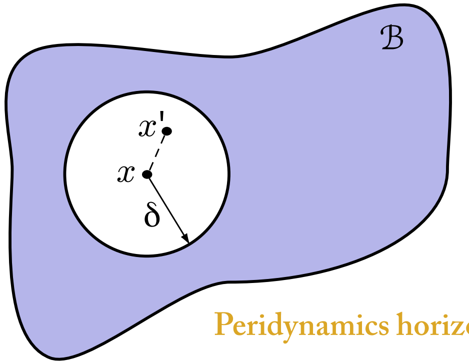
Flow across a porous tensile specimen

Peridynamics formulation

- Equation of motion

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \mathbf{L_u}(\mathbf{x},t) + \mathbf{b}(\mathbf{x},t) \qquad \forall\, \mathbf{x} \in \mathscr{B},\quad t \geq 0,$$

$$\mathbf{L_u}(\mathbf{x},t) = \int_{\mathscr{B}} \{\underline{\mathbf{T}}[\mathbf{x},t]\langle \mathbf{x}' - \mathbf{x}\rangle - \underline{\mathbf{T}}[\mathbf{x}',t]\langle \mathbf{x} - \mathbf{x}'\rangle\}\, \mathrm{d}V_{\mathbf{x}'}$$



Peridynamics horizon

- Discretized equation of motion

Cells in neighborhood of x (horizon)

Bond

$$\rho(\mathbf{x})\ddot{\mathbf{u}}_h(\mathbf{x},t) = \sum_{i=0}^{N} \left\{\underline{\mathbf{T}}[\mathbf{x},t]\left\langle \mathbf{x}_i' - \mathbf{x}\right\rangle - \underline{\mathbf{T}}'[\mathbf{x}_i',t]\left\langle \mathbf{x} - \mathbf{x}_i'\right\rangle\right\} \Delta V_{\mathbf{x}_i'} + \mathbf{b}(\mathbf{x},t)$$

Force state (associates bond with force density per unit volume)

- Material model

Unit vector pointing from x to x'

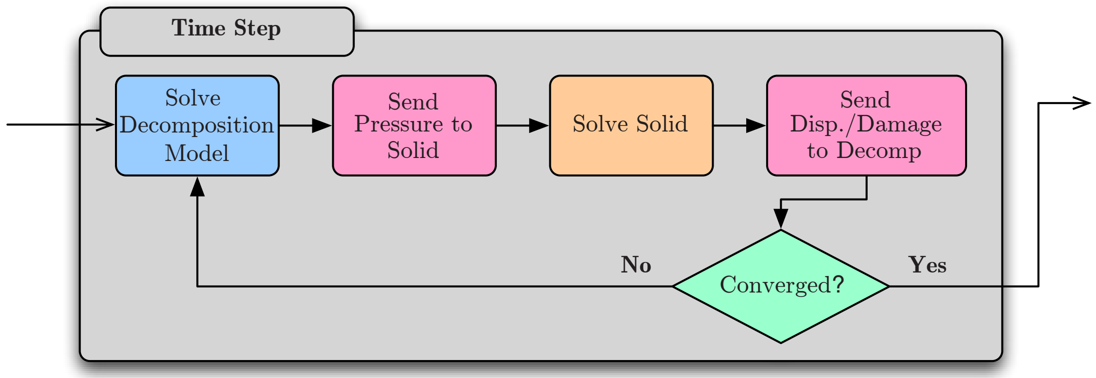
$$\underline{\mathbf{T}}[\mathbf{x},t]\left\langle \mathbf{x}_i' - \mathbf{x}\right\rangle = \underline{t}\ \underline{\mathbf{M}}[\mathbf{x},t]\left\langle \mathbf{x}_i' - \mathbf{x}\right\rangle$$

Pairwise force based on the deformation of all cells in the neighborhood of x

$$t_e = \underline{t} + \tilde{t}(p^{(f)})$$

Effective stress contribution

Solution procedure



Lockstep solution procedure

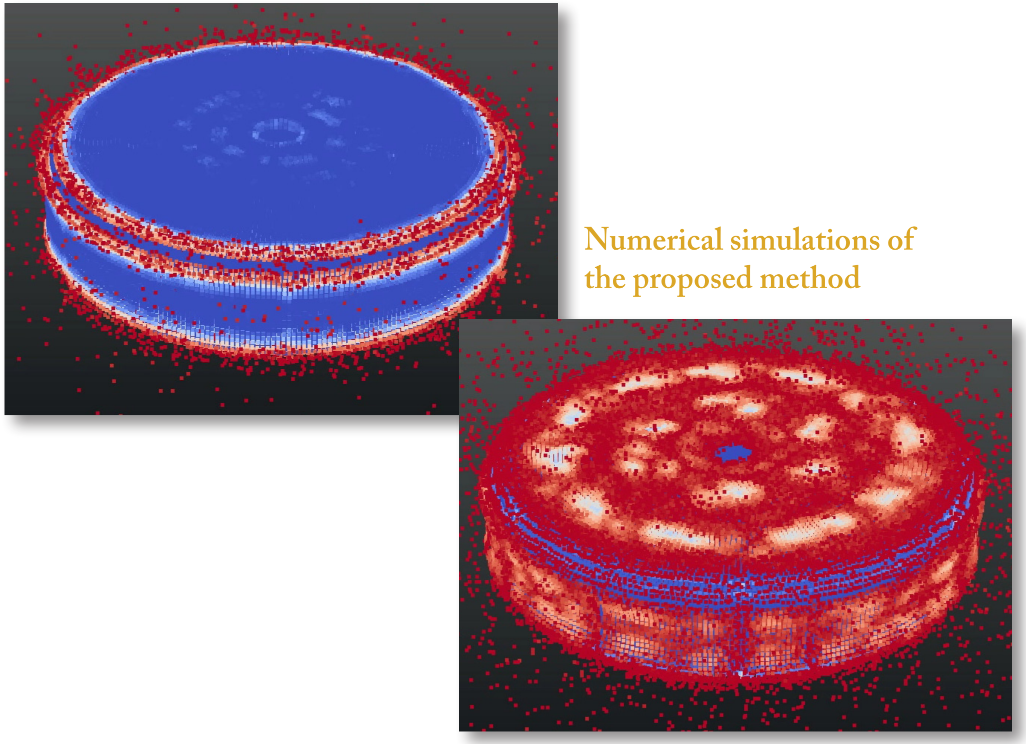
```
Begin Solution Control Description

   Use System Main
   Begin System Main
      Begin Transient The_Time_Block
         Advance AriaRegion
         Transfer Aria_to_Presto
         Transfer Aria_to_Presto_Bond
         begin subcycle PrestoSubcycle
           Advance PrestoRegion
         end
         Transfer Presto_to_Aria
      End
   End
```

Sierra solution control input block

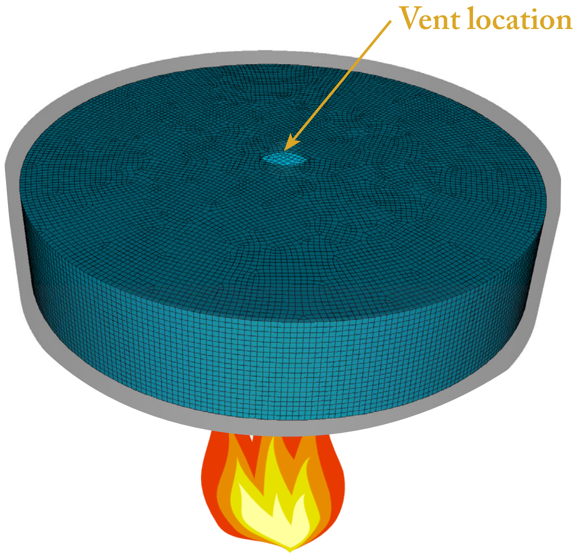
Slow cookoff

Questions for accident scenarios

- Will ignition occur? Or will the reaction gases escape before pressurizing or reacting?
- How might the enclosure fragment and with how much energy will the pieces be projected?
- Does damage to the energetic material change the ignition location or the volume that simultaneously ignites?
- How can safety mechanisms like vents be designed to ensure insensitive munitions without inadvertently encouraging reaction violence?
- How does ullage effect reaction violence if at all?



Numerical simulations of the proposed method

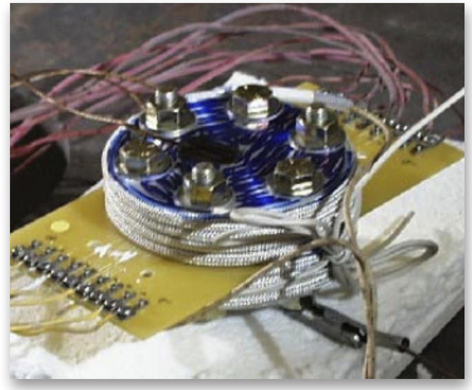


Experiment Description

Problem description

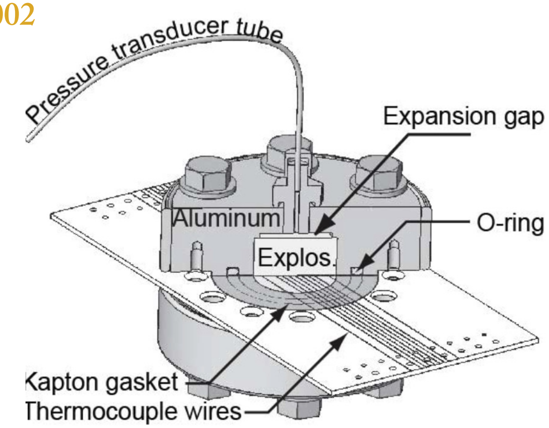
- Heating drives the reaction rate which may or may not run away
- Pressure causes material damage which allows for both pressure relaxation and transport of heat via fluid through the cracks
- Eclosure breach or seal damage allows gas to escape potentially stalling reaction

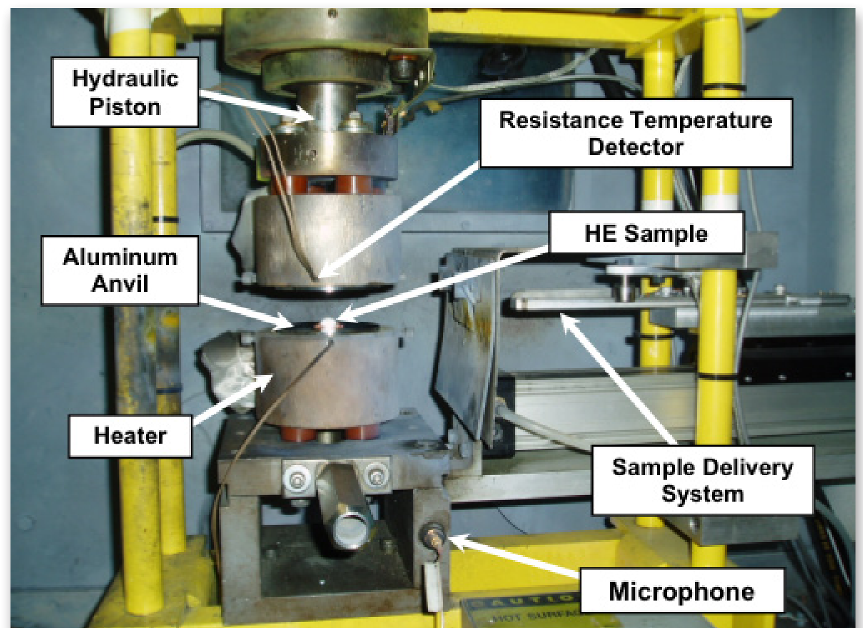
- Multiphysics coupling:
  mass balance (pressure)
  energy (temperature)
  species transport (concentration)
  peridynamics (displacements)



SITI device

Kaneshige, Renlund, Schmidtt, and Erikson, 2002





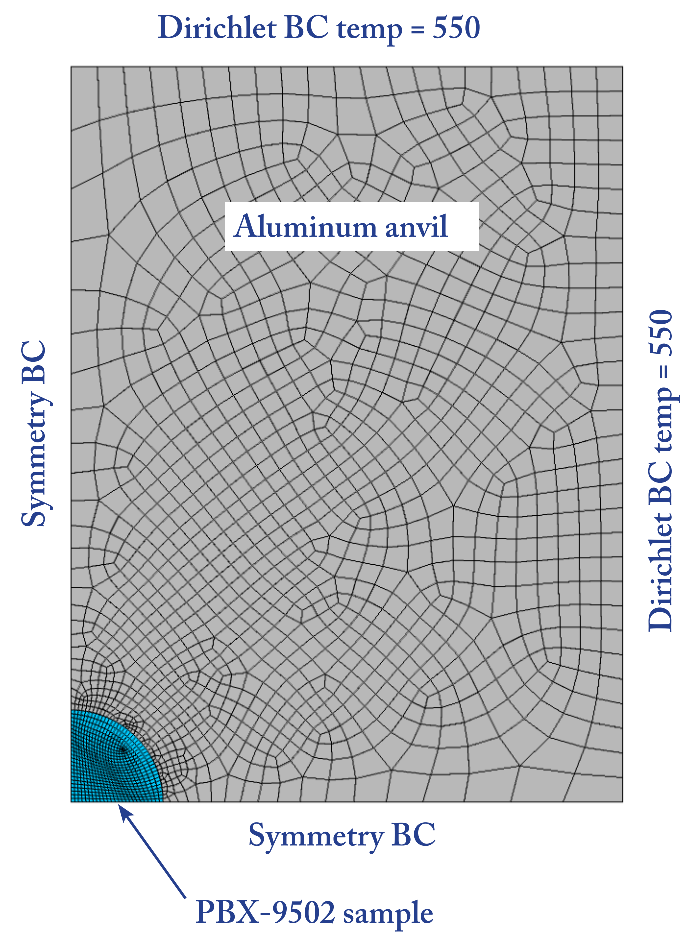
Koerner, Maienschein, Burnham, and Wemhoff, UCRL-CONF-232590

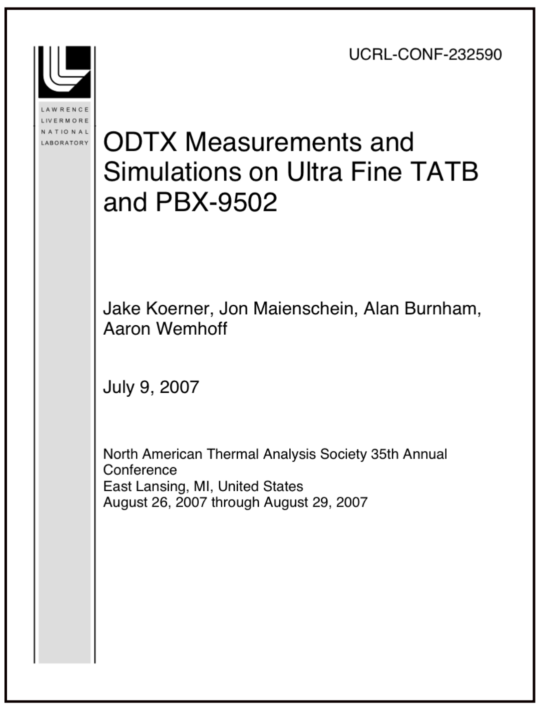
ODTX device

Decomp Model Validation (No Damage)

ODTX with PBX-9502

- Vary anvil temperature measure time to ignition
- No pressure dependence
- No damage model
- No enclosure deformation
- Assuming sealed confinement




UCRL-CONF-232590

LAWRENCE LIVERMORE NATIONAL LABORATORY

ODTX Measurements and Simulations on Ultra Fine TATB and PBX-9502

Jake Koerner, Jon Maienschein, Alan Burnham, Aaron Wemhoff

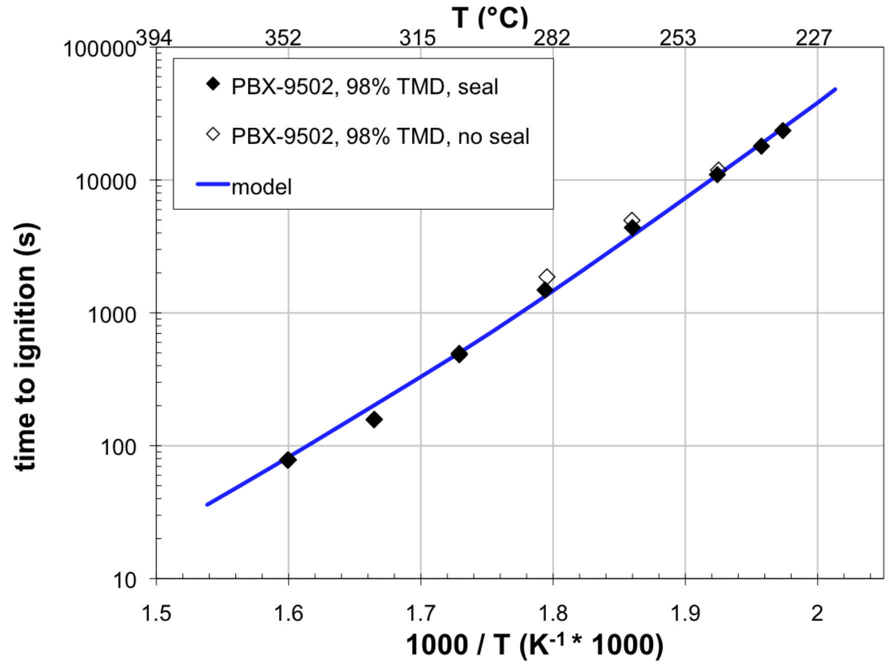
July 9, 2007

North American Thermal Analysis Society 35th Annual Conference
East Lansing, MI, United States
August 26, 2007 through August 29, 2007

$$S = A\exp\left(-\frac{E}{RT}\right)X^n(1-wX)^m$$

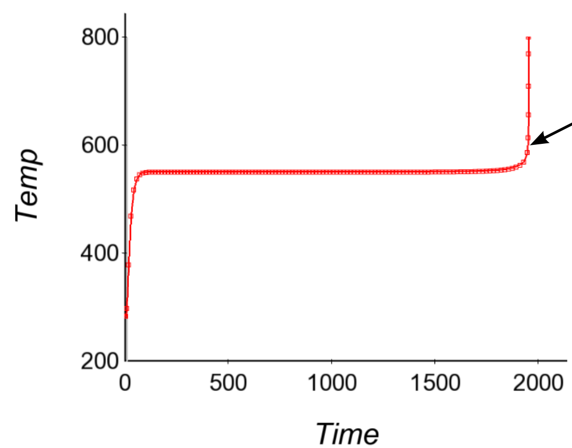
Reaction rate model for source, S

Decomp Model Validation (No Damage)

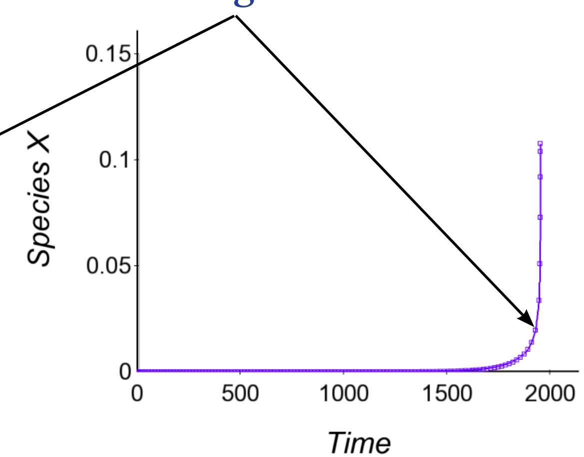


Time to ignition vs. anvil temperature

Ignition



Temperature vs. time



Species X vs. time

Permeability Changes Due to Damage

Unconfined PBX-9501

- Leading prediction is that permeability chages are mainly due to phase change
- Pressure dependent rate model
- Random initialization of bond strength
- Measure average flux/pressure and back calculate the permeability
- Specific permeability K/μ

Reaction rate model for source, S

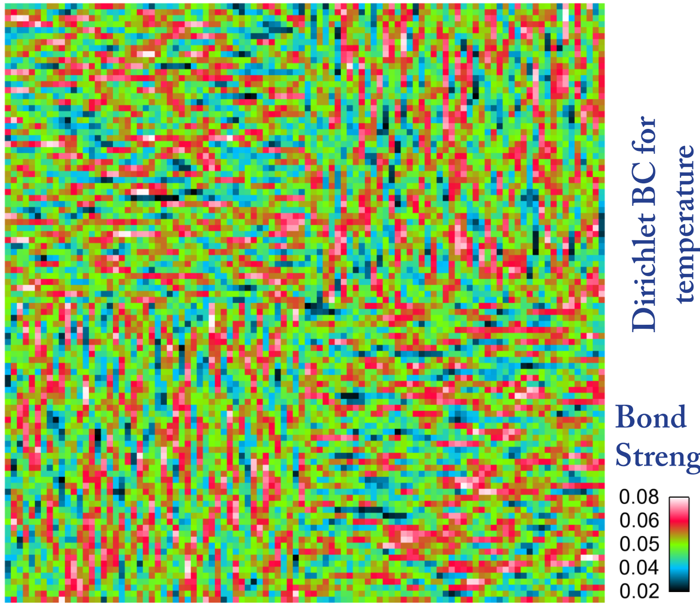
$$S = A\exp\left(-\frac{E}{RT}\right)\left(\frac{p}{p_0}\right)^r X^n(1 - wX)^m$$

Darcy Flow

$$\boldsymbol{v} = -\frac{\boldsymbol{K}}{\mu}\mathrm{grad}[p]$$

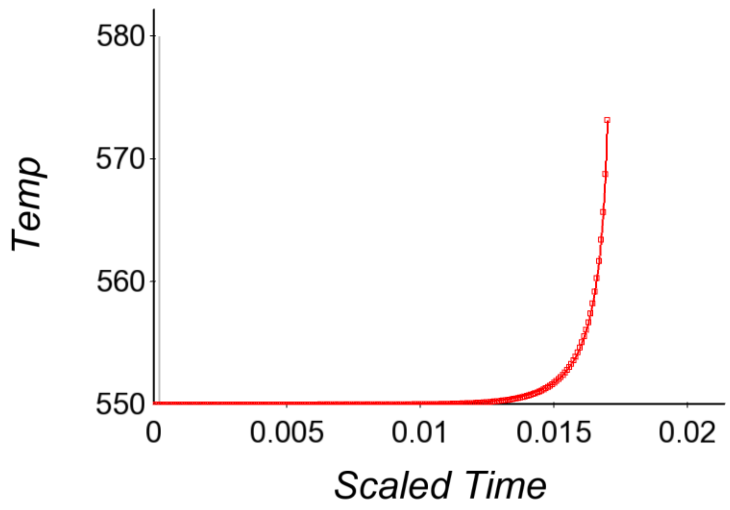
Local permeability model

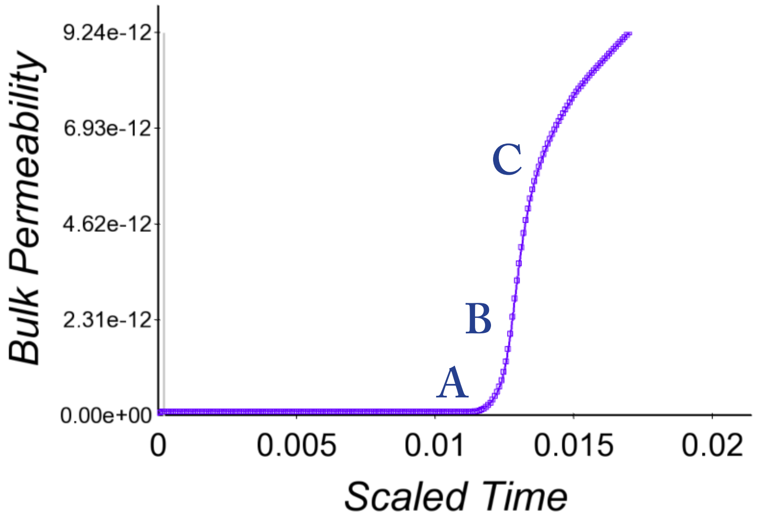
$$\boldsymbol{K} = f(\mathrm{damage})$$



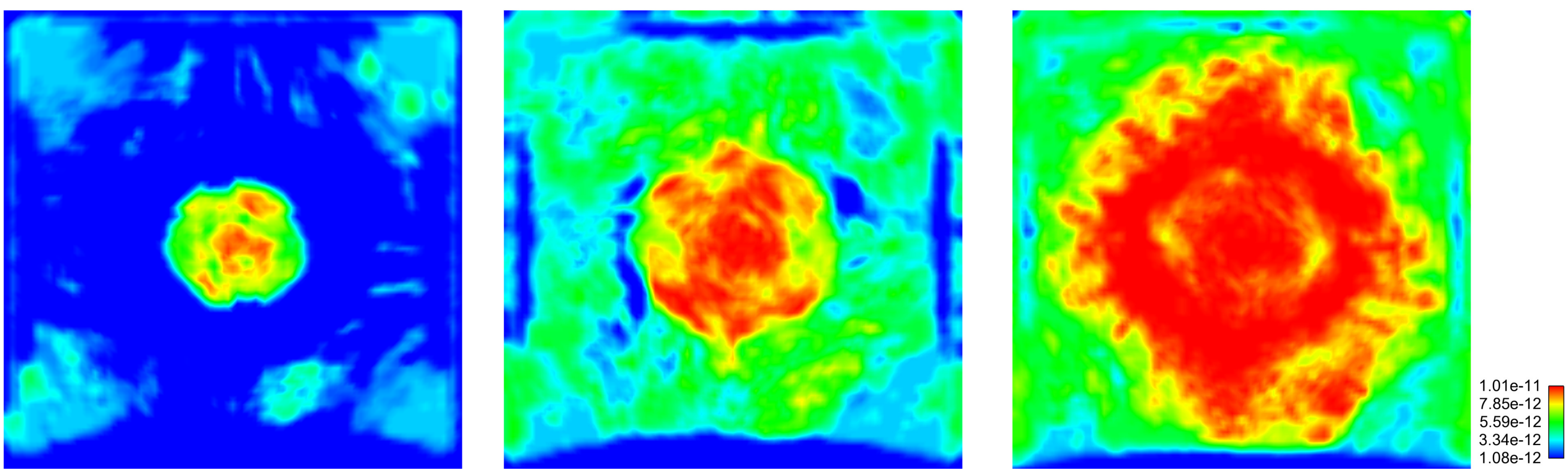
Schematic of unconfined PBX-9501 sample showing random particle bond strength

Permeability Changes Due to Damage



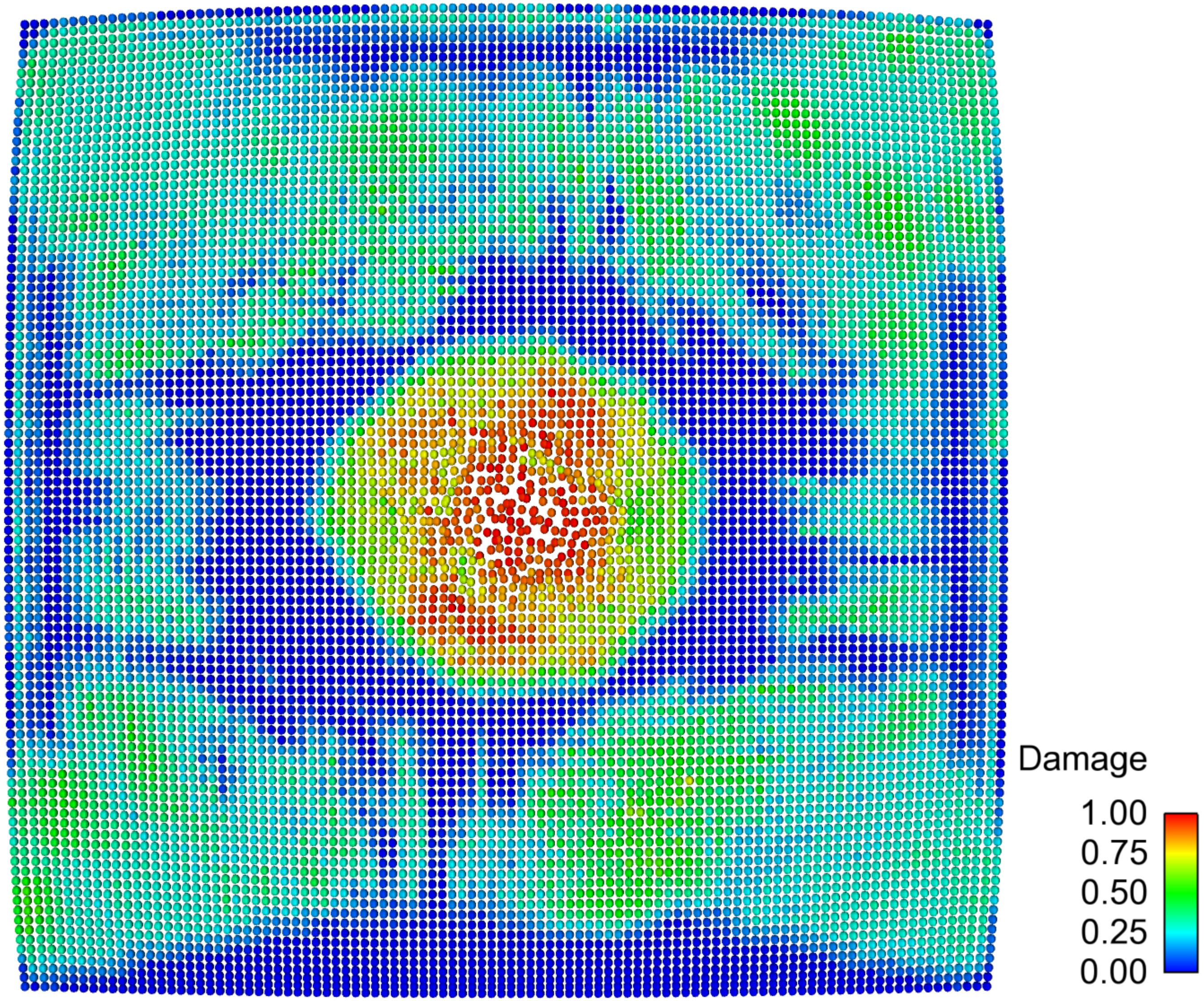


A B C



Plots of local permeability due to damage
for various points in time

Permeability Changes Due to Damage



Deformed configuration of PBX-9501 sample
immediately prior to ignition (point B)

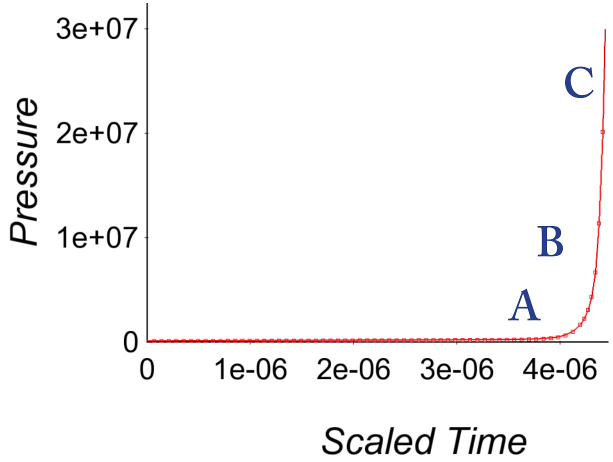
Stalling ignition

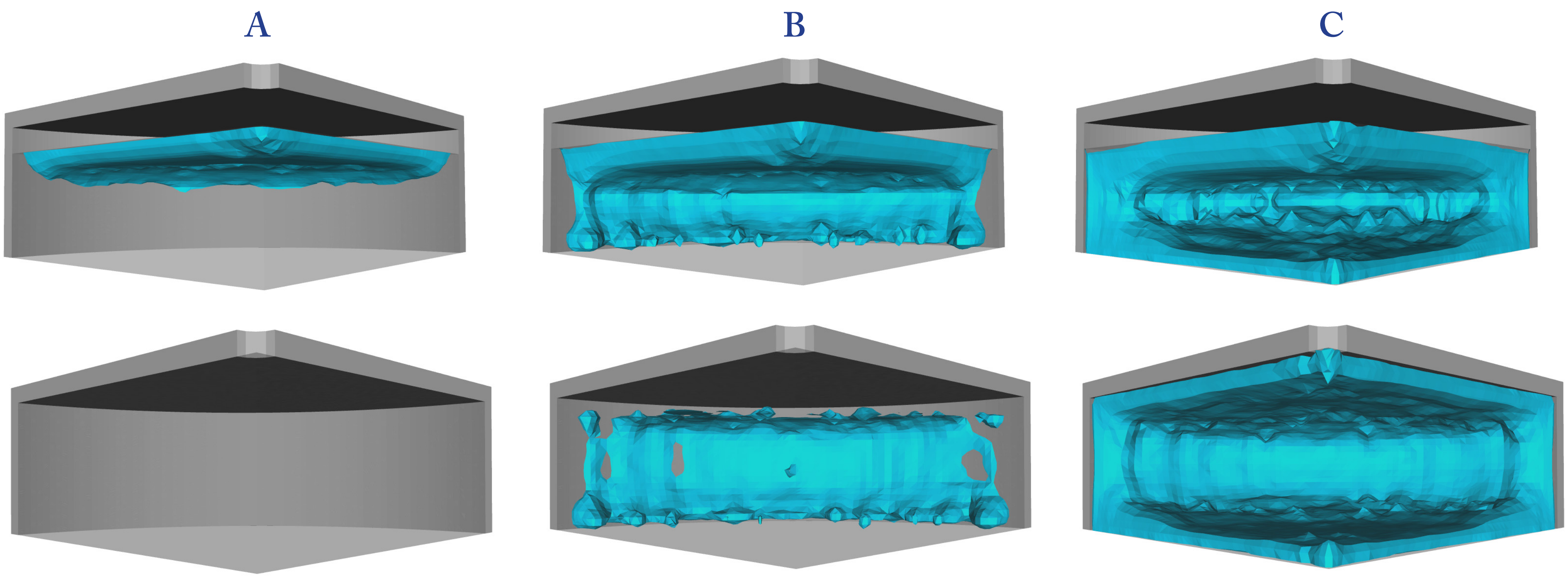
- For certain cases an explosion may or may not occur depending on the integrity of the confinement
- If reaction gases escape during heating, the confinement may depressurize leading to slower reaction rates

Damage Evolution Characteristics

Damage evolution characteristics

- How does the material decompose inside the confinement at ignition?
- How does damage propegate inside the energetic material?

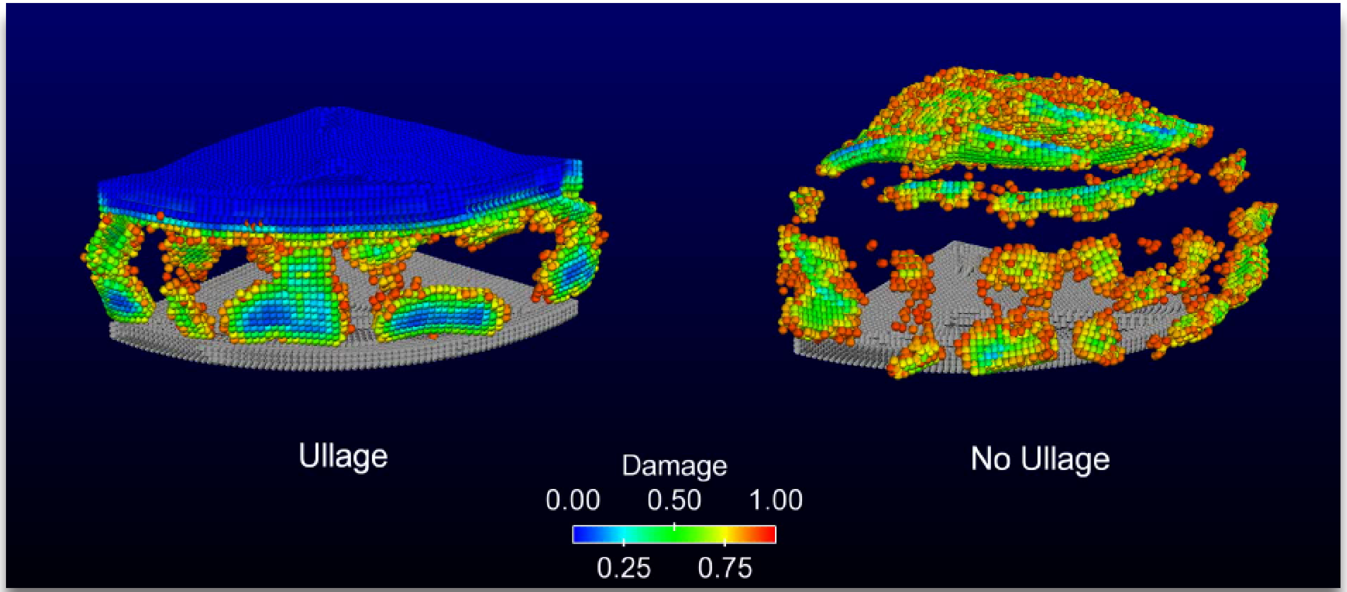




Isosurface of damage in (top) confinement with ullage
(bottom) confinement with no ullage
at various times during ignition

Fragmentation and projectile energy

- How does ullage in the confinement affect the resulting fragmentation?
- For a given scenario, how large will the fragments be and with how much energy will they project?



Summary and Future Work

Overview of numerical approach

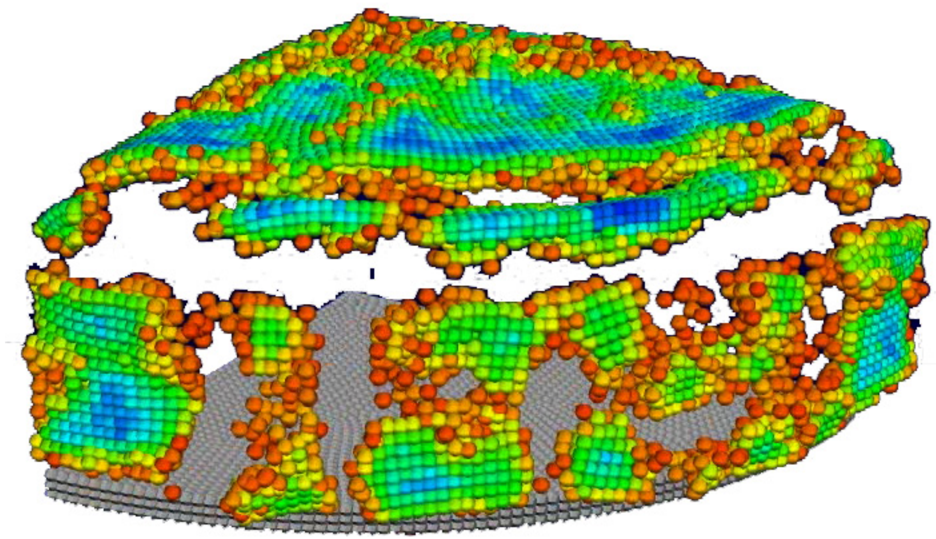
- Pore pressure / effective stress addition to peridynamics
- Modified permeability based on peridynamics damage criteria

Problems of interest

- Enclosure breach
- Permeability changes due to damage
- Fragmentation of confinement

Future work

- Experimental validation
- Model development
- Justification for peridynamics effective stress from first principles



Fragmentation pattern for simple confinement at ignition

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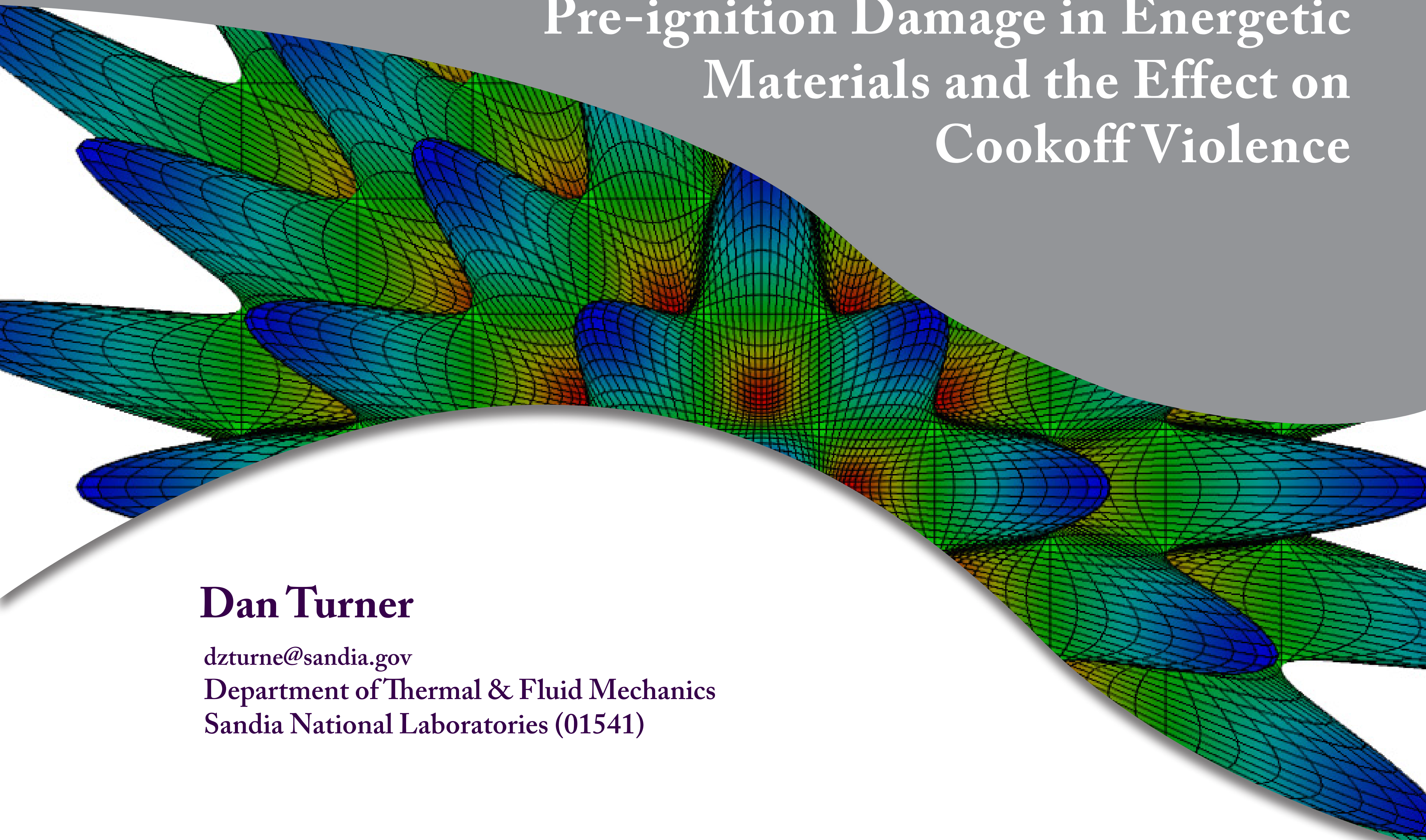

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