SAND2023-04577C

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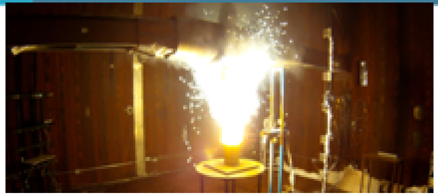
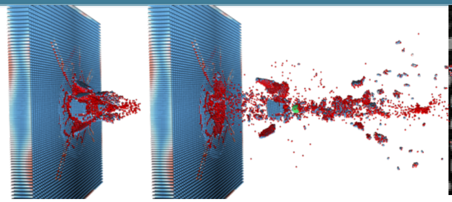
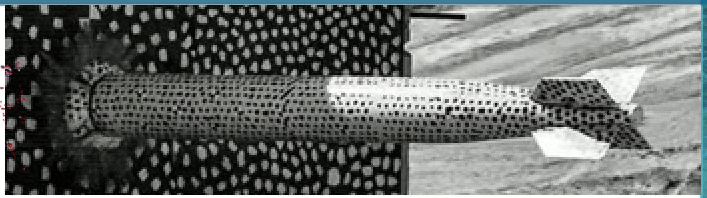
Meshfree modeling of coupled thermal-mechanical-chemical phenomena in energetic aggregates

LDRD
LABORATORY DIRECTED RESEARCH & DEVELOPMENT
WHERE INNOVATION BEGINS







Judith A. Brown[1], Frank Beckwith[1], Ki Tae Wolf[1], Joel Clemmer[1]

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

X International Congress of Computational Methods for Coupled Problems in Science and Engineering (COUPLED)

June 5-7, 2023, Chania, Crete, Greece

U.S. DEPARTMENT OF ENERGY NNSA

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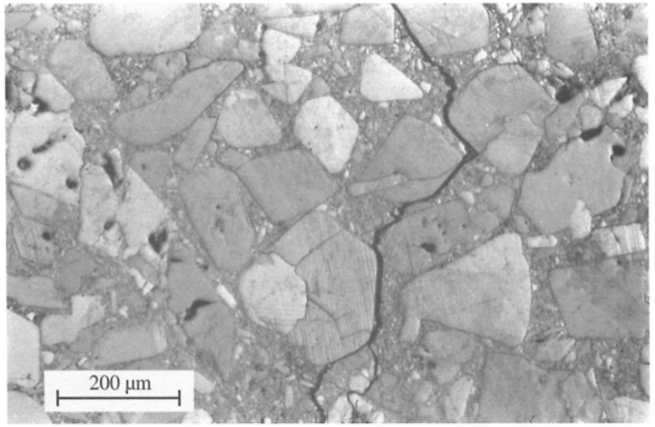
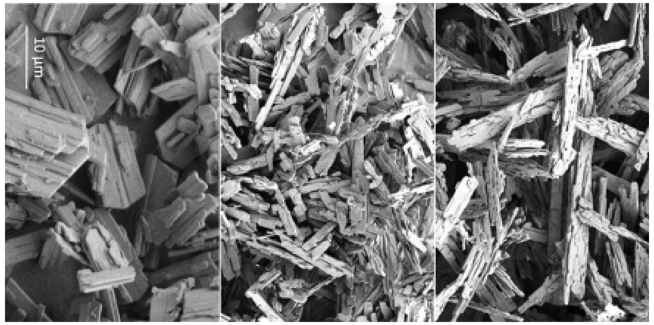
Energetic Materials: A Modeling Challenge

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

} Multi-Physics!

Plastic Bonded Explosive [Rae, 2002]





Energetic Crystals [Yarrington, 2018]

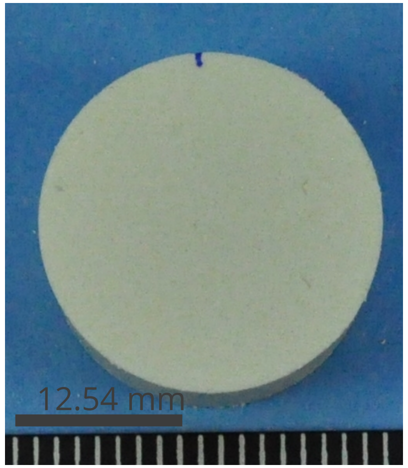
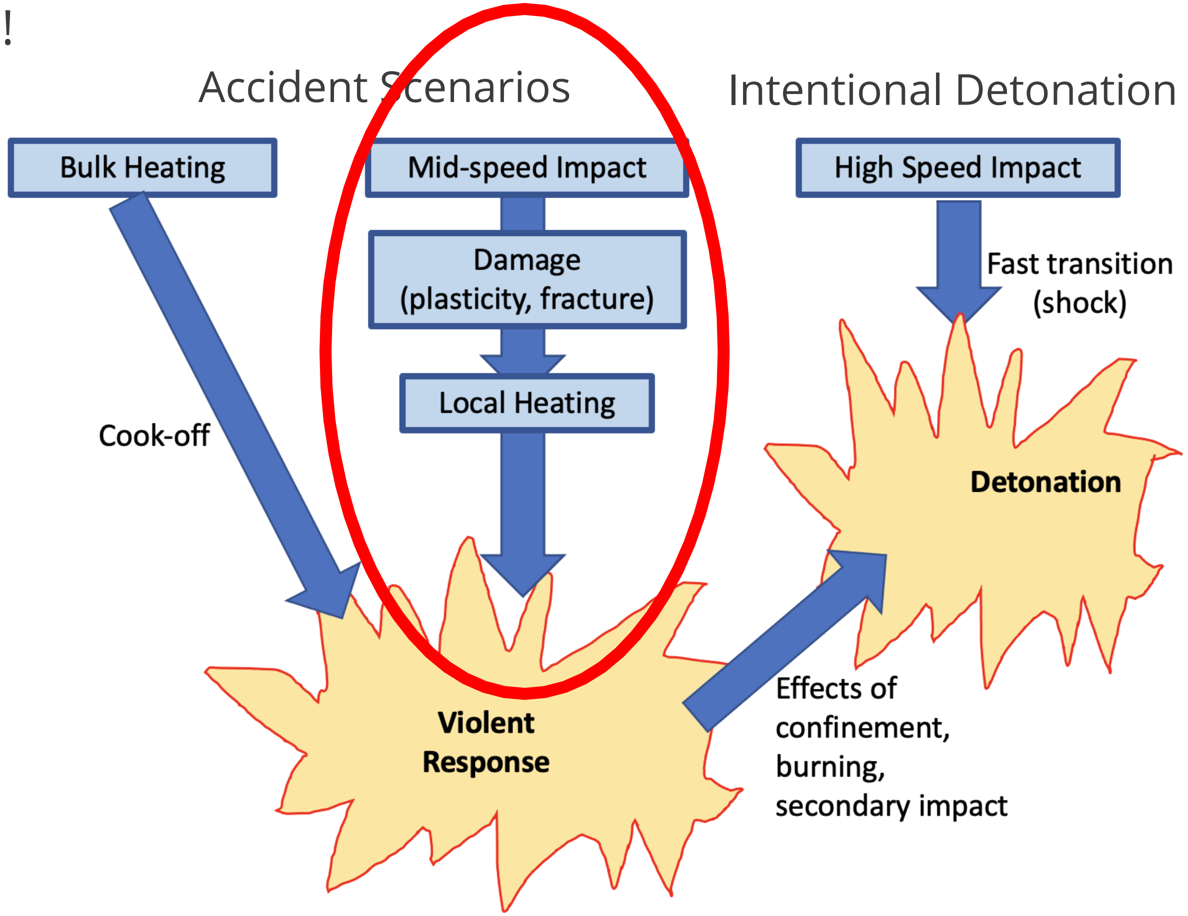


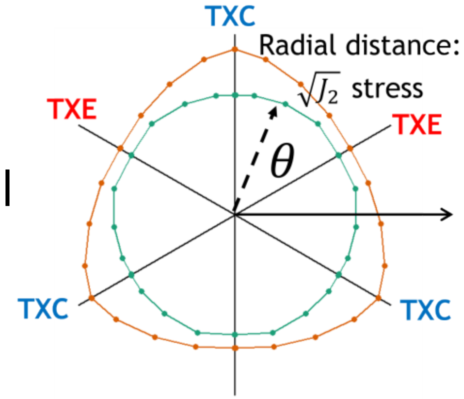
Image: courtesy Marcia Cooper

A few different ways to get an explosion…

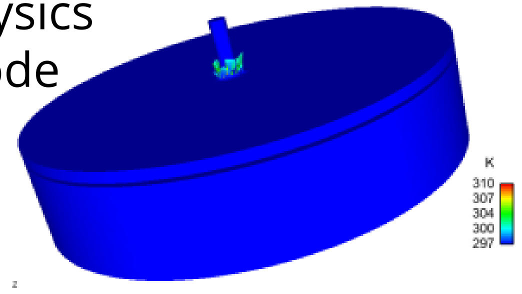


Overall Multiscale Approach

Continuum Constitutive Model



Multiphysics CRK code



Impact Event

Mechanical Deformation & Damage

Local Hotspot Formation

Heat Conduction

Thermally Activated Chemistry

Go

?

No Go

Interface Debonding

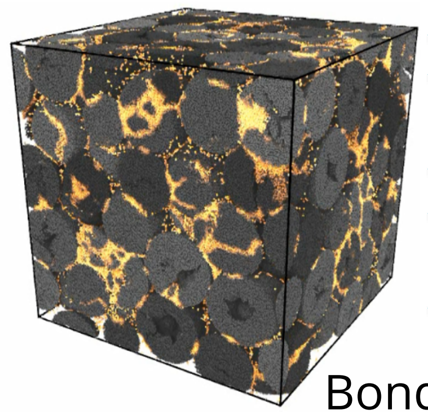
Crystal Fracture

Particle Rotation

Plasticity

Friction

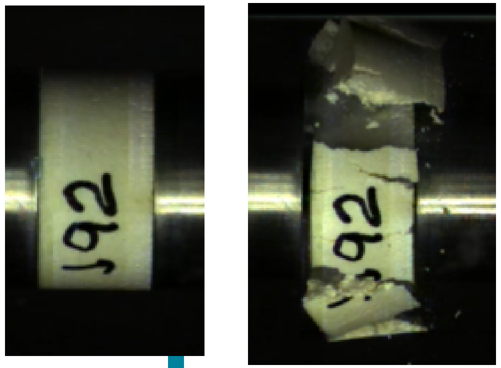
Viscoelastic Heating



Bonded Particle Methods

The Case for Meshfree Methods

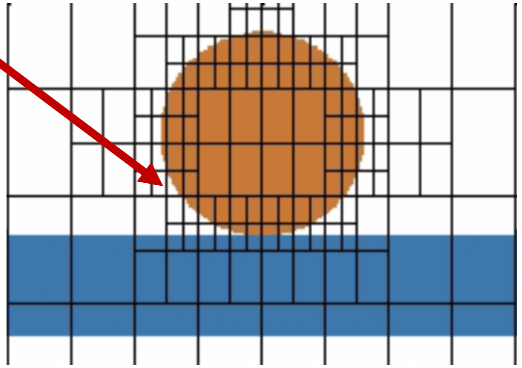
Numerical Method Should Accurately Predict:
- Capture transition from solid to rubble
- Deformation-induced heating, chemistry

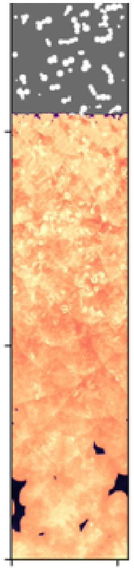


Example: Impact Test, Marcia Cooper

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

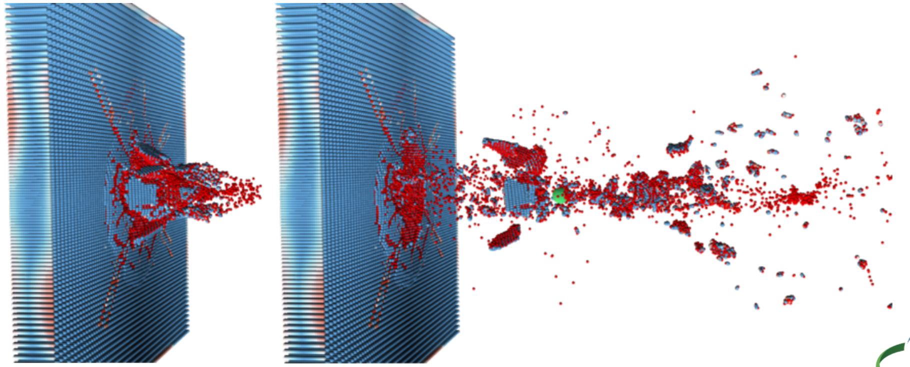
Hydrocode Methods





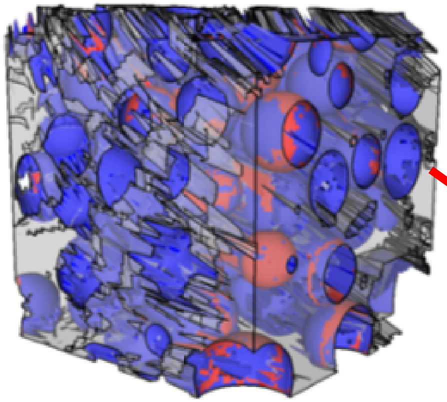
Meshfree Methods

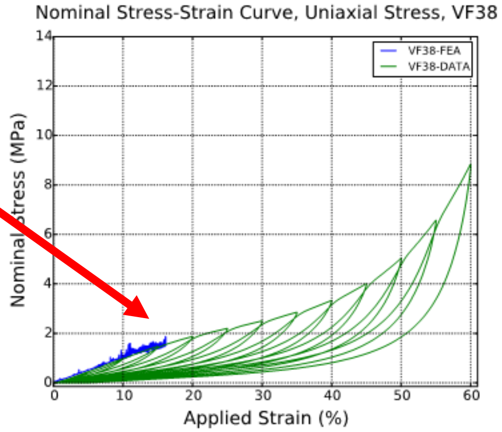
Show promise in overcoming these problems at both meso and macro scales



Mesh-based Methods (FEA)

Problem: Mesh entanglement at large deformations



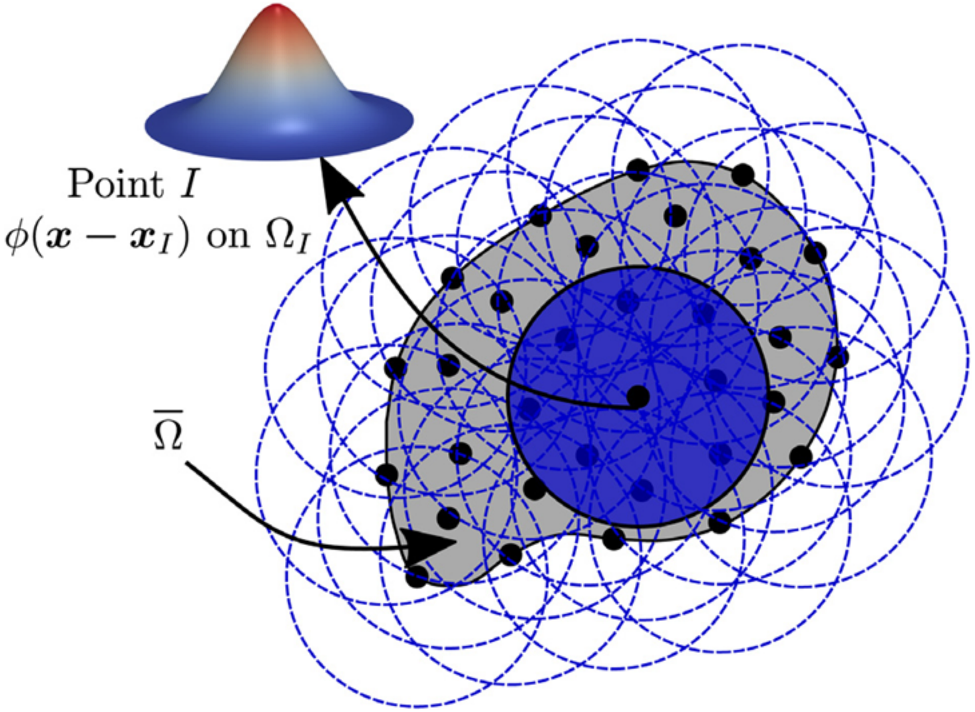


Meshfree Conforming Reproducing Kernel Method

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

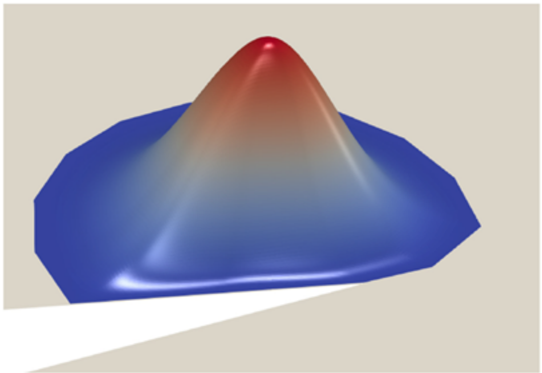
$$u^h(x) = \sum_{I=1}^{NP} \Psi_I d_I; \qquad \Psi_I = C(x; x - x_I)\Phi_a(x - x_I)$$



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

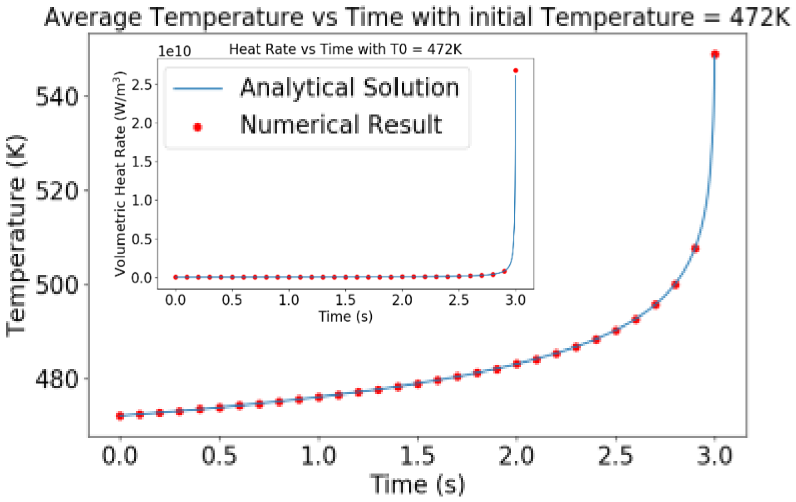
CRK-Thermal implemented to simultaneously solve momentum

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

and conservation of energy

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

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

LDRD

Thermo-chemical coupling verification

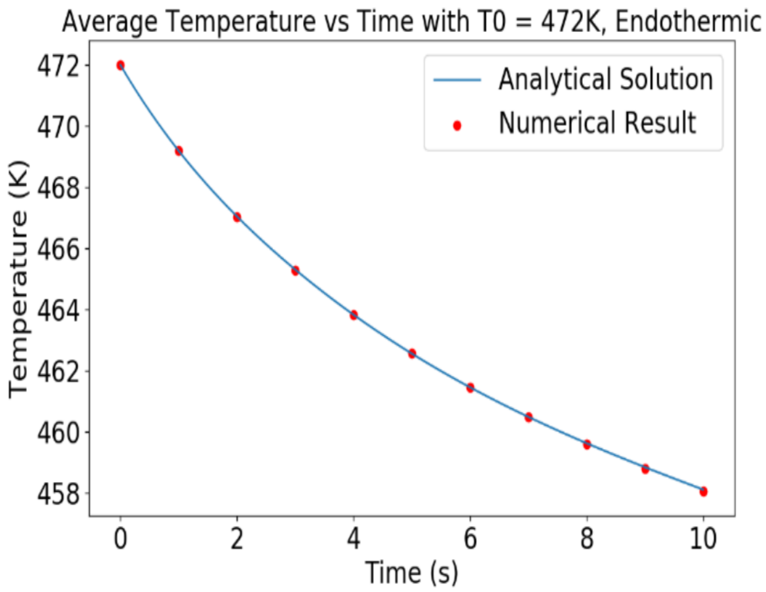
- Temporal verification based on Frank-Kamenetskii equation[1]:

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

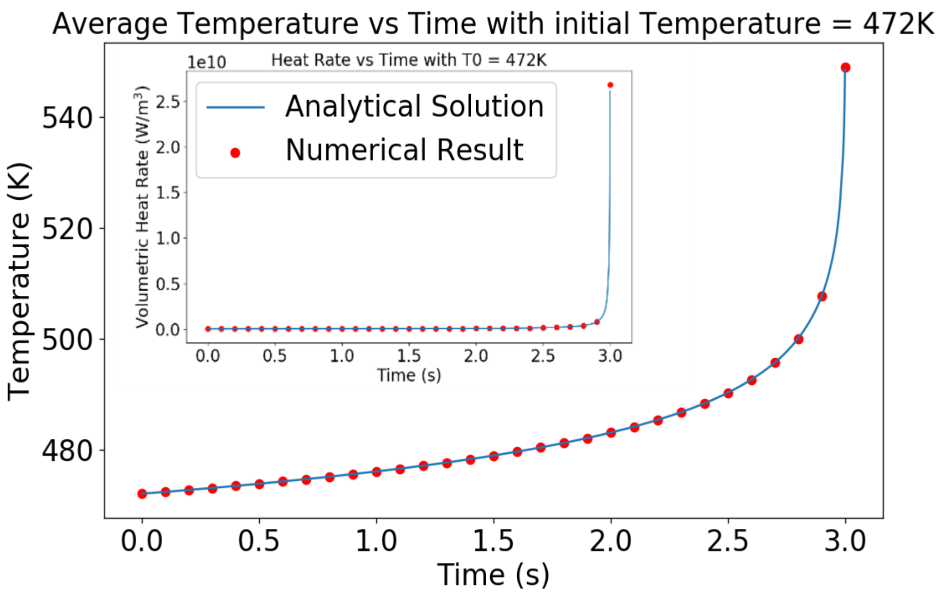
Uniform temperature change
(temporal variation only)

$$\rho C\frac{dT}{dt} = \rho\Delta H Z e^{-E_a/RT}$$

Endothermic Process



Exothermic Process



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

Thermo-chemical coupling verification

- Verification test based on Frank-Kamenetskii critical temperature[1]:

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

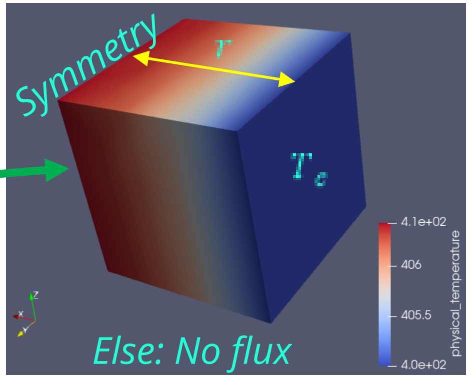
Steady state solution (spatial variation only)

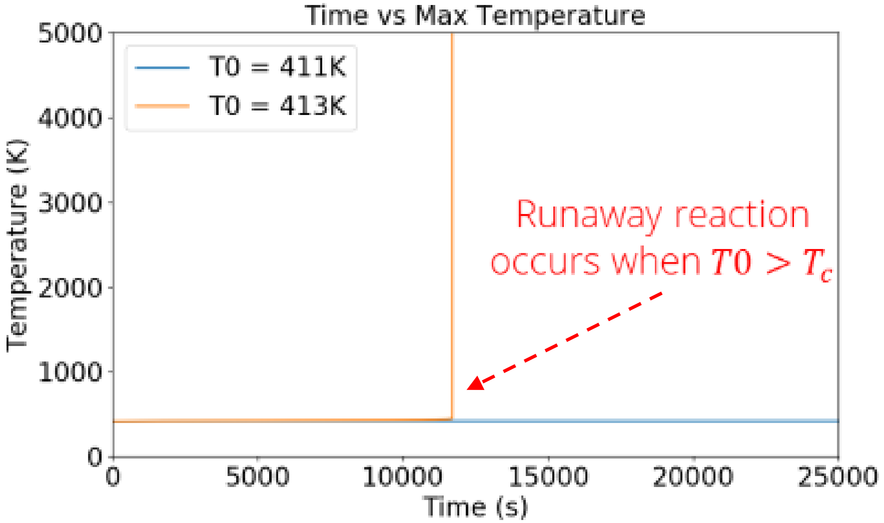
$$-\lambda\nabla^2 T = \rho \Delta H Z e^{-E_a/RT}$$

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

Cubic domain with no flux boundary except one surface with constant T_c (infinite slab)

Max. Temperature at symmetry boundary





Solve for critical ambient temperature (T_c) before runaway reaction[1]

Analytical Critical Temperature: ~412K

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

Shear-Induced Heating in Steel

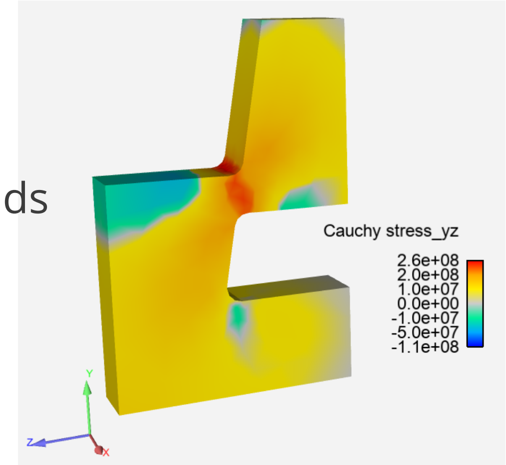
- Top-hat geometry designed to induce high localized shear
- Material properties: steel

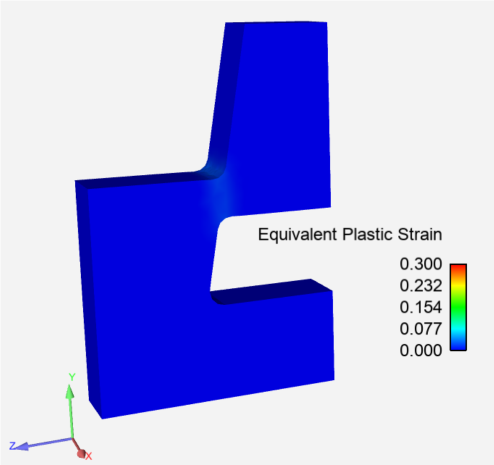
Shear Stress

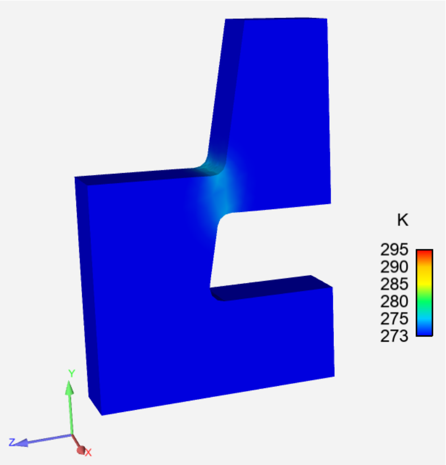
Equivalent Plastic Strain

Temperature

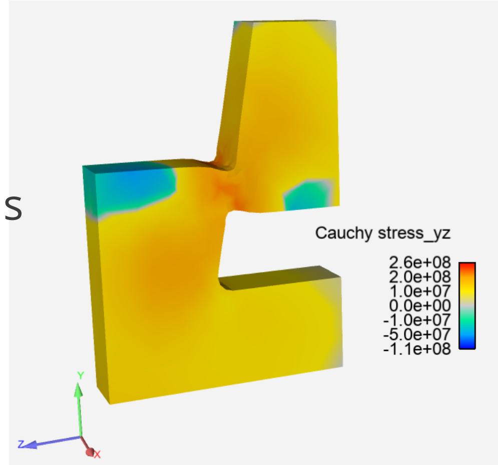
Time = 65 microseconds

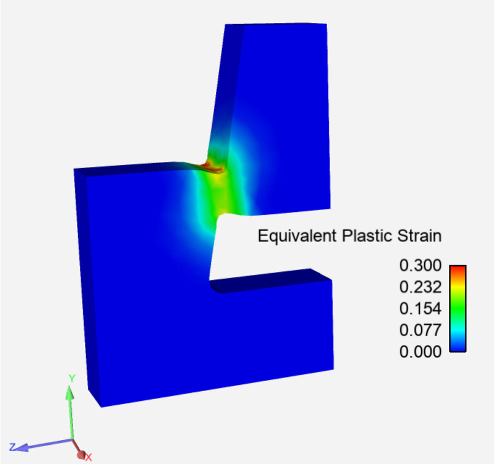


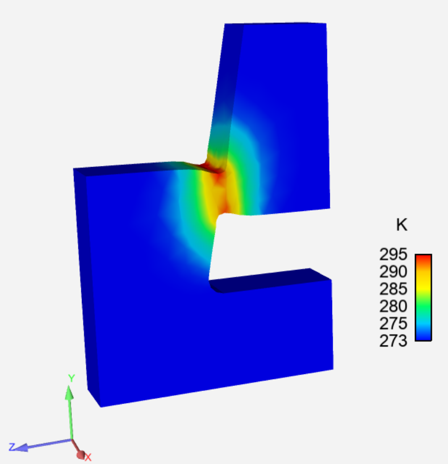




Time = 250 microseconds



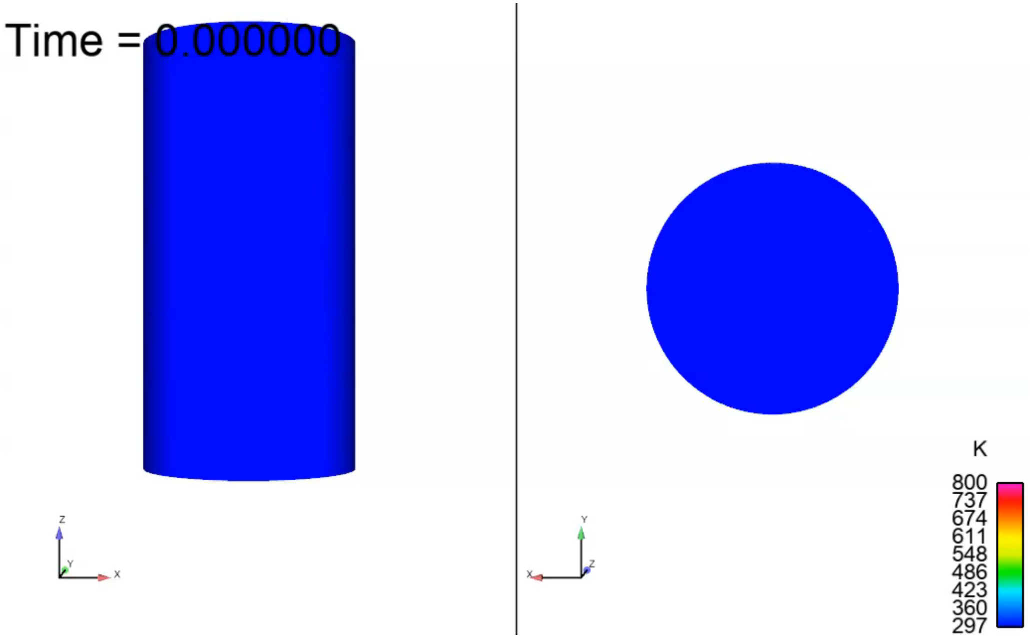




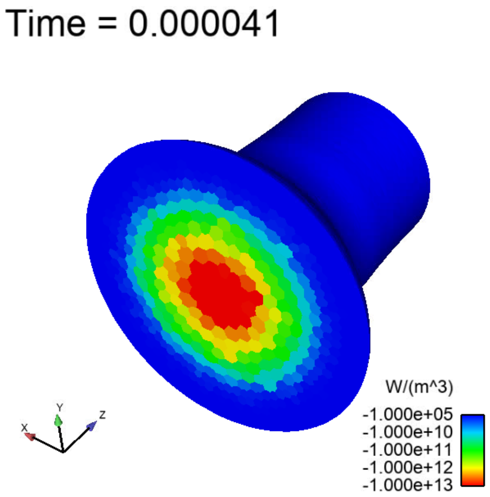
Thermal Runaway in Taylor Bar Impact: 450 m/s

- Material properties: pure energetic crystals
- Energy dissipated due to plastic deformation raises temperature enough to start runaway chemistry

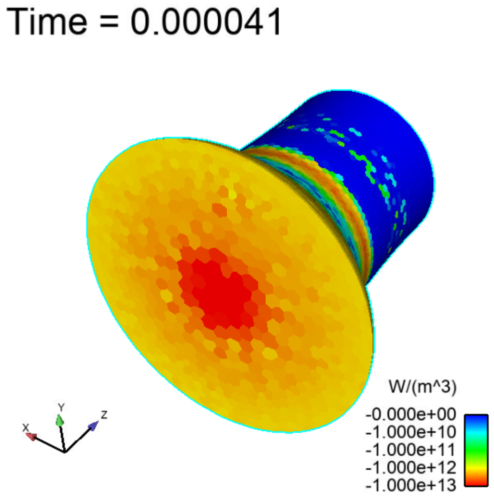
Temperature (K)



Chemistry Heating Rate

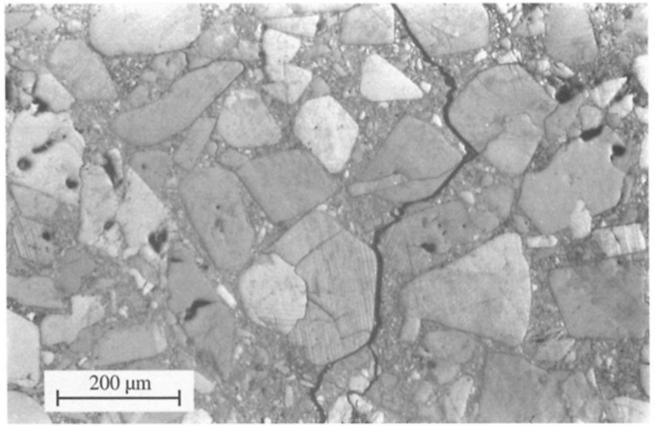


Plasticity Heating Rate



Now we consider energetic aggregate materials

- Composite mechanical behavior is complex:
  - Strain rate dependent
  - Temperature dependent
  - Pressure dependence
  - Tension-Compression Asymmetry
  - Many inelastic deformation mechanisms: Viscoelasticity (binders), Cracking (intra- and inter-granular), Porosity opening, dislocation slip, twinning (some energetic crystals)



Plastic Bonded Explosive [Rae, 2002]

How to represent various inelastic mechanisms in a macroscale model?

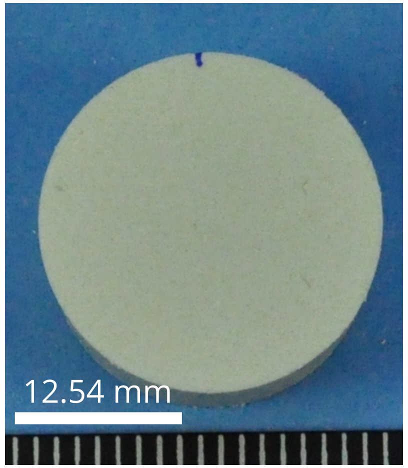
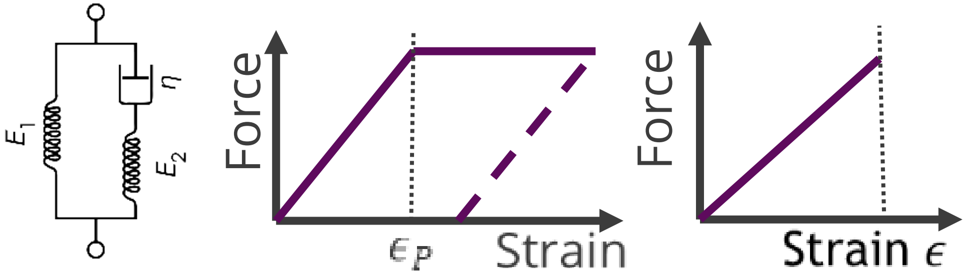


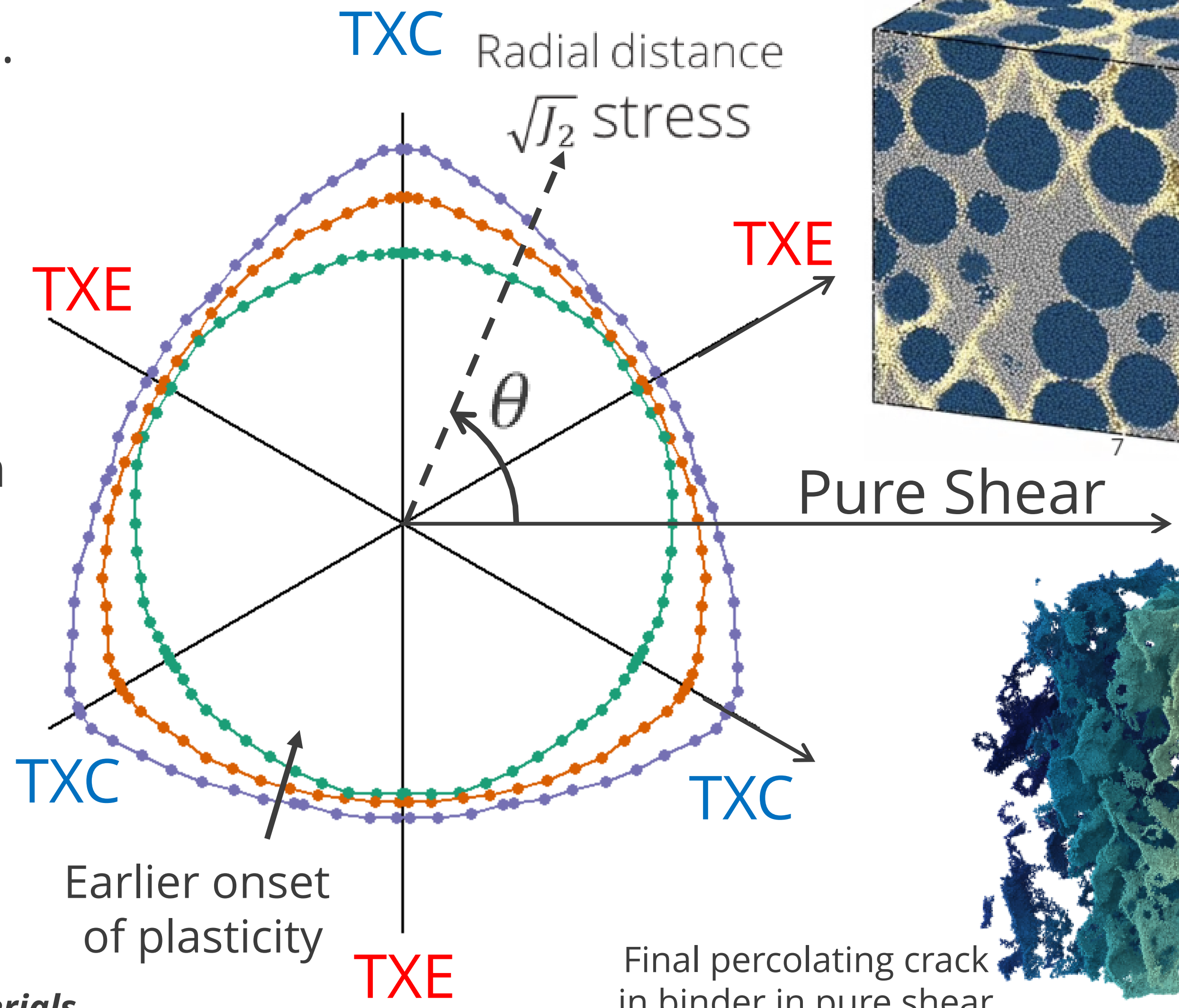
Image: courtesy Marcia Cooper

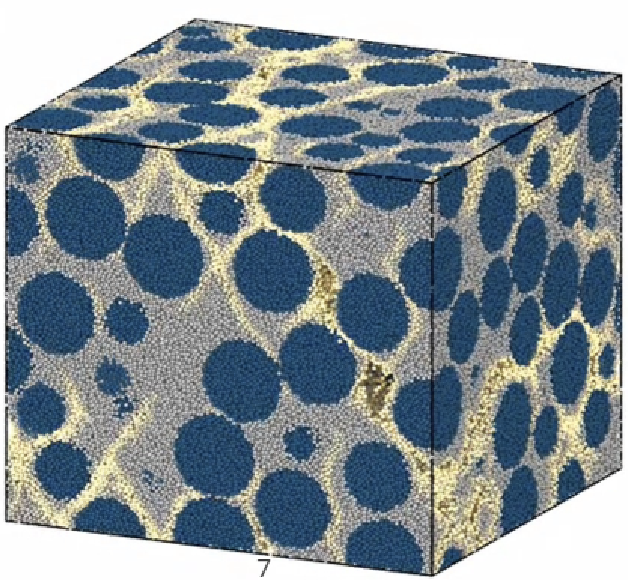
Mesoscale studies to inform continuum models

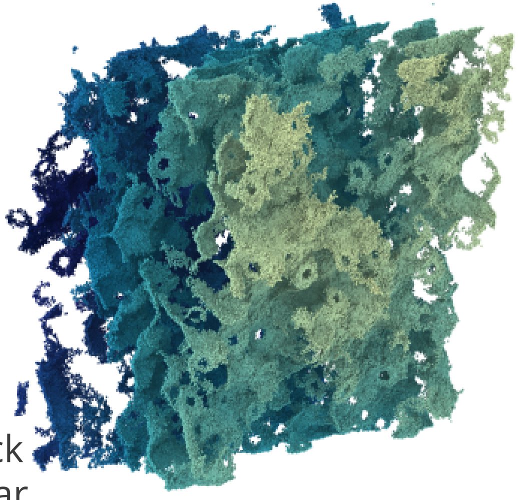
- Map out yield surfaces, often assumed to have simple shape (e.g. Drucker-Prager)

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







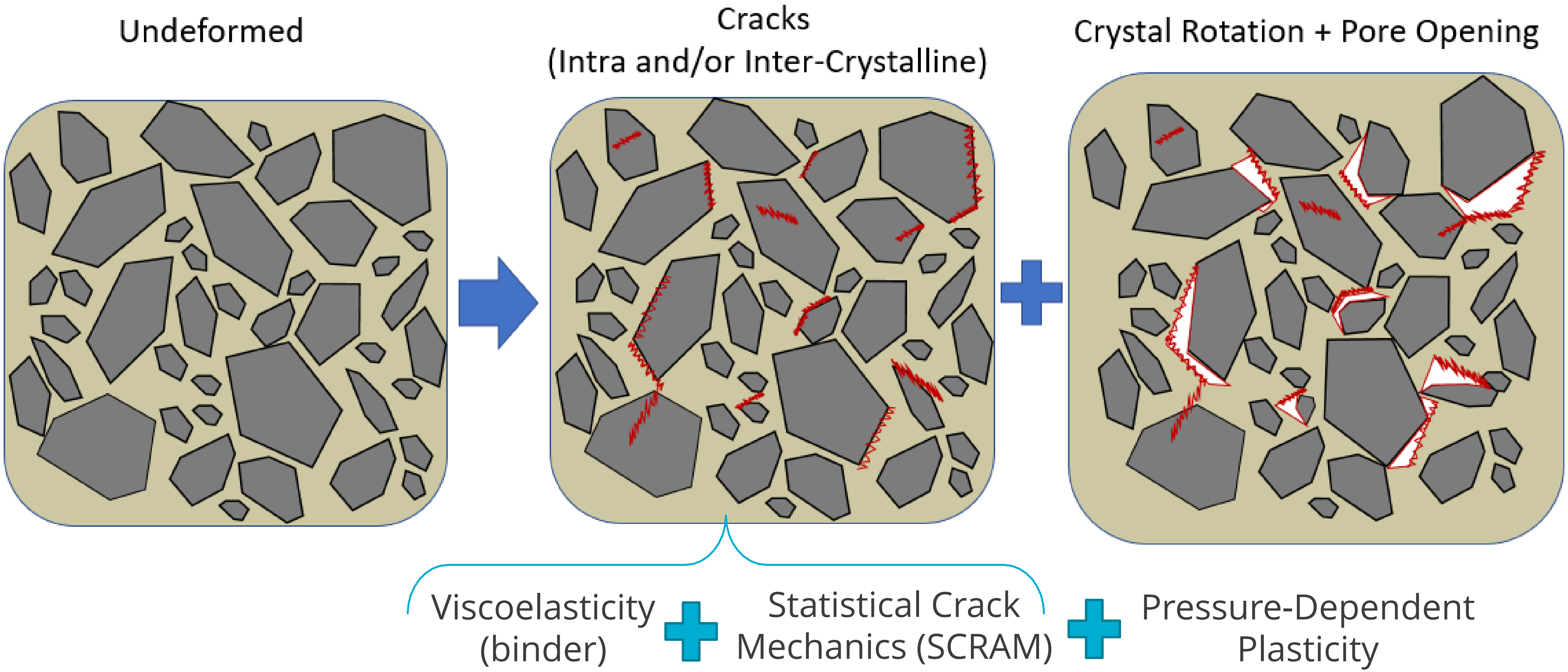


Final percolating crack in binder in pure shear

JT Clemmer, KN Long, JA Brown, Mechanics of Materials, 2023, https://doi.org/10.1016/j.mechmat.2023.104693

Hypothesized Mesoscale Deformation Mechanisms

- Simplified view of mesoscale processes and macroscale interpretation



ViscoPlastic-ViscoSCRAM Model Theory

- Kinematics:

$$\boldsymbol{\epsilon} = \boldsymbol{e} + \frac{1}{3}\epsilon_{\text{vol}}\boldsymbol{I} \qquad \sigma_{\text{m}} = K\epsilon_{\text{vol}}$$

$$\boldsymbol{e} = (\boldsymbol{e}^{ve} + \boldsymbol{e}^{D}) + \boldsymbol{e}^{p}$$

- Viscoelasticity

$$\dot{\boldsymbol{s}} = 2G^{\infty}\dot{\boldsymbol{e}}^{ve} + \sum_{\kappa=1}^{N}\left(2G^{(\kappa)}\dot{\boldsymbol{e}}^{ve} - \frac{\boldsymbol{s}^{(\kappa)}}{\tau^{(\kappa)}}\right)$$

Prony series of shear moduli and relaxation times

- SCRAM Damage

$$\boldsymbol{e}^{D} = \frac{1}{2G_0}\left(\frac{c}{a}\right)^3\boldsymbol{s}$$

$$\dot{c} = \begin{cases} v_{res}\left(\frac{K_I}{K_1}\right)^m & \text{for } K_I < K' \\ v_{res}\left[1 - \left(\frac{K_{0\mu}}{K_I}\right)^2\right] & \text{otherwise} \end{cases}$$

$$\dot{s}^{(\kappa)} = 2G^{(\kappa)}(\dot{e} - \dot{e}^{p}) - \frac{s^{(\kappa)}}{\tau^{(\kappa)}} - \frac{G^{(\kappa)}}{G_0}\left[\frac{3}{a}\left(\frac{c}{a}\right)^2\dot{c}s + \left(\frac{c}{a}\right)^3\dot{s}\right] \qquad D = \frac{\left(\frac{c}{a}\right)^3}{1 + \left(\frac{c}{a}\right)^3}$$

M.A. Buehler, D.J. Luscher, Int. J. Num. Meth. Eng. 2014

- Drucker-Prager Plasticity

$$f(\sigma_{ij}) = \sigma_e + A\cdot\sigma_m - \sigma_y$$

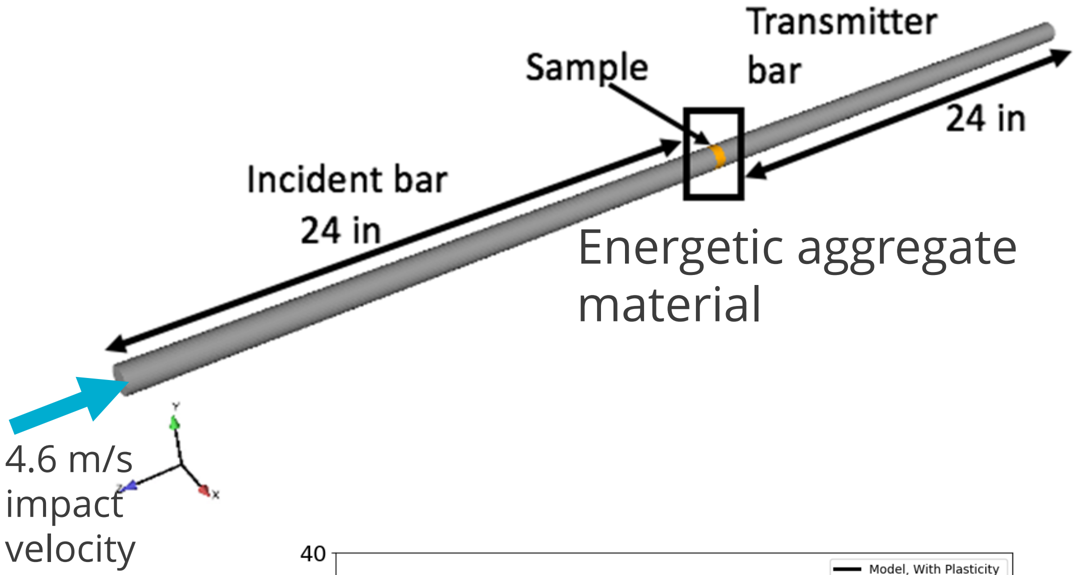
$$g(\sigma_{ij}) = \sigma_e + B\cdot\sigma_m - \sigma_y$$

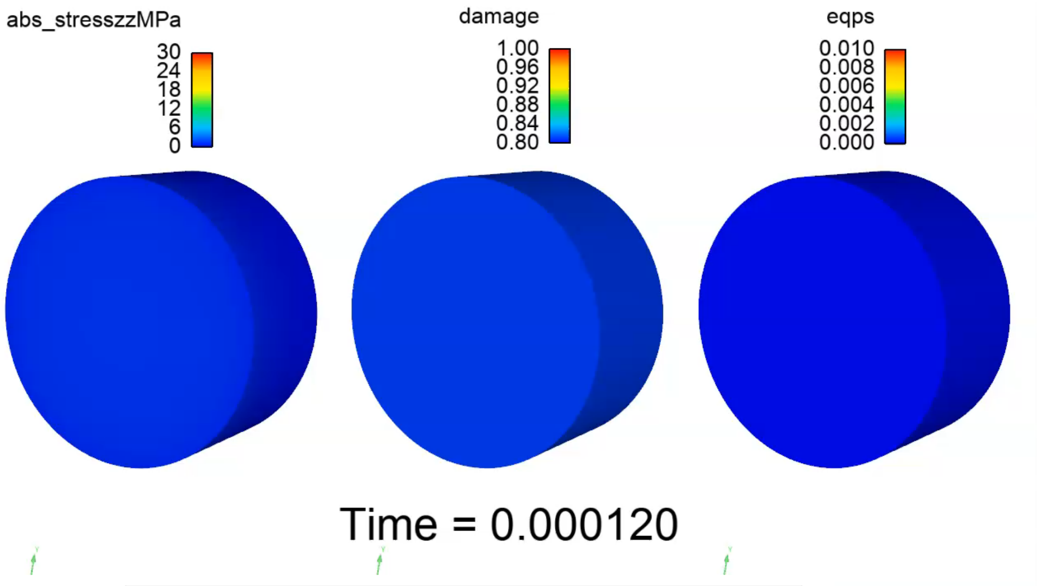
$$\dot{\boldsymbol{\epsilon}}^{p} = \dot{\lambda}\frac{\partial g}{\partial \boldsymbol{\sigma}}$$

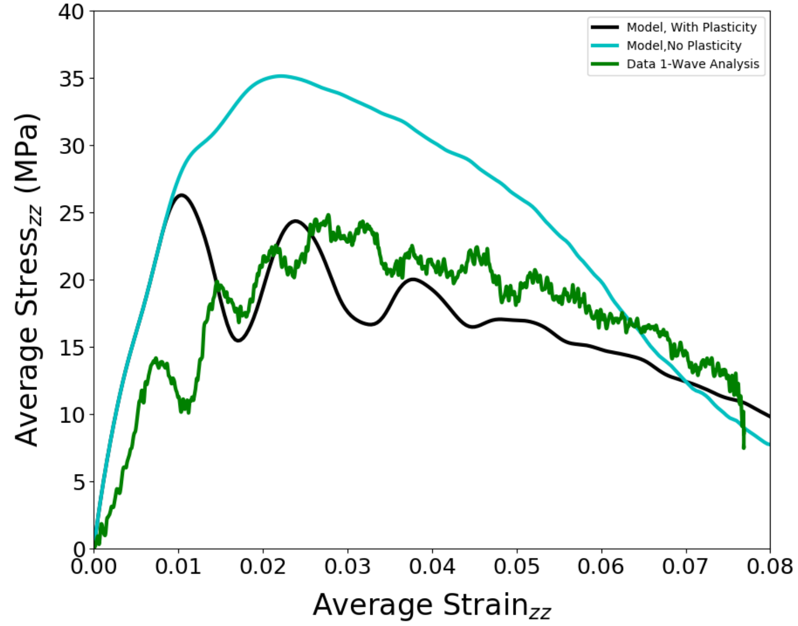
$$\dot{\lambda} = \frac{1}{\tilde{\tau}}\langle\frac{f(\sigma_{ij})}{\sigma_0}\rangle^{\tilde{m}} \qquad \sigma_e = \sqrt{\frac{3}{2}s_{ij}s_{ij}}$$

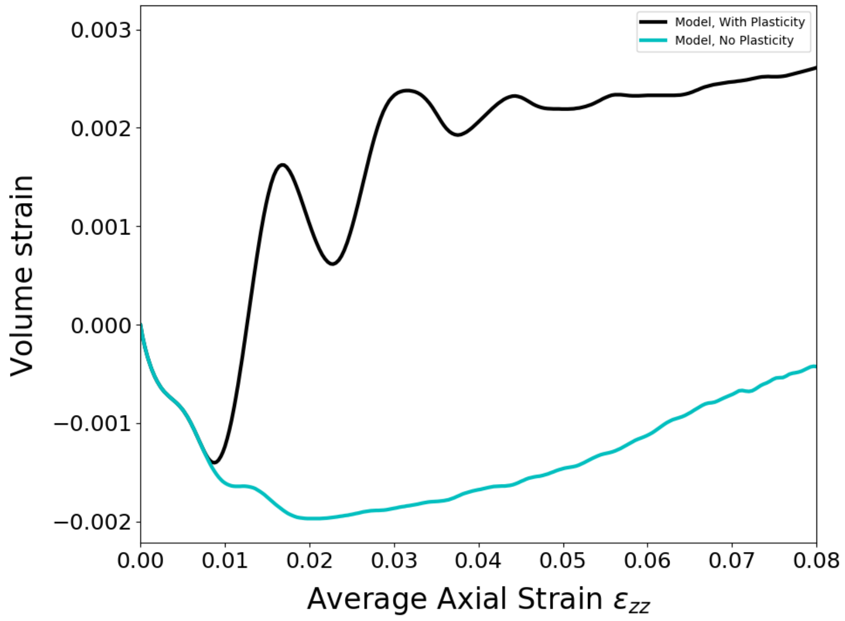
LDRD

Mechanical Model Validation: Split Hopkinson Pressure Bar

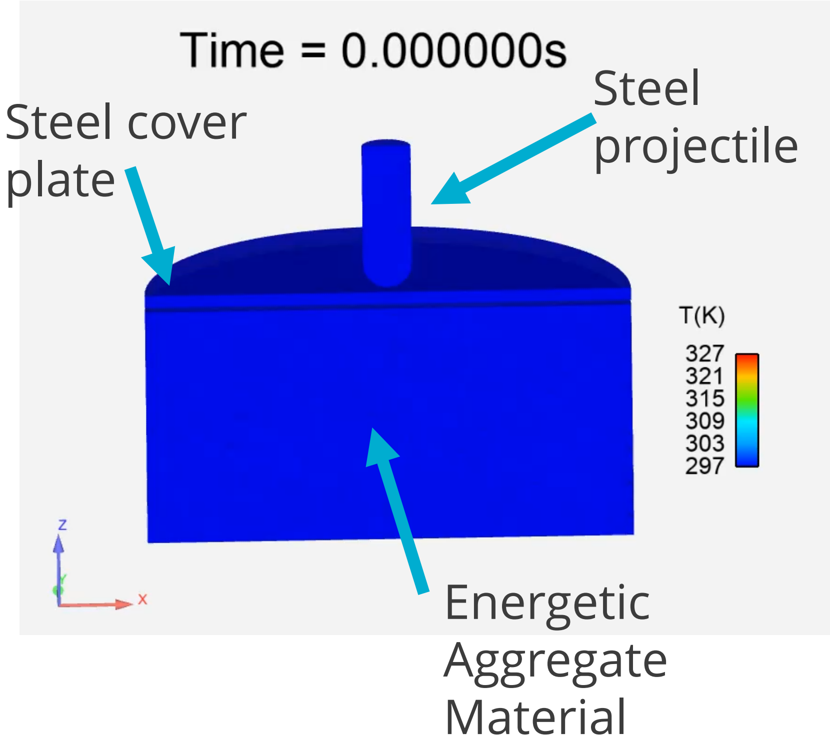




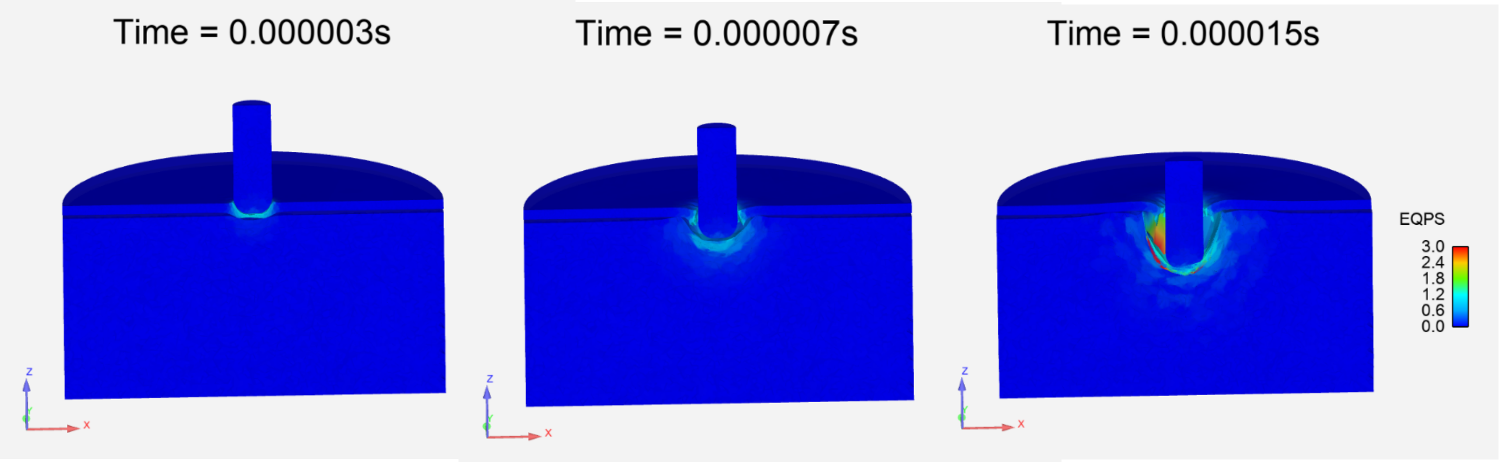




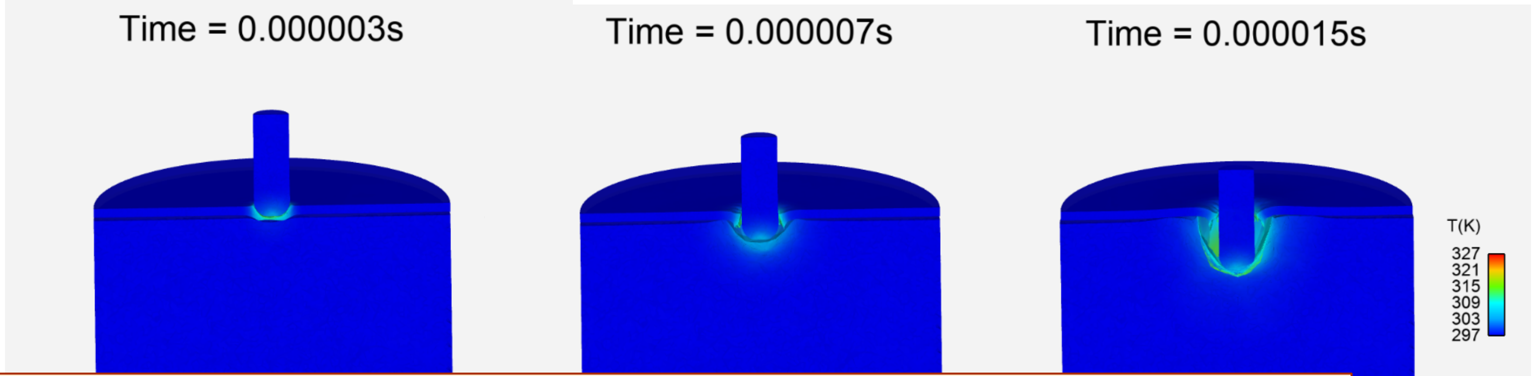
Multi-material impact example



Equivalent Plastic Strain



Temperature



Extreme numerical robustness coupled with multiphysics enables new simulation capability

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 evolution)
- Macroscale, Multiphysics predictions of impact-induced runaway temperatures
- Conforming Reproducing Kernel (CRK) Method as a powerful tool for *Lagrangian* continuum mechanics at massive strains and coupled physics

Thank You!