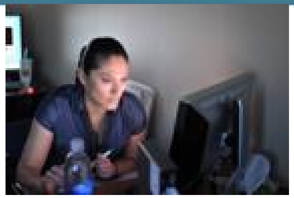
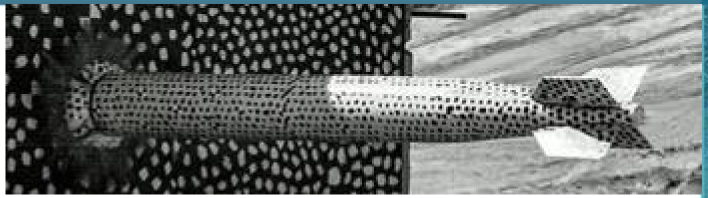
SAND2022-7410C

Sandia National Laboratories

Meshfree modeling of coupled mechanical-thermal-chemical phenomena in energetic aggregates at multiple length scales

LDRD LABORATORY DIRECTED RESEARCH & DEVELOPMENT WHERE INNOVATION BEGINS

Judith A. Brown[1], Frank Beckwith[1], Ki Tae Wolf[1], Joel Clemmer[1], Caleb Overstreet[2], Marcial Gonzalez[2]

[1]Sandia National Laboratories, Albuquerque, NM, USA

[2]Purdue University, West Lafayette, IN, USA

8th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS)

June 5-9, 2022, Oslo, Norway

U.S. DEPARTMENT OF ENERGY NNSA National Nuclear Security Administration

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

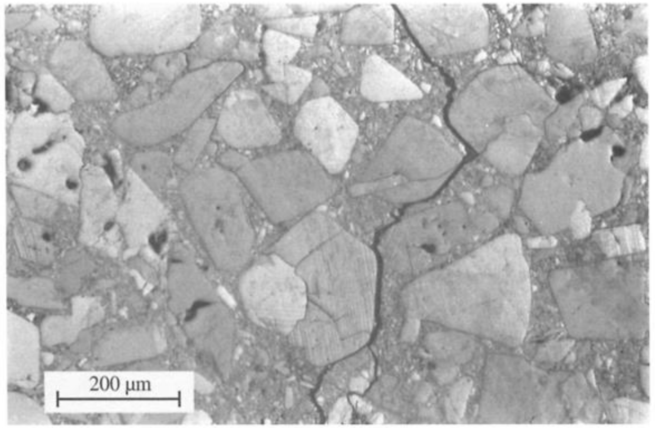
Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

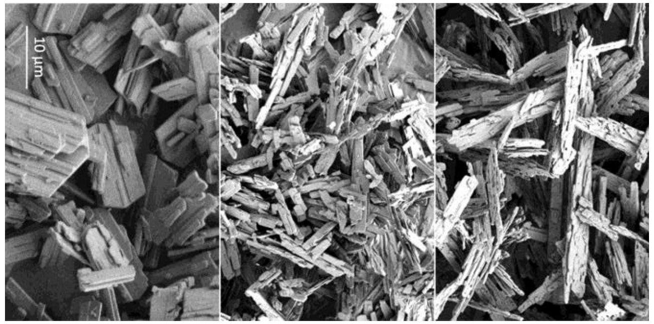
Energetic Materials: A Modeling Challenge

- Complex material structure
- Chemically reactive (fast, exothermic)
- Everything is a function of temperature

Multi-Physics!

Plastic Bonded Explosive [Rae, 2002]





Energetic Crystals [Yarrington, 2018]

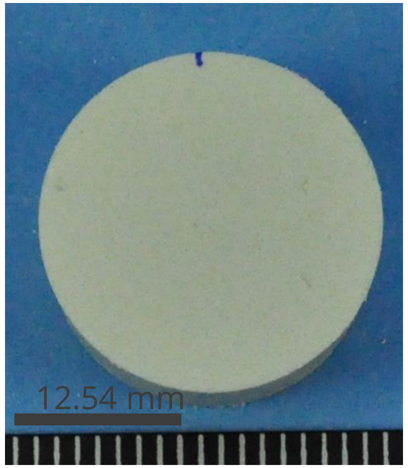
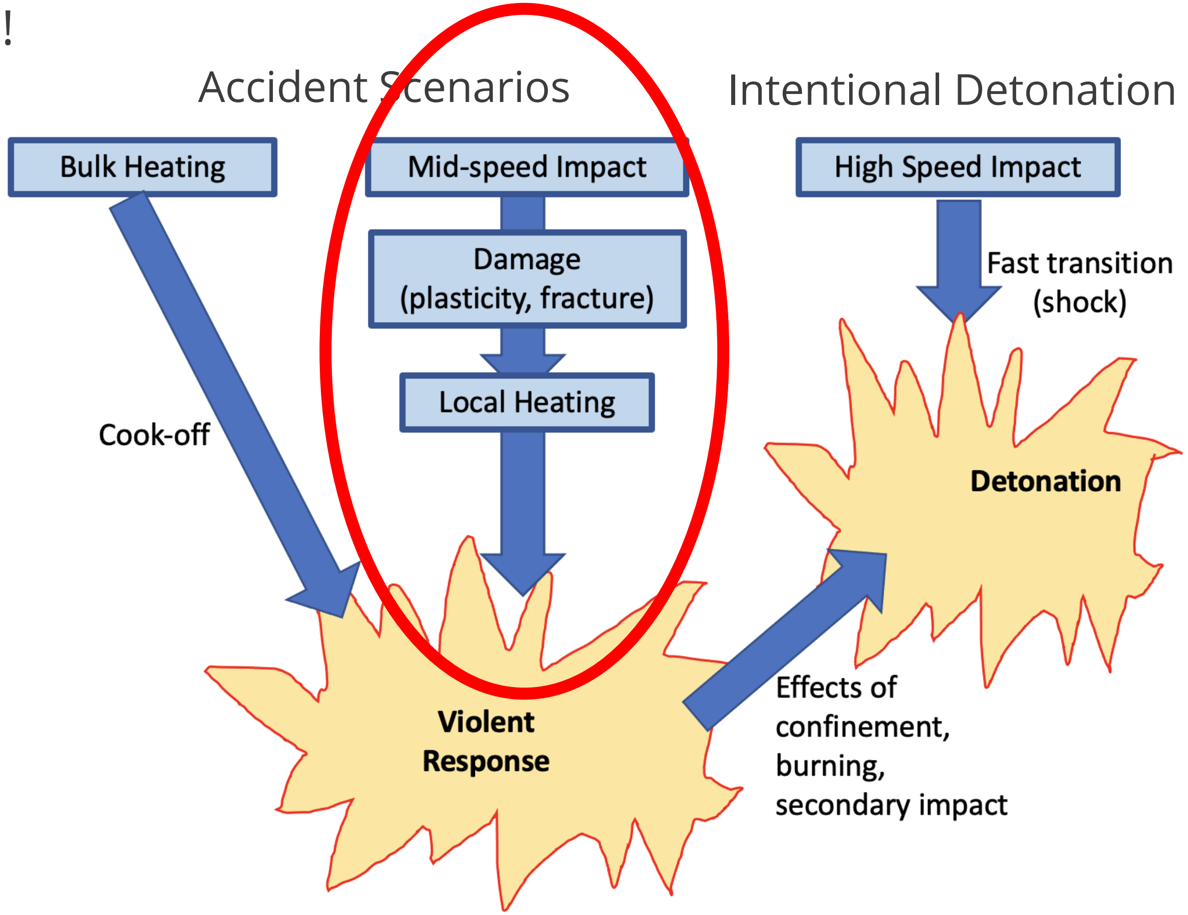


Image: courtesy Marcia Cooper

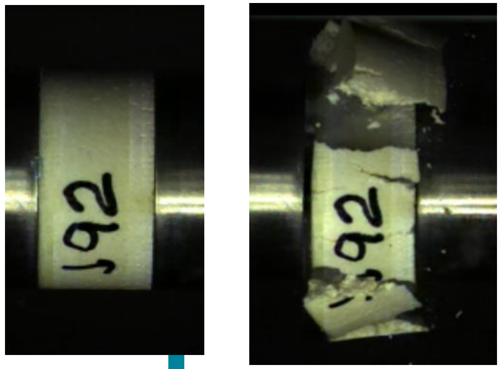
A few different ways to get an explosion...



The Case for Meshfree Methods

Numerical Method Should Accurately Predict:

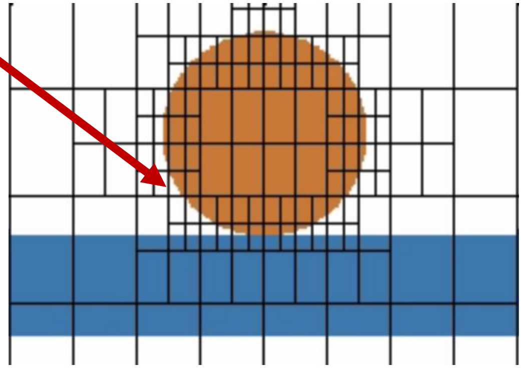
- Capture transition from solid to rubble
- Deformation-induced heating, chemistry

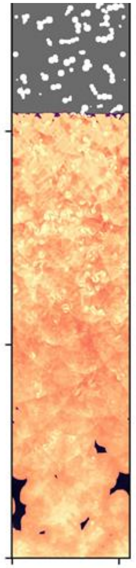


Example: Impact Test, Marcia Cooper

Problem: poorly resolved strain fields and interface physics, averaging in mixed material cells

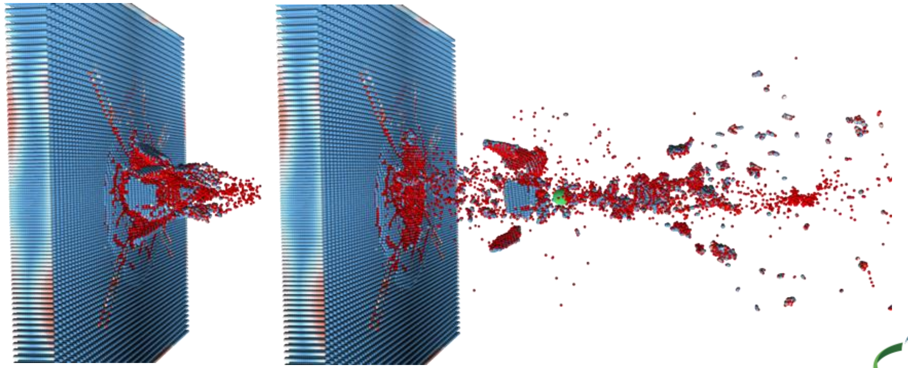
Hydrocode Methods





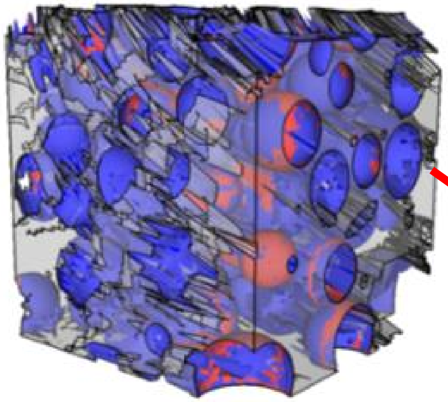
Meshfree Methods

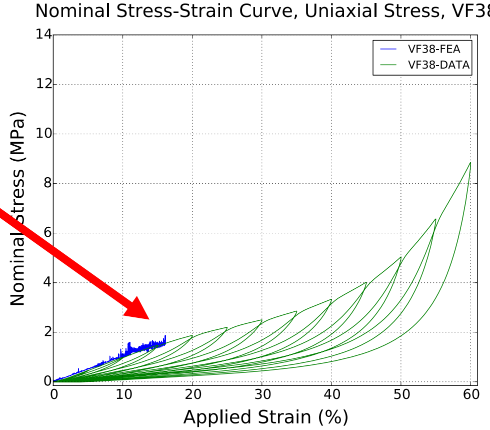
Show promise in overcoming these problems at both meso and macro scales



Mesh-based Methods (FEA)

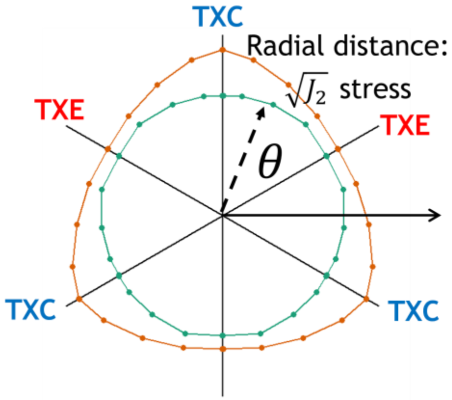
Problem: Mesh entanglement at large deformations



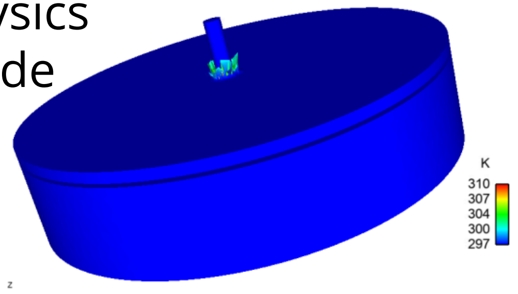


Overall Multiscale Approach

Continuum Constitutive Model



Multiphysics CRK code



Impact Event

Mechanical Deformation & Damage

Local Hotspot Formation

Heat Conduction

Thermally Activated Chemistry

Go

?

No Go

Interface Debonding

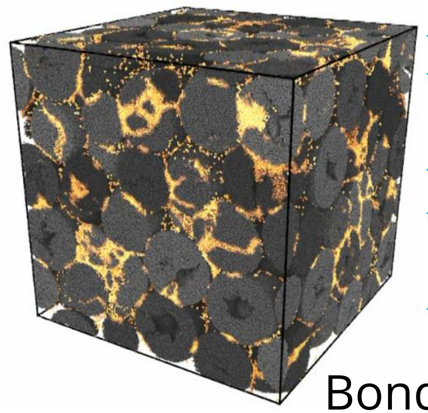
Crystal Fracture

Particle Rotation

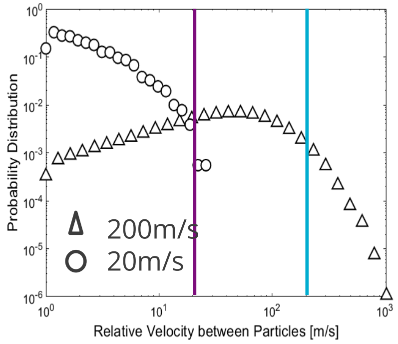
Plasticity

Friction

Viscoelastic Heating



Bonded Particle Methods



Mesoscale Response statistics

Meshfree Mesoscale Models

Give insight to mechanical deformation and damage mechanisms under many different stress states

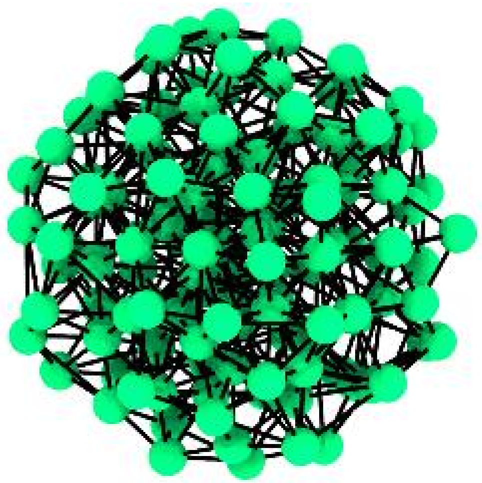
Bonded Particle Models (BPMs)

- BPMs are minimalistic particle-based models for fragmentation – ideal for studying trends/testing theories

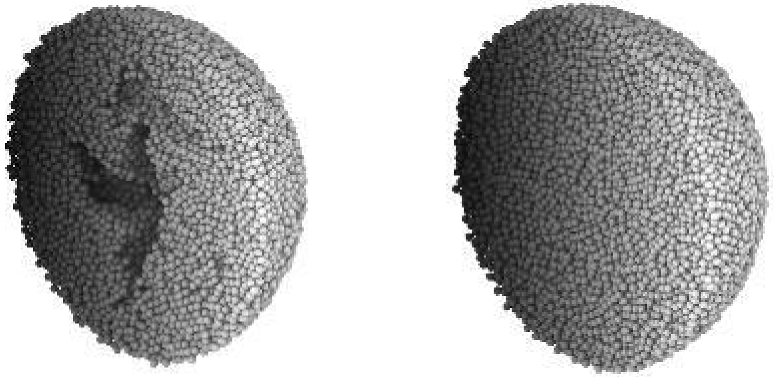
- Very efficient, can simulate large systems, $\sim 10^3$ grains, at high resolutions, $\sim 10^4$ particles/grain

- In BPMs, grain = collection of repulsive particles connected by network of (typically) pairwise bonds
- Bonds break under specific criteria – e.g. stretch threshold
- Functional form of bond controls material properties:
  moduli, fracture toughness, plasticity, viscoelasticity, …

- Open-sourced models available in recently released LAMMPS package



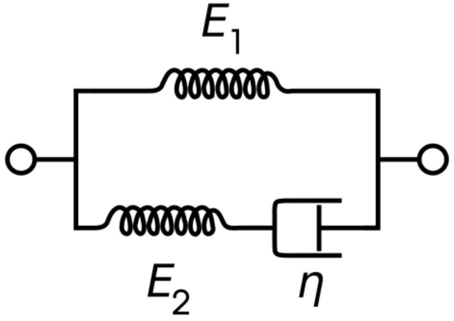
Grain consisting of $\sim 10^2$ particles



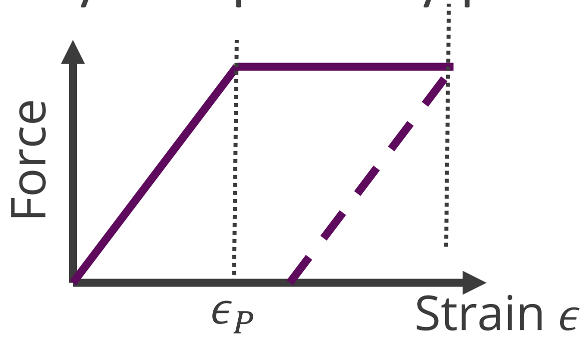
Mesoscale Models of Energetic Composites

BPMs can be easily generalized to support new physics by changing bond construction (~10 new lines of code)

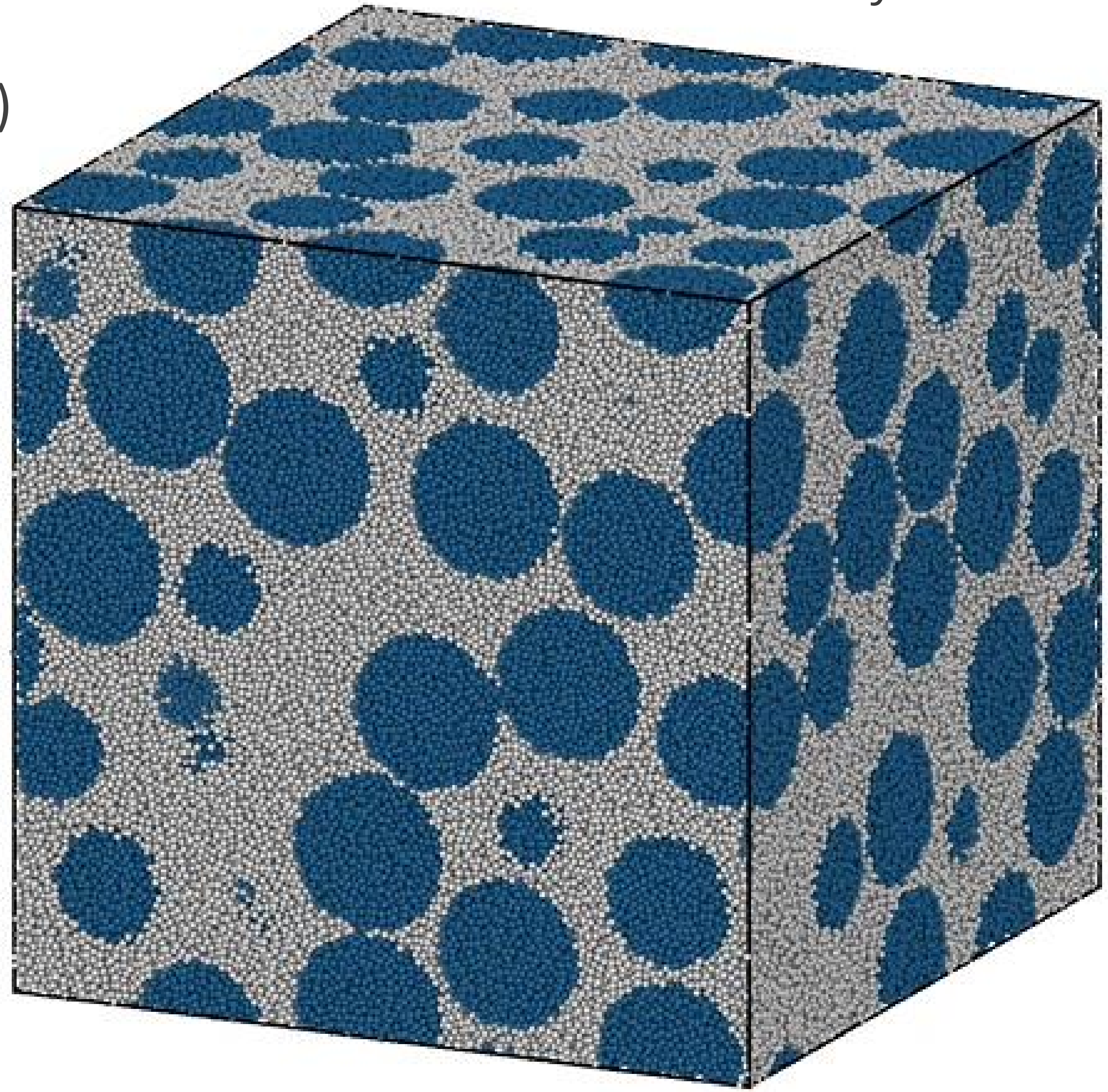
Using Zener bonds gives viscoelasticity
Can generalize to Prony series (Kaiske 1997)



Model plasticity with perfectly-plastic bonds



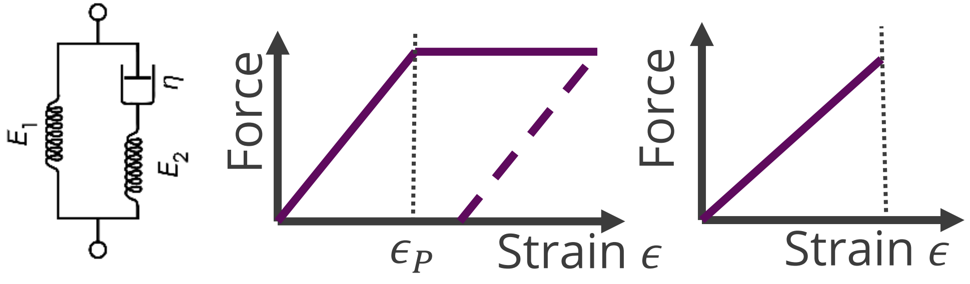
1/8th of studied system size

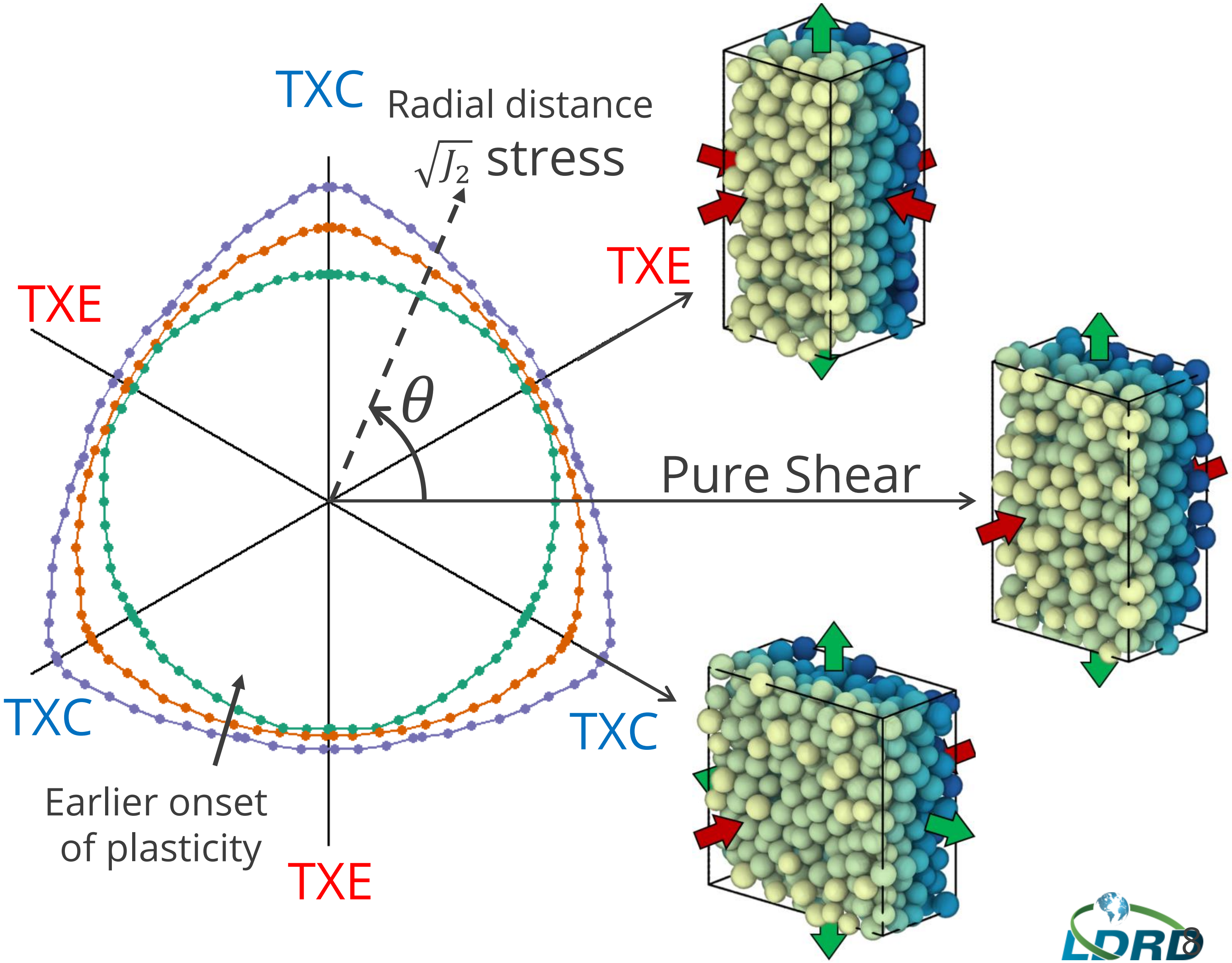


Identifying yield surface shape to inform continuum models

- Many possible loading paths, all have unique failure stress. Map out yield surfaces, often assumed to have simple shape (e.g. Drucker-Prager)

- **Testing how changes in binder's material properties impact yield surface**
  - better understanding of inelastic yielding for continuum models



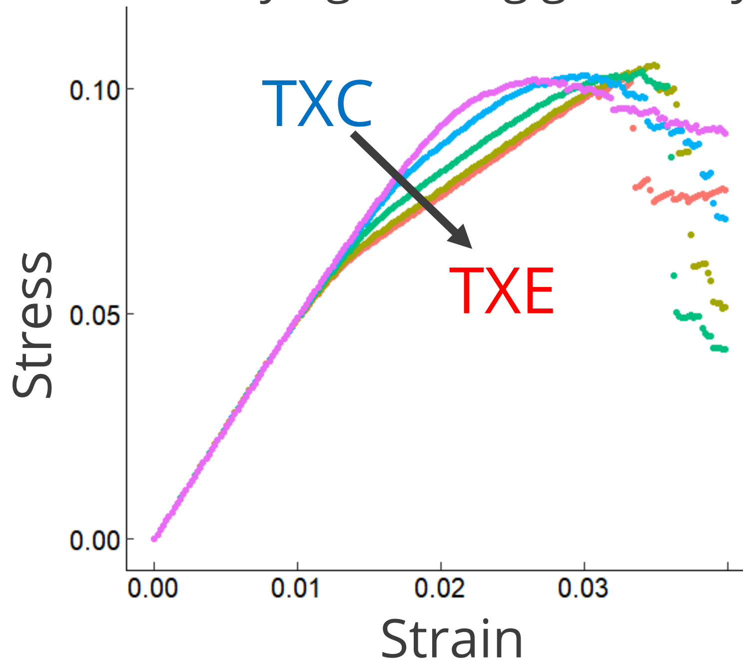


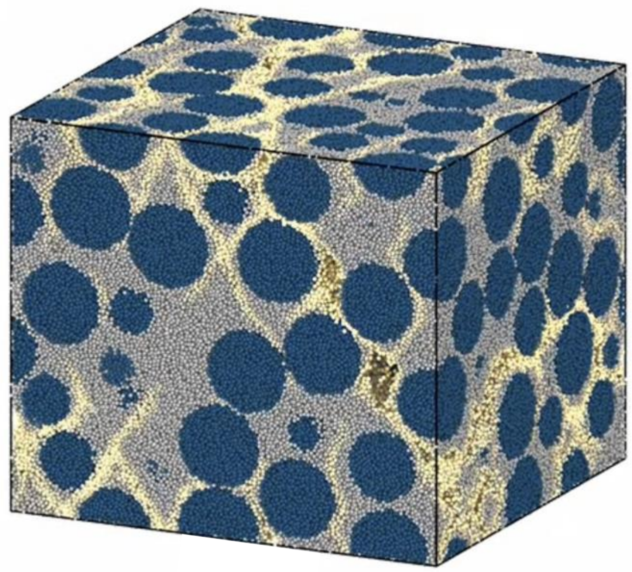
Extending framework to capture damage and crack percolation

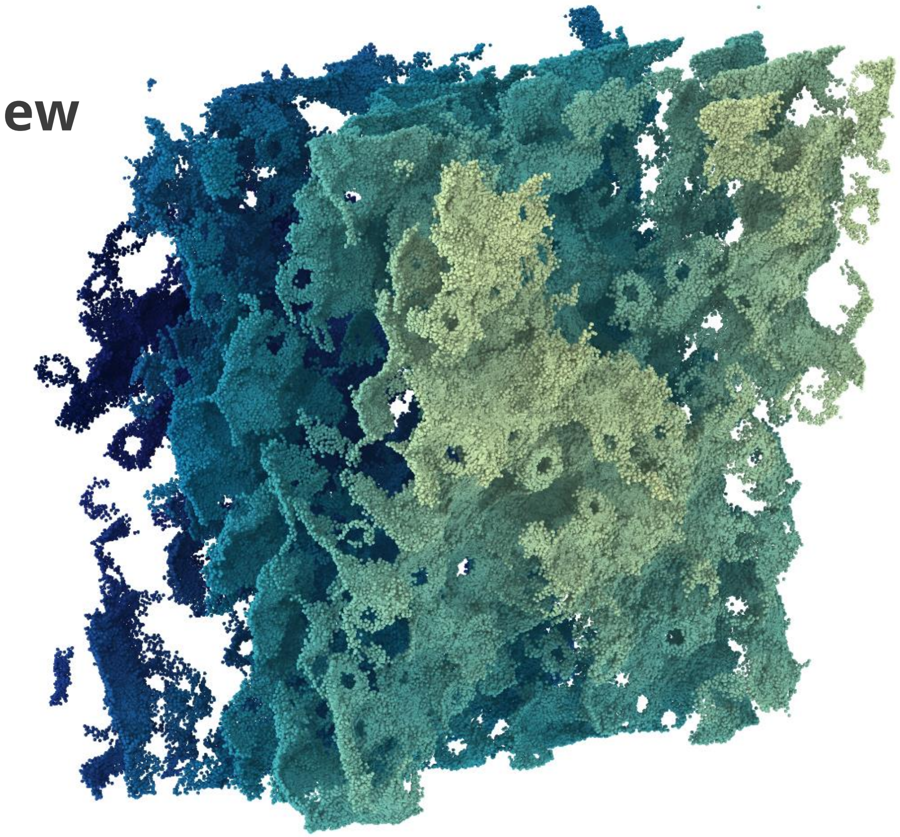
Simulations allow us to identify yield while simultaneously tracking crack growth in binder & quantifying damage

Complete spatial-temporal history of damage provides a new perspective on complex mechanical problems

See emergence of damaged modulus by varying loading geometry





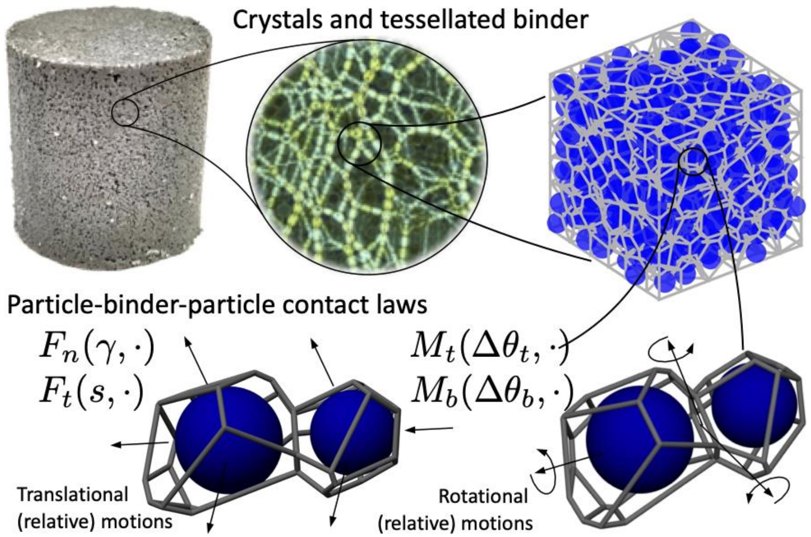


Final percolating crack in binder in pure shear

Statistical Descriptors of Mesoscale Response

PURDUE UNIVERSITY

- **Working hypothesis:** Hot spots are rare events function of distribution tails of mesoscopic statistical descriptors (e.g., inter-particle velocity, contact pressure)



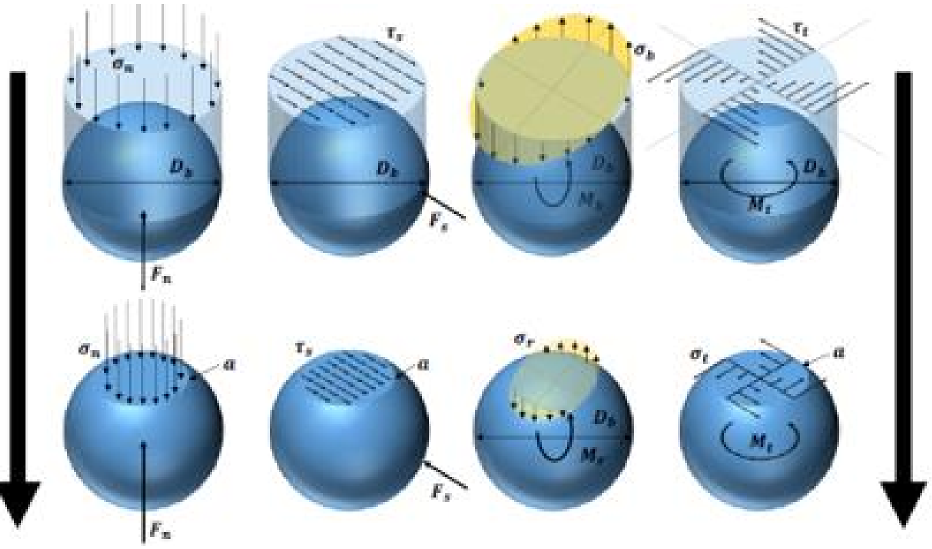
- Particle-based numerical method that includes binder behavior in particle contact laws

Compression

Binder and particles share the compressive load

Transition from particle-binder-particle to particle-particle

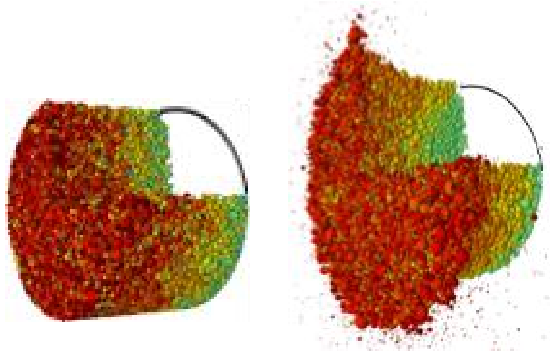
Binder failure in compression. Hertz contact in effect



Tension

Binder alone supports tension

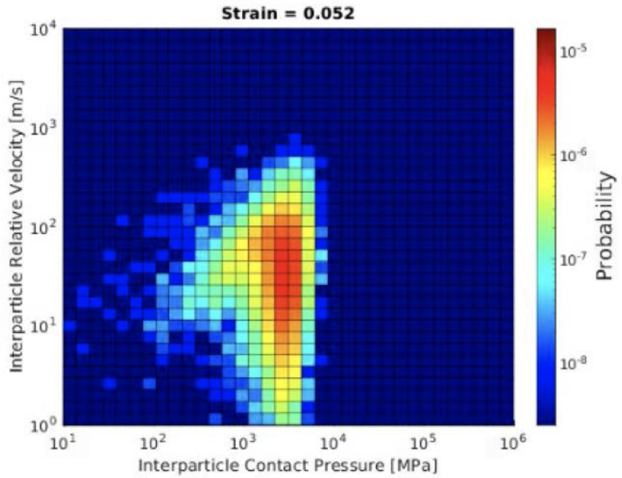
Binder rupture
OR
Binder debonding (depending on properties, initial debonding, and particle sizes)



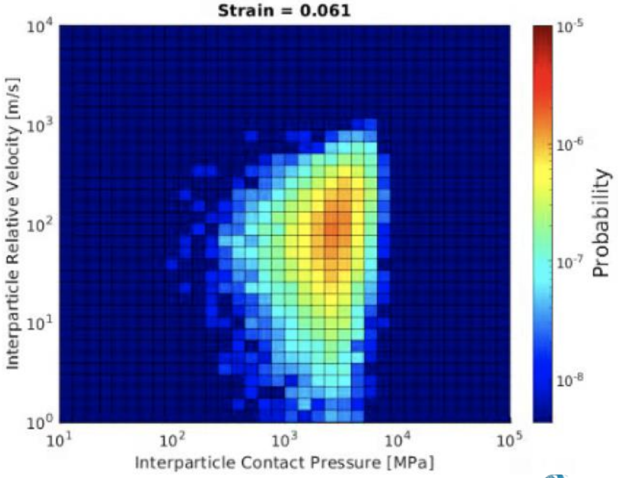
Statistical Descriptors of Mesoscale Response

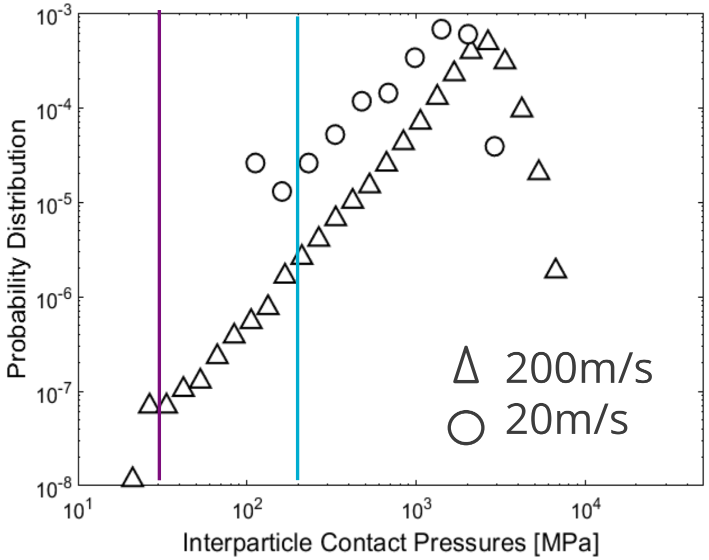
- Interparticle Contact Pressure—indicator for particle fracture
- Relative velocity between particles—indicator for debonding/binder failure
- Explore probability distributions/likelihood of different failure mechanisms to inform failure modes in macroscale model

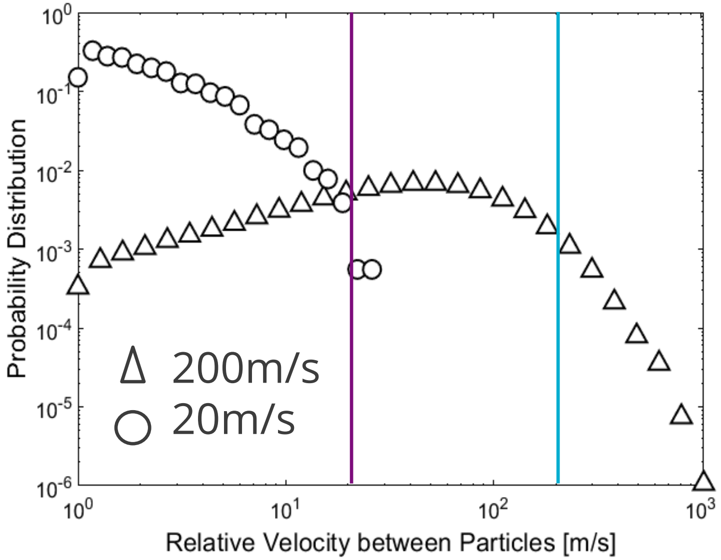
Stiff binder (200m/s)



Soft binder (200m/s)







Macroscale Multiphysics Model

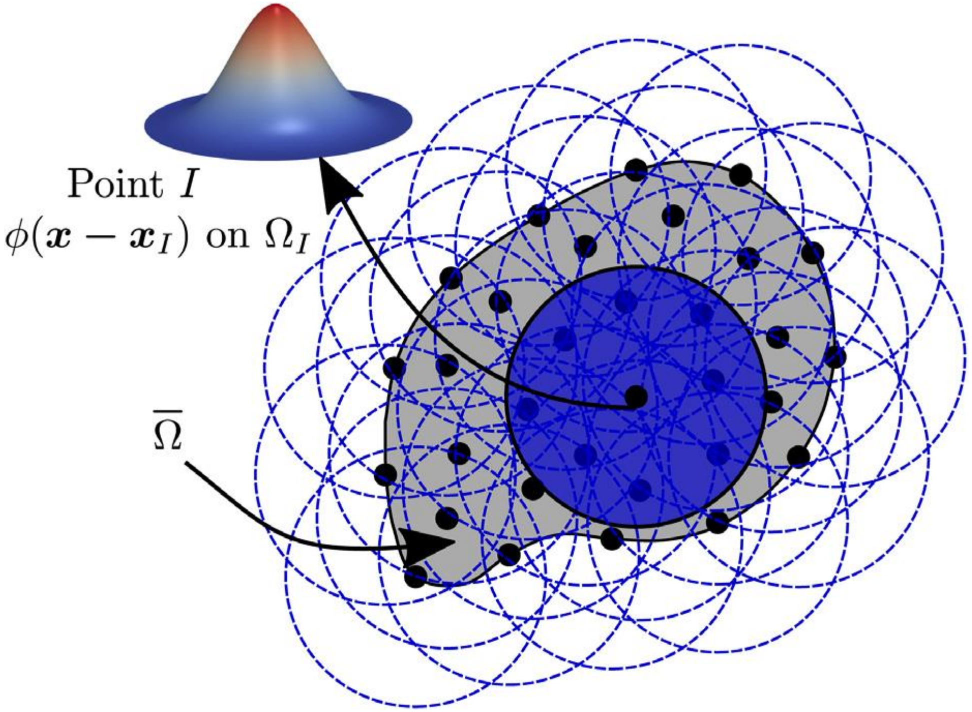
Predict coupled mechanical-thermal-chemistry events

Meshfree Conforming Reproducing Kernel Method

Reproducing Kernel Particle Method

- Galerkin-based variational method using the reproducing kernel discretization
- Shape functions are the product of a window/kernel function and correction function

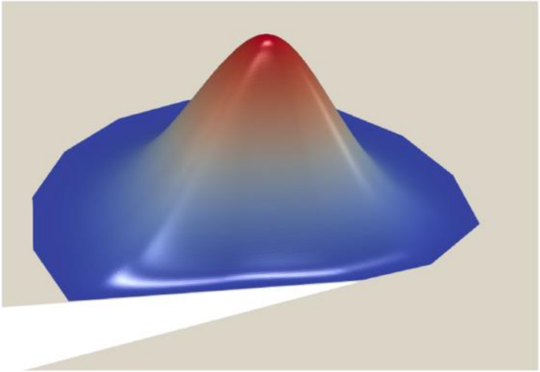
$$u^h(x) = \sum_{I=1}^{NP} \Psi_I d_I; \qquad \Psi_I = C(x; x - x_I)\Phi_a(x - x_I)$$



J. Koester, J.S. Chen, Comput. Methods Appl. Mech. Engrg. 347 (2019) 588–621

Conforming Reproducing Kernel

- Graph distance informed window/kernels replace traditional Euclidian kernels to provide improved accuracy and robustness for nonconvex geometries and essential boundary conditions



Thermo-mechanical-chemical coupling in CRK Multiphysics

CRK-Thermal implemented to simultaneously solve momentum

$$\int_\Omega \mathbf{w} \cdot \rho \ddot{\mathbf{u}} d\Omega + \int_\Omega \mathbf{F}(\nabla \mathbf{w}) : \mathbf{P}(\nabla \mathbf{u}) d\Omega = \mathbf{f}^{\text{ext}}(\mathbf{u}),$$

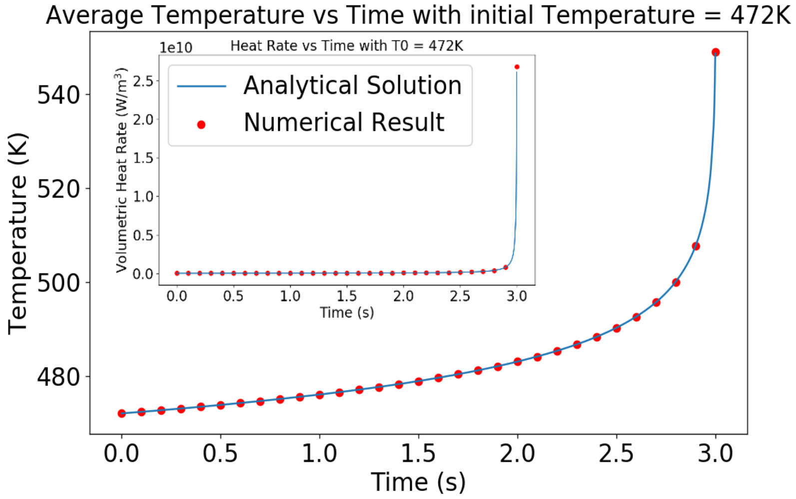
and conservation of energy

$$\int_\Omega w \rho C_P \dot{T} d\Omega + \underbrace{\int_\Omega \nabla w \cdot K \nabla T d\Omega}_{} = \int_\Omega w \left(\dot{q}^{\epsilon^P} + \dot{q}^{\text{species}} \right) d\Omega + \int_{\partial\Omega} w h d\Gamma.$$

Thermal conduction

Adiabatic heating from material plasticity

Chemical heating



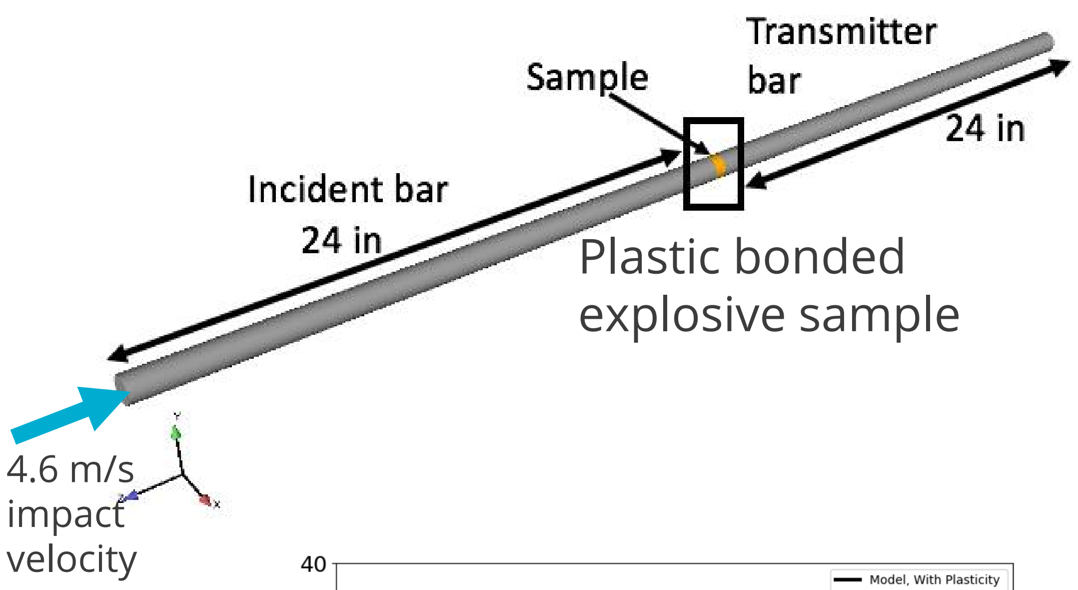
$$Q = \rho \Delta H Z e^{-E_a/RT}$$

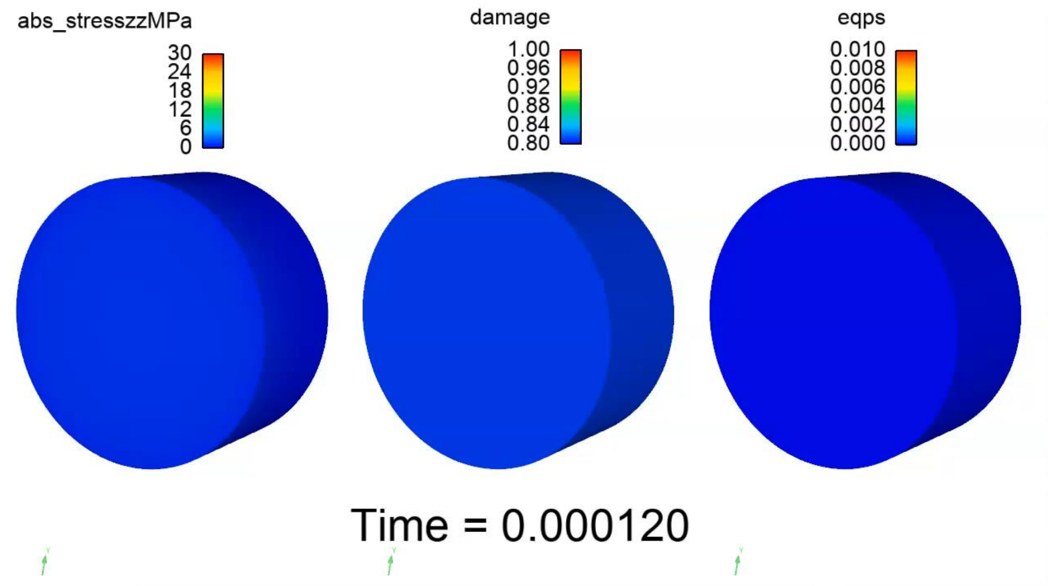
- **Viscoplastic-ViscoSCRAM constitutive model**
  - Viscoelasticity
  - Cracking damage (Statistical Crack Mechanics)
  - Pressure-dependent viscoplasticity with Drucker-Prager yield surface

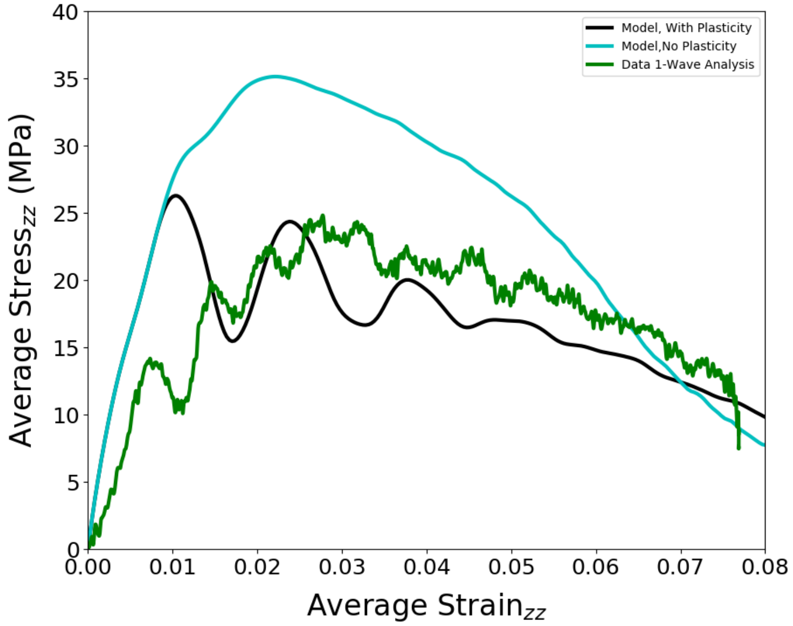
- Chemical heating from exothermic decomposition
  - Currently restricted to Arrhenius rate
  - More sophisticated models in progress

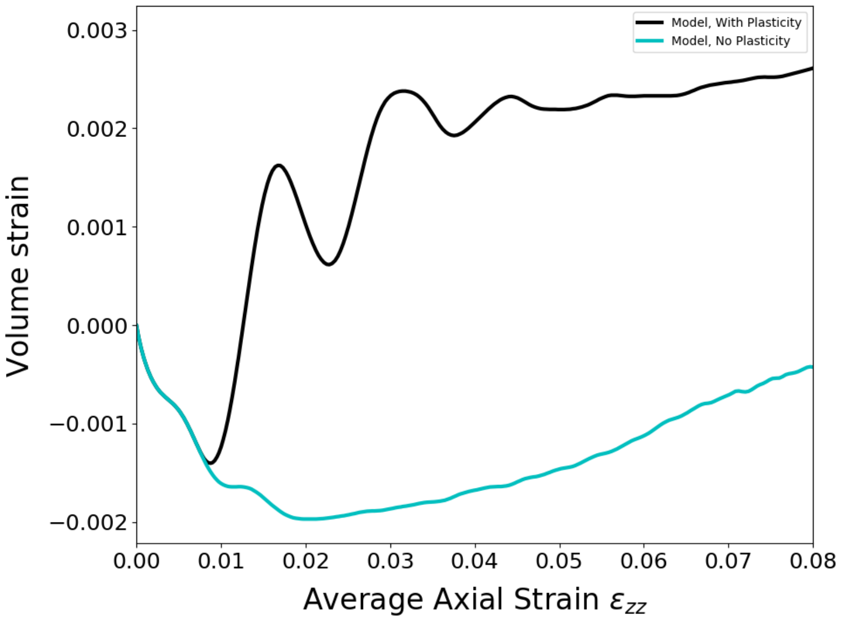
LAMÉ Team, *Library of Advanced Materials for Engineering (LAMÉ) 5.4*, Sandia Report SAND2021-16079

Model Validation: Split Hopkinson Pressure Bar





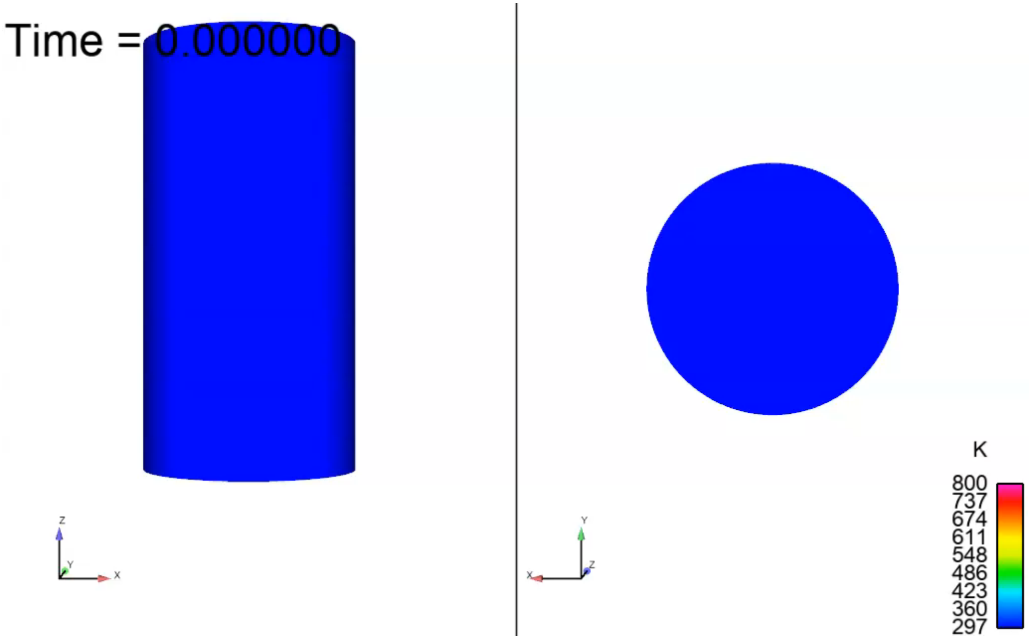




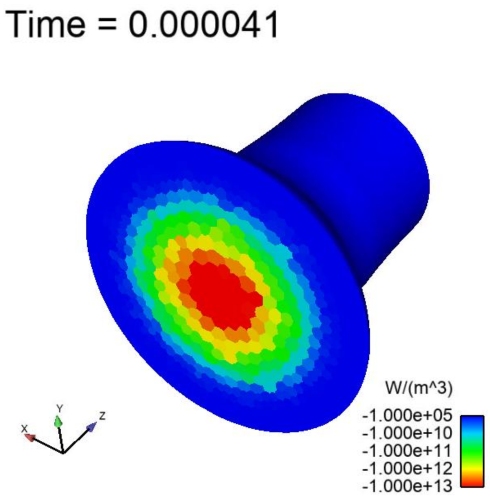
Thermal Runaway in Taylor Bar Impact: 450 m/s

- Energy dissipated due to plastic deformation raises temperature enough to start runaway chemistry

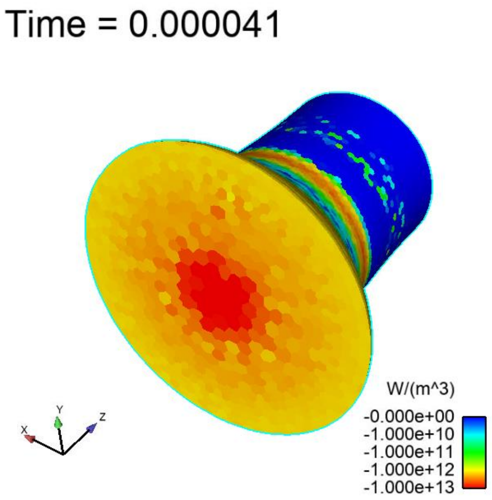
Temperature (K)



Chemistry Heating Rate



Plasticity Heating Rate



Conclusions & Ongoing Work

- Multifaceted effort to understand and model mechanically induced reaction in energetic materials
  - Meshfree numerical methods (continuum and mesoscale)
  - Understanding damage and heat generation mechanisms
  - Upscaling to macroscale constitutive models (yield surface, damage, statistical signatures)
  - Macroscale, Multiphysics predictions of impact-induced runaway temperatures

- Next Steps:
  - Linking additional damage mechanisms to heat generation
  - Best methods for representing localized hot spots in macroscale model?
  - Complex ignition test geometries (Stevens test, Spigot test, etc.)

Thank You!

Extra Slides

Thermo-chemical coupling in CRK

Arrhenius equation-based chemical heat generation

$$Q = \rho \Delta H Z e^{-E_a/RT}$$

Two verification tests based on Frank-Kamenetskii equation

- Temporal verification test

$$-\lambda \nabla^2 T + \rho C \frac{dT}{dt} = \rho \Delta H Z e^{-E_a/RT} \rightarrow \rho C \frac{dT}{dt} = \rho \Delta H Z e^{-E_a/RT}$$

Uniform temperature change (temporal variation only)

$$-\lambda \nabla^2 T + \rho C \frac{dT}{dt} = \rho \Delta H Z e^{-E_a/RT} \rightarrow -\lambda \nabla^2 T = \rho \Delta H Z e^{-E_a/RT}$$

- Verification test based on critical temperature

Steady-state solution (spatial variation only)

$$\frac{E_a}{T_c} = R\, ln\left(\frac{r^2 \rho \Delta H Z E_a}{T_c^2 \lambda \delta R}\right)$$

Critical ambient temperature (T_c) before runaway reaction[1]

[1]Cooper, Paul W.. Explosives Engineering, John Wiley & Sons, Incorporated, 1996.