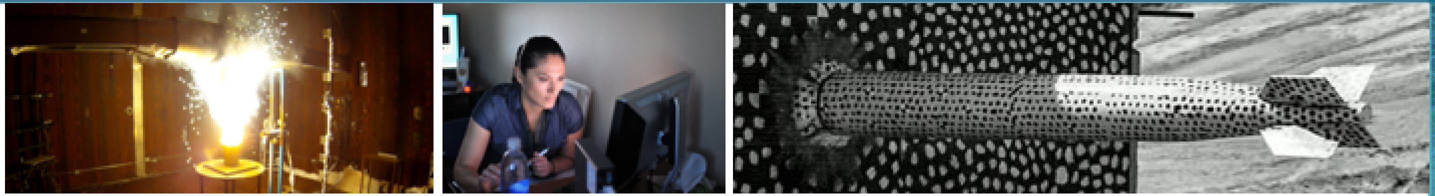
SAND2024-07566C

Meshfree Modeling of Thermo-Mechanical Behavior and Damage Evolution in Binderized Energetic Materials



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

GRC Energetic Materials

June 2-7, 2024, Newry, ME

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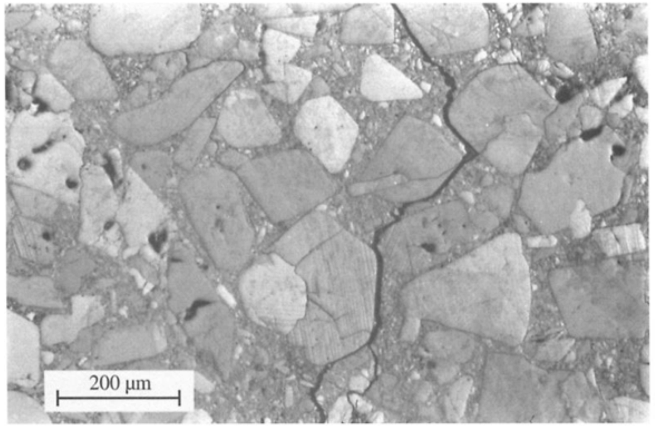
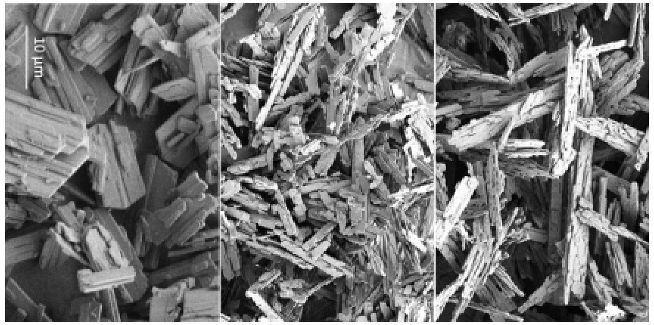
- Abhay Kumar

Energetic Materials: A Modeling Challenge

- Complex material structure
- Chemically reactive (fast, exothermic)
- Inherently multi-physics

Plastic Bonded Explosive [Rae, 2002]





Energetic Crystals [Yarrington, 2018]

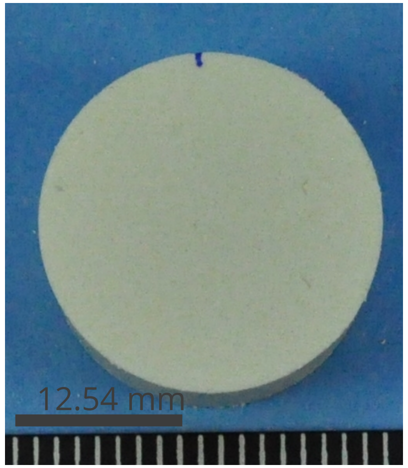
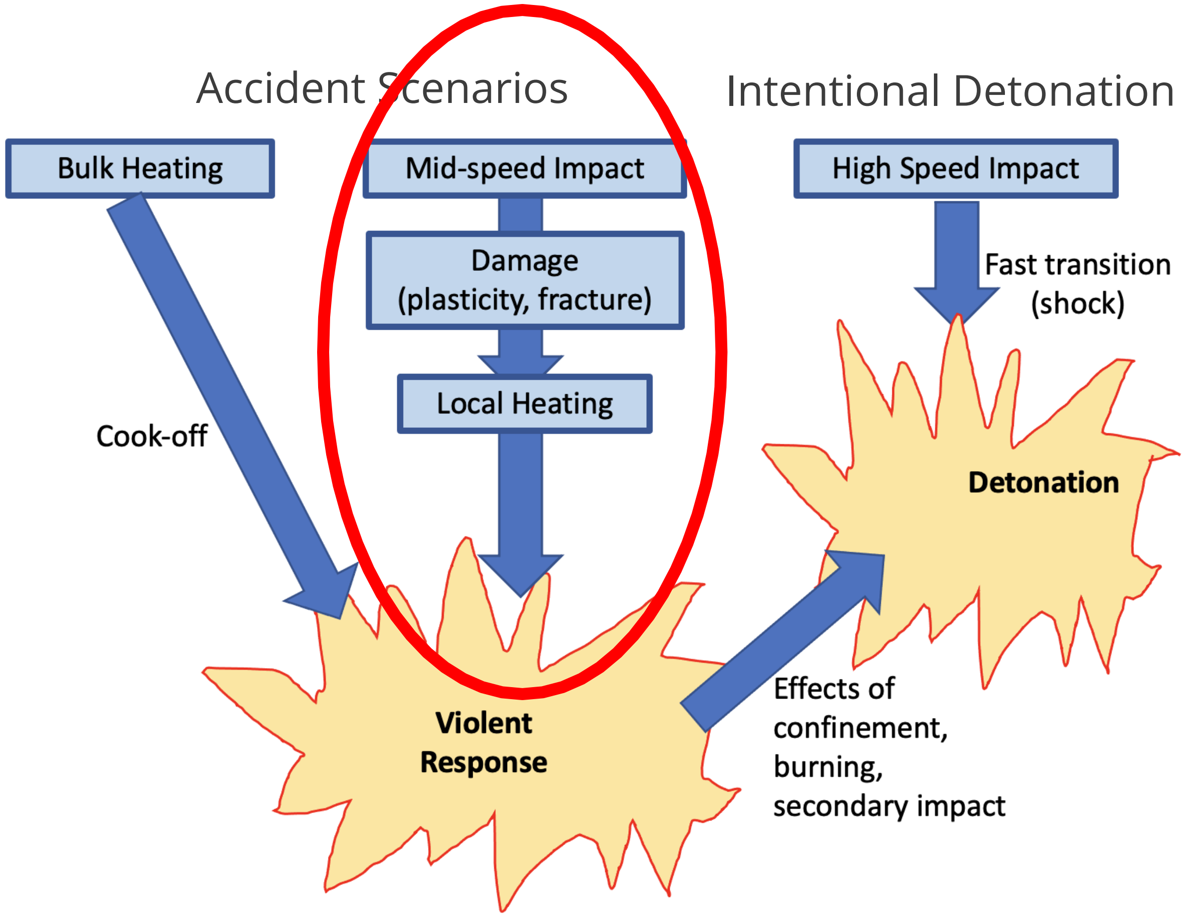
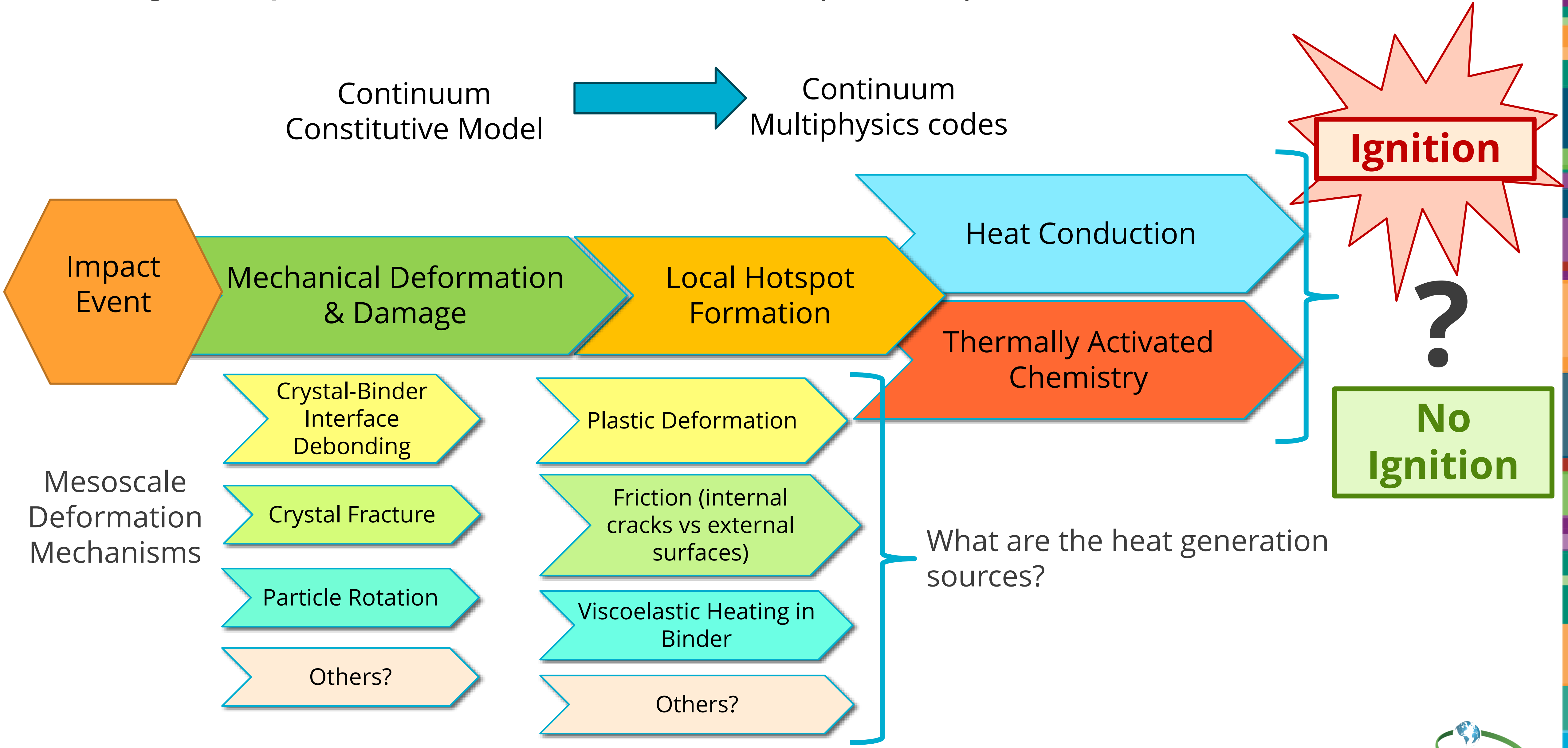


Image: courtesy Marcia Cooper

A few different ways to get an explosion…



High Explosive Violent Reaction (HEVR)



Continuum Constitutive Model

Continuum Multiphysics codes

Impact Event

Mechanical Deformation & Damage

Local Hotspot Formation

Heat Conduction

Thermally Activated Chemistry

Ignition

?

No Ignition

Mesoscale Deformation Mechanisms

- Crystal-Binder Interface Debonding
- Crystal Fracture
- Particle Rotation
- Others?

- Plastic Deformation
- Friction (internal cracks vs external surfaces)
- Viscoelastic Heating in Binder
- Others?

What are the heat generation sources?

Many Outstanding Modeling Challenges

1. Large Deformation (Global and/or localized) and Pervasive Damage/Fracture
    - Numerical method challenges
2. Complex mechanical behavior, requires unique constitutive models
    - Mesoscale mechanisms vs. macroscale effects
    - What are the heat generation mechanisms? What drives hot spots & ignition?
3. Multi-physics nature of HEVR event
    - Governing physics change throughout the event
    - Initially mechanics dominated, localized heat generation and transfer, transition to material flow and reactive burn

We are exploring meshfree numerical methods as a computational tool to study mechanically induced HEVR

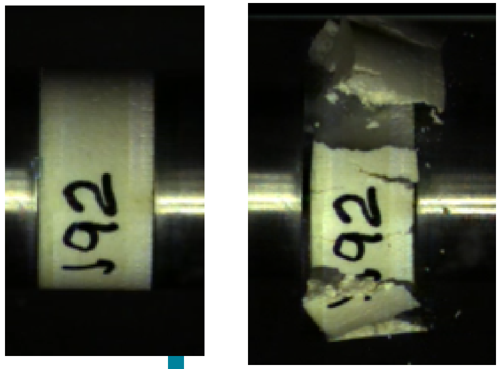
1. Large Deformation and Pervasive Fracture:

The Case for Meshfree Numerical Methods

The Case for Meshfree Methods: Macroscale

Numerical Method Should Accurately Predict:

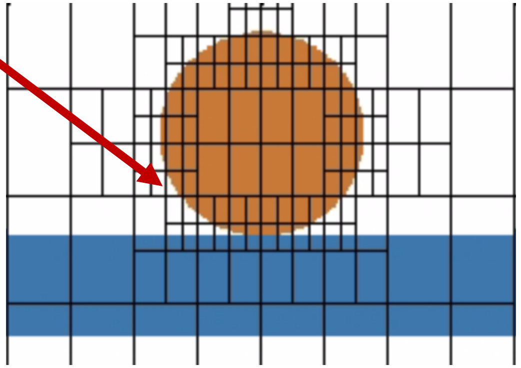
- Capture transition from solid to rubble
- Deformation-induced heating, chemistry

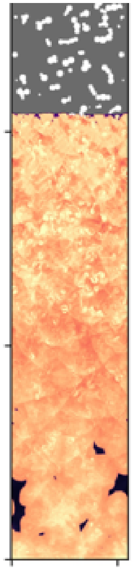


Example: Impact Test, Marcia Cooper

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

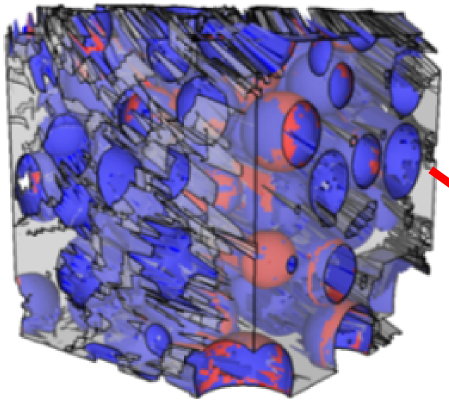
Hydrocode Methods

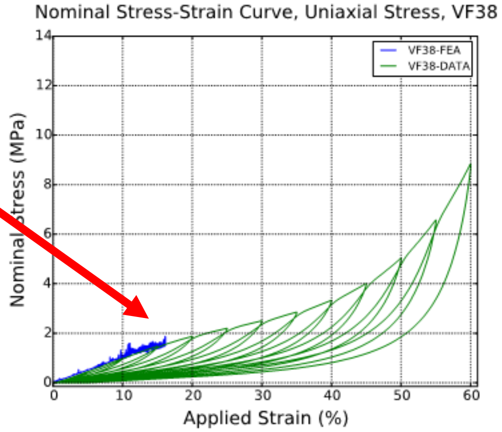




Mesh-based Methods (FEA)

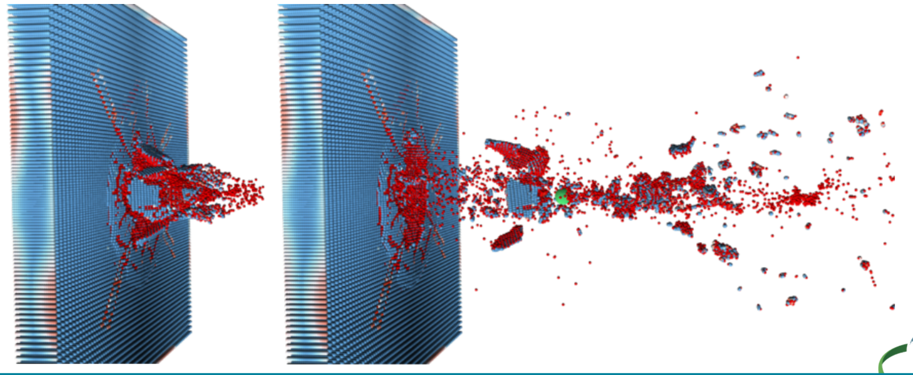
Problem: Mesh entanglement at large deformations





Meshfree Methods

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

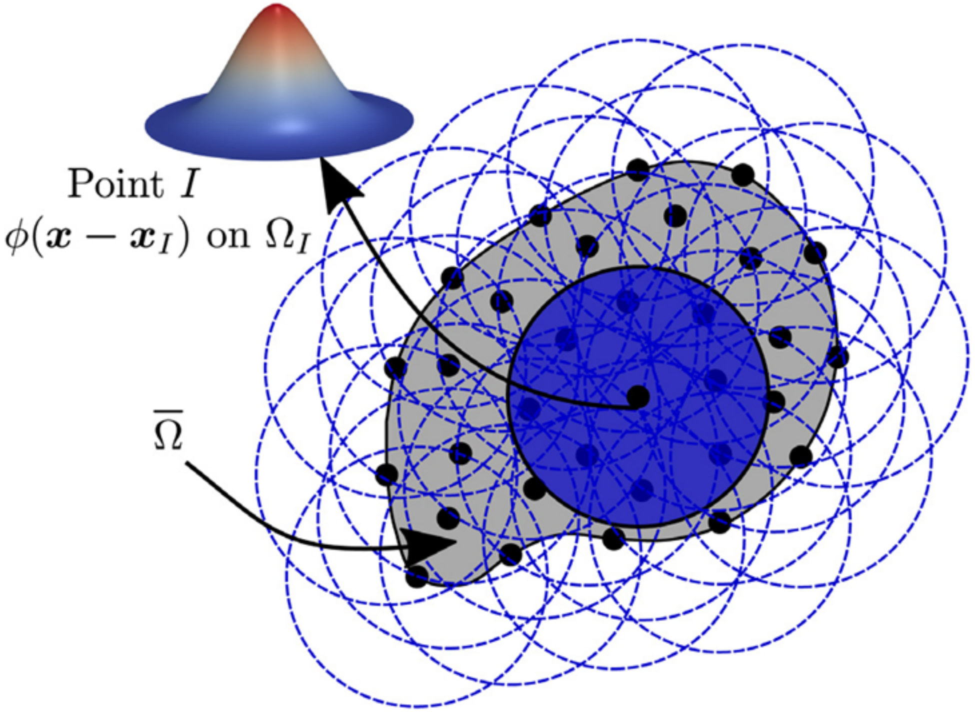


Macroscale: Meshfree Conforming Reproducing Kernel Method

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

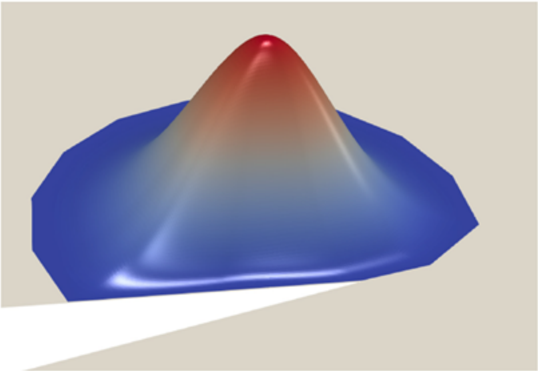
$$u^h(x) = \sum_{I=1}^{NP} \Psi_I d_I; \qquad \Psi_I = C(x; x - x_I)\phi_a(x - x_I)$$



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

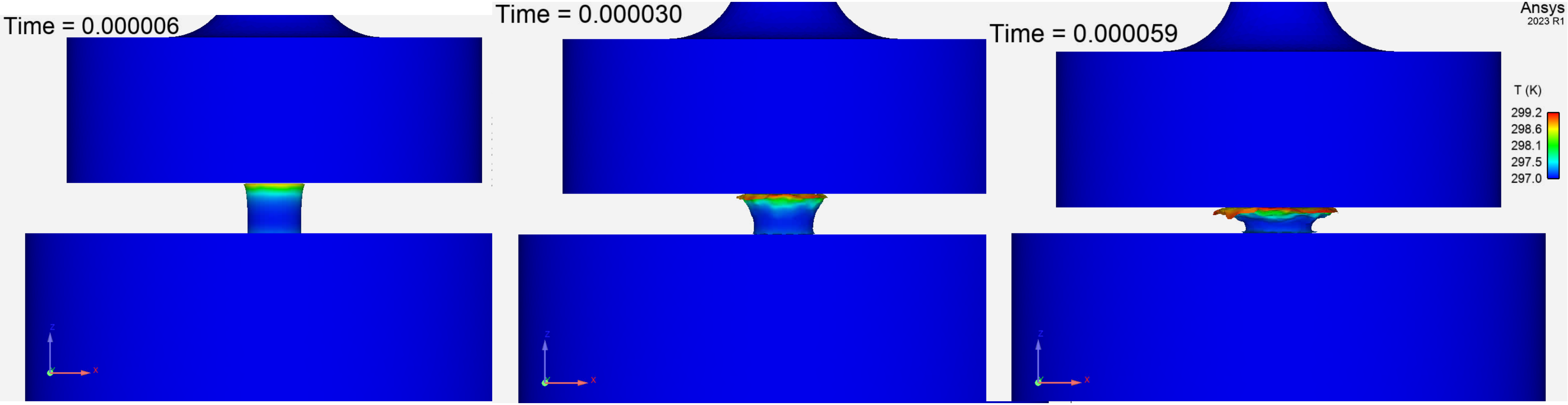
Conforming Reproducing Kernel

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

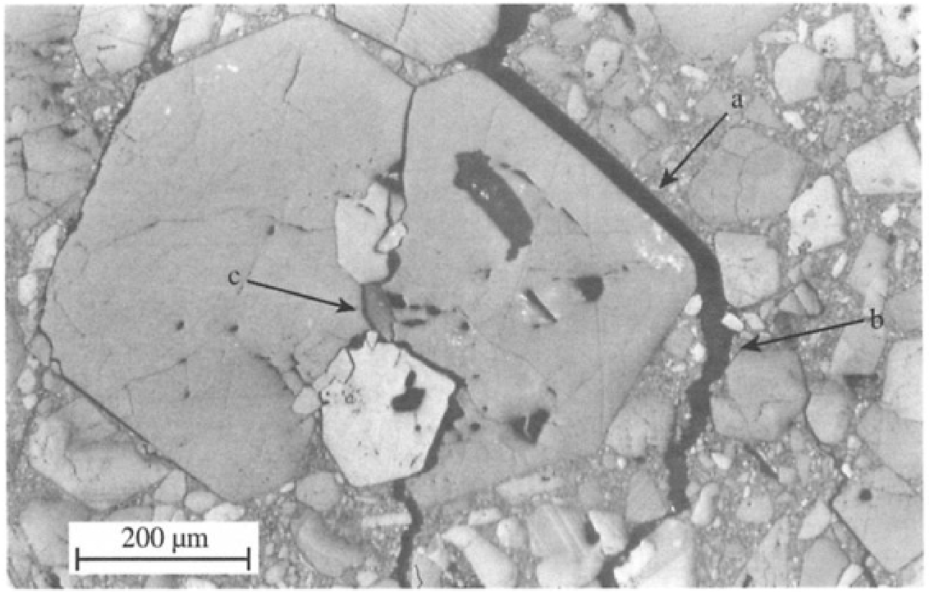


CRK Example: Dynamic Crushing of a PBX Material

- Impact of top anvil at 60 m/s
- Method is numerically robust at very large deformations



The case for meshfree methods: Mesoscale



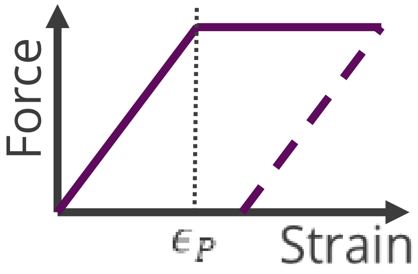
PJ Rae Proc. R. Soc. Lond. A. 2002

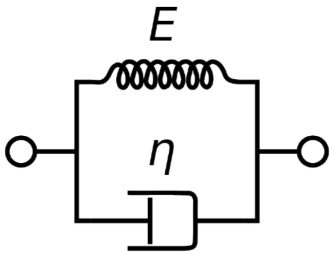
- Many physical mechanisms:
  - Plasticity/viscoelasticity in binder (or grains)
  - Rotation/delamination/friction in grains
  - Crack nucleation, growth, coalescence
- Variety of length scales
  - Failure often dominated by binder phase: Can be much smaller/thinner than grains
  - Macro response depends on 100s-1000s of grains
  - Need to simulate an representative sample
- Mechanics of micron-sized grains may be dominated by defects, not well described by bulk continuum model
- Microcracks create many discontinuities

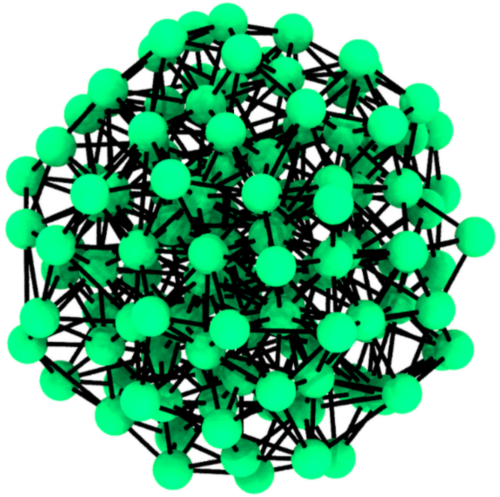
Need a flexible and cheap modeling approach!

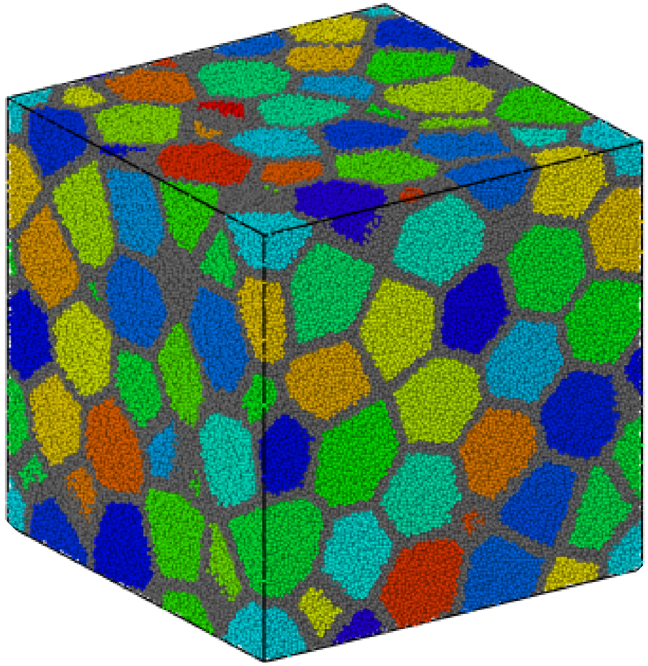
Bonded Particle Model (BPM)

- Lagrangian material points connected by a breakable network of bonds, AKA a spring network
- Solve Newtonian equations while obeying symmetries ⇒ ***Physics-based approach, focus on emerging behavior***
- Ideal for studying trends in abstract material classes, vary details of bond forces to capture different physics







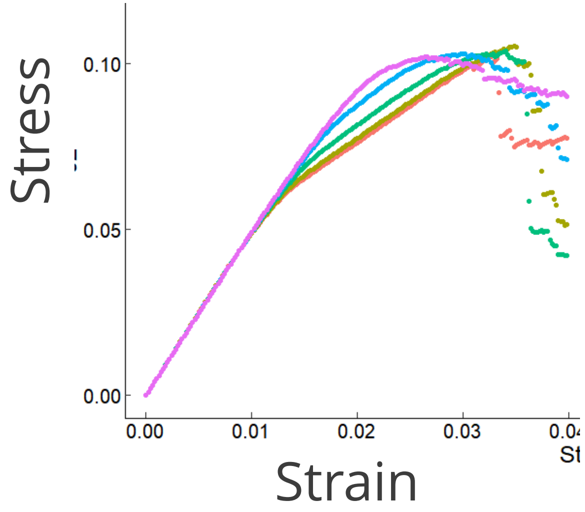


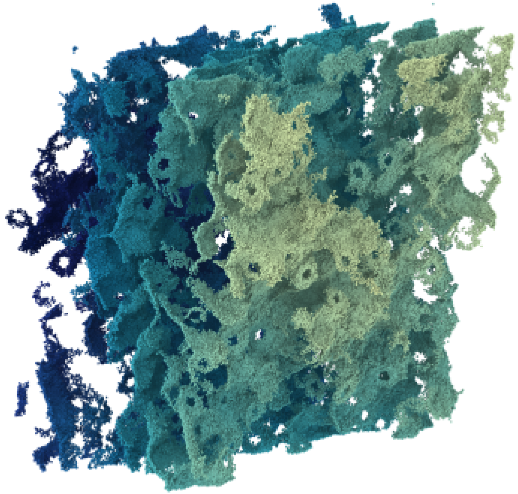
- **Simple and computationally cheap** – can simulate large domains at high resolution
- **Stably handles large deformation**, complex cracking, etc.

www.lammps.org

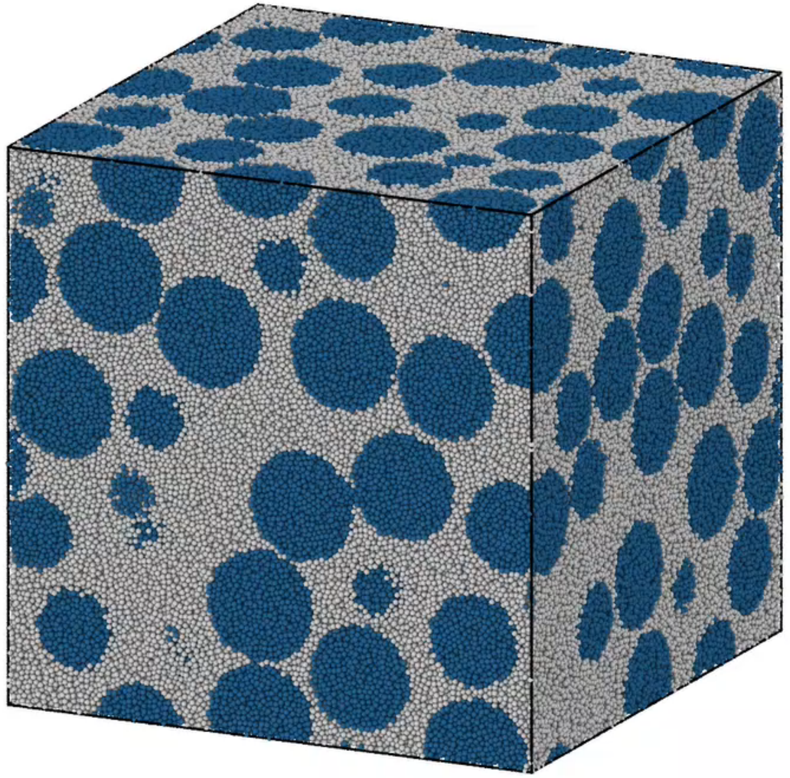
BPM example: Compression of Crystals in Binder

- Spherical, rigid crystals
- Elastic Binder, Ebinder << Ecrystals
- Volume Fractions: Crystals ~64%, Binder ~36%
- Simulation Outputs:
    - Global homogenized stress/strain
    - Time-evolution of damage metrics: crack size, connected crack networks, etc.




Final percolating crack networks in binder

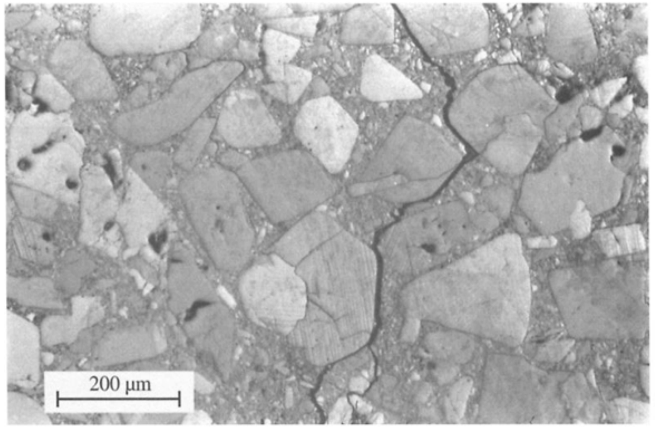
Uniaxial Compression



2. Complex mechanical behavior requires unique constitutive models

Mechanical Response Characteristics

- Mechanical behavior of Binderized Energetics is complex:
  - Strain rate dependence
  - Temperature dependence
  - Pressure dependence
  - Tension-Compression Asymmetry
  - Loss of Stiffness (Damage)
  - Permanent Strains (Plasticity)
  - Shear-induced dilation
- Many inelastic deformation mechanisms driving these macroscopic behaviors:
  - Viscoelasticity (binders)
  - Cracking (intra- and inter-granular)
  - Porosity opening
  - Dislocation slip within crystals
  - Twinning (some energetic crystals)



Plastic Bonded Explosive [Rae, 2002]

Macroscopic behavior (e.g. permanent strain) is produced by a combination of mesoscale mechanisms

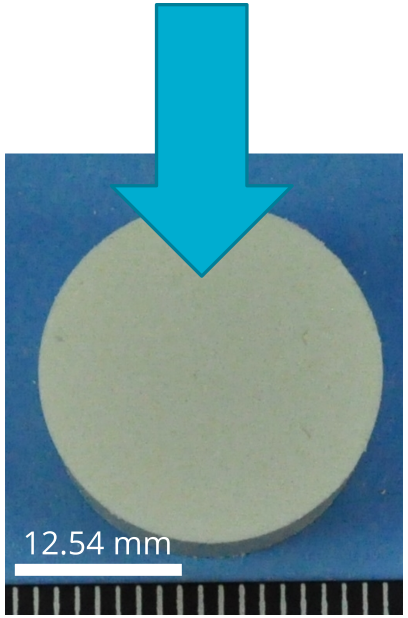
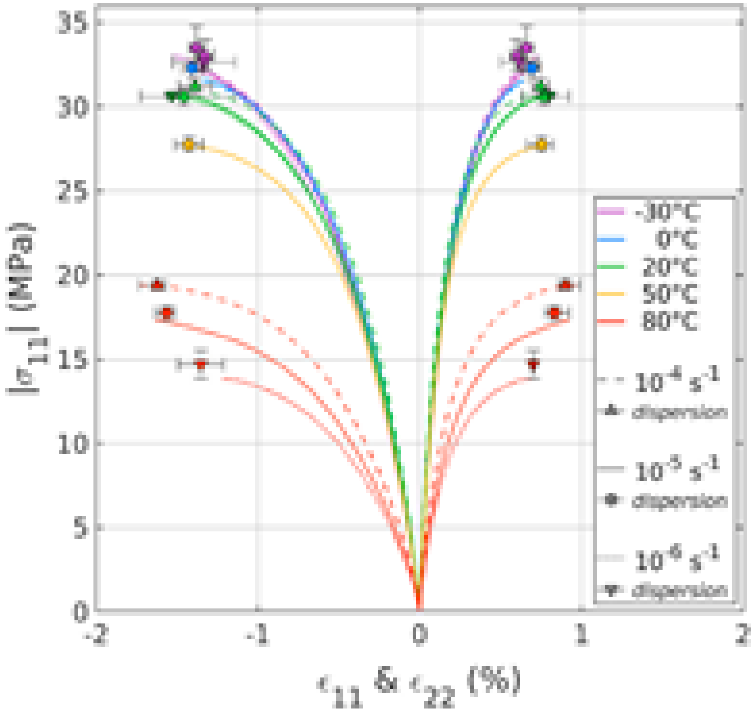


Image: courtesy Marcia Cooper

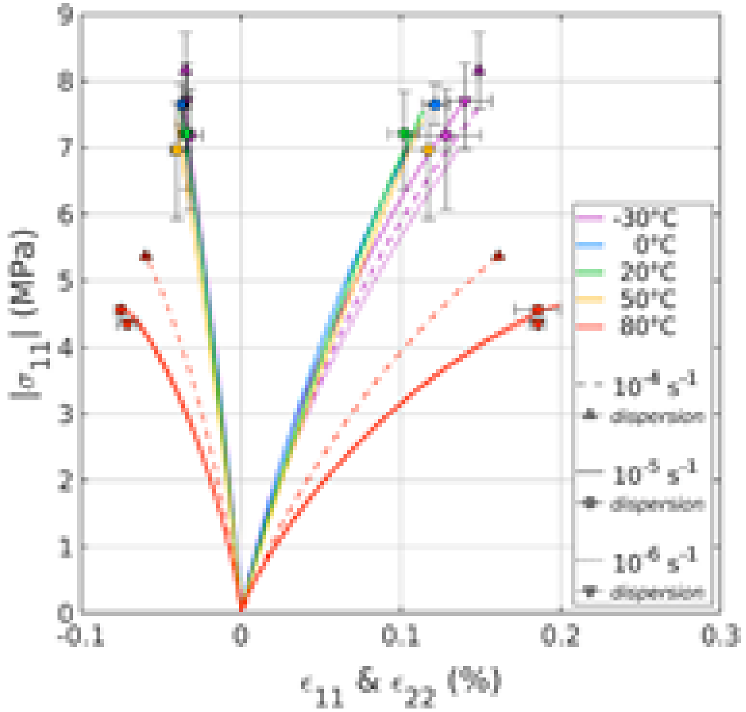
Example Data from the Literature

- Excellent review paper by *Plassart et al., Mech. Mat., 150 (2020) 103561.*

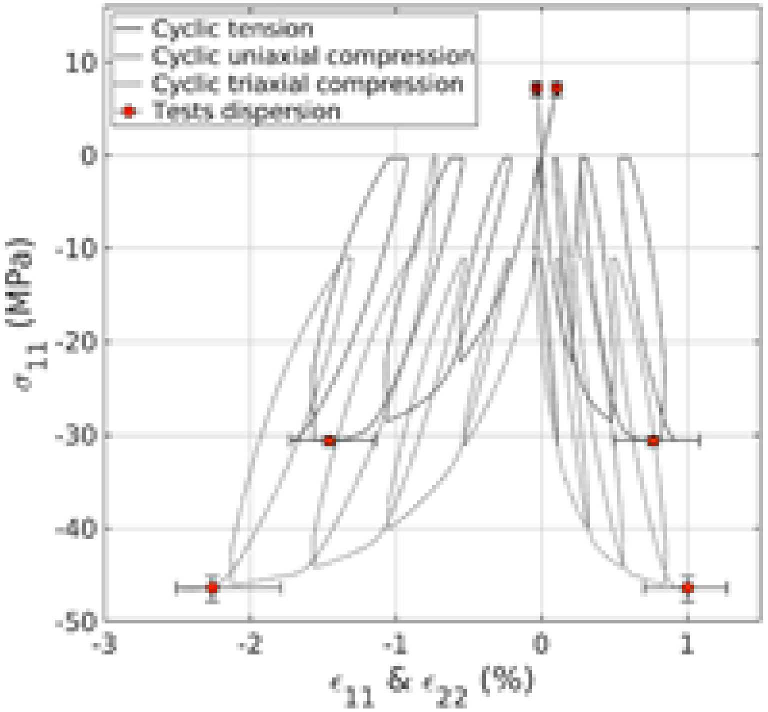
Uniaxial Compression



Uniaxial Tension

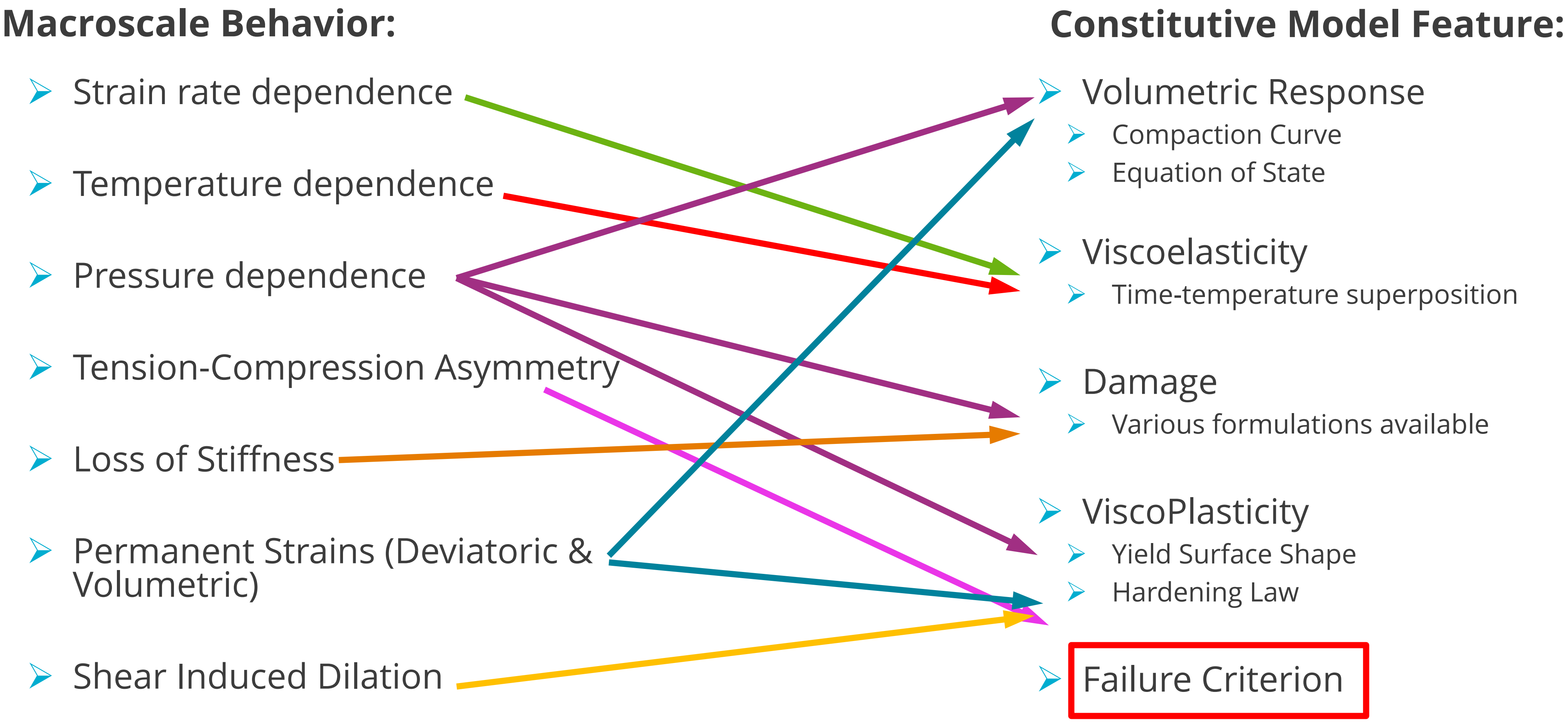


Cyclic Compression



Monotonic uniaxial stress tests induce response governed by many deformation mechanisms—thus these are not enough to fully characterize behavior in an arbitrary stress state

Mapping observed macroscale behaviors to constitutive model features



Macroscale Behavior:

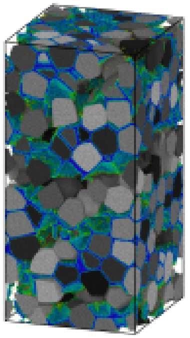
- Strain rate dependence
- Temperature dependence
- Pressure dependence
- Tension-Compression Asymmetry
- Loss of Stiffness
- Permanent Strains (Deviatoric & Volumetric)
- Shear Induced Dilation

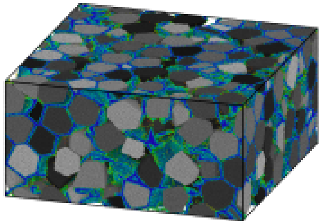
Constitutive Model Feature:

- Volumetric Response
  - Compaction Curve
  - Equation of State
- Viscoelasticity
  - Time-temperature superposition
- Damage
  - Various formulations available
- ViscoPlasticity
  - Yield Surface Shape
  - Hardening Law
- Failure Criterion

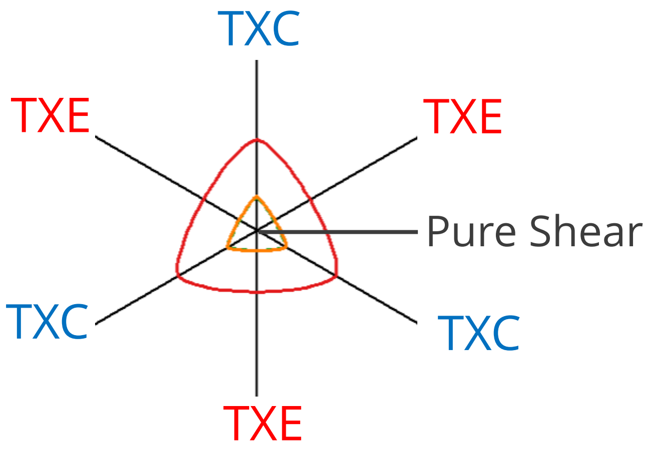
Mesoscale Studies of Failure Surfaces in Multiaxial Stress Space

- Study Parameters: Binder deformation (elastic vs. elastic-plastic), Crystal-binder bond strength



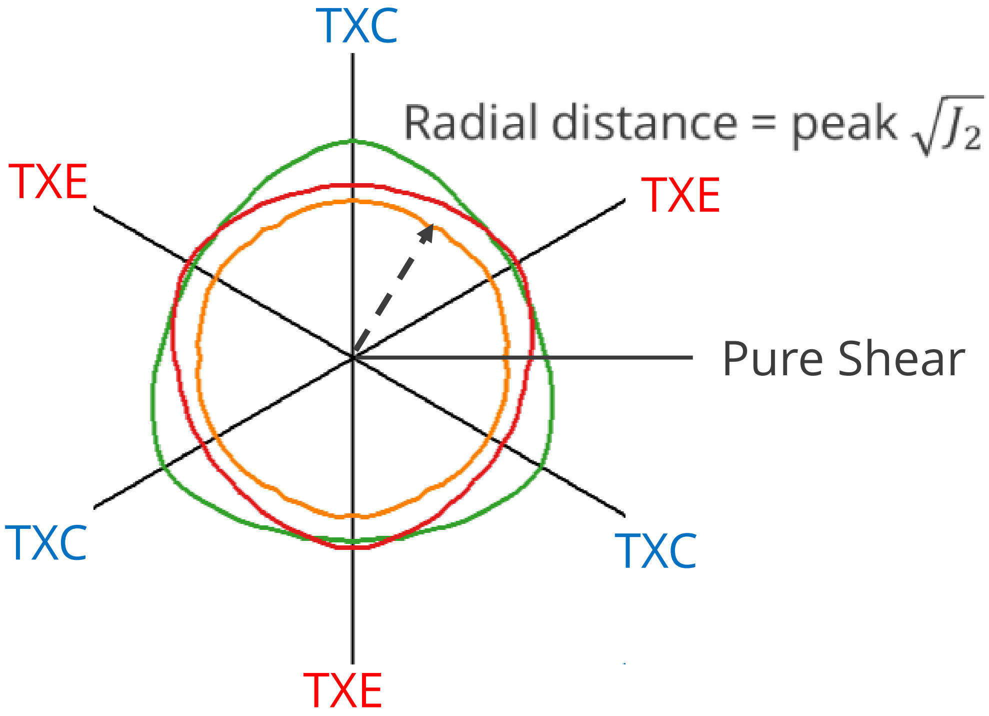


Unconfined, mean P = 0



- All cases are angular, Mohr-Coulomb-like, with strong tensile-compressive asymmetry

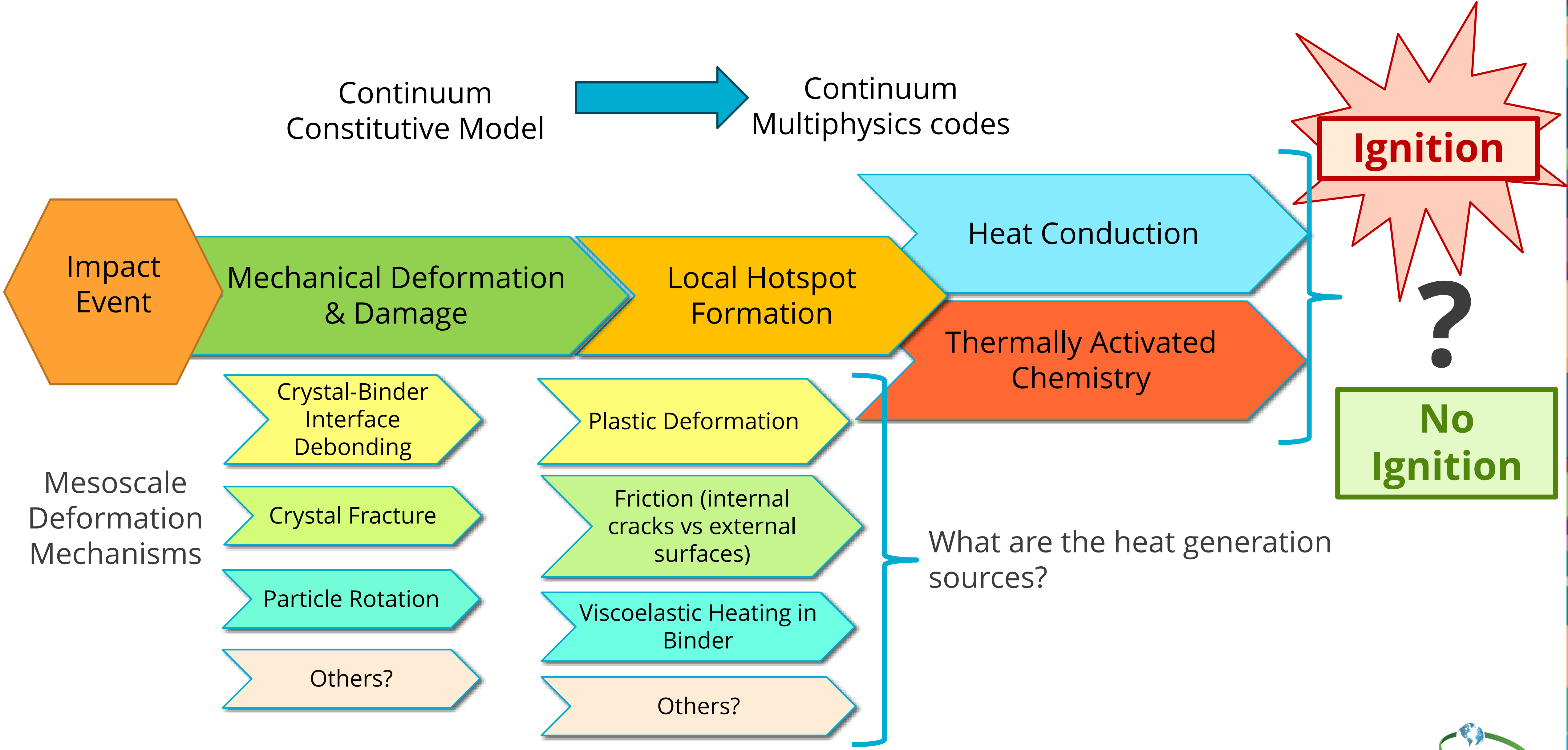
Confined with mean P = 0.3



- All cases show hardening (larger yield surface) with confining pressure

3. High Explosive Violent Reaction is a Multi-Physics, Multi-Scale Event

Revisiting the Full HEVR Event



Continuum Constitutive Model

Continuum Multiphysics codes

Impact Event

Mechanical Deformation & Damage

Local Hotspot Formation

Heat Conduction

Thermally Activated Chemistry

Ignition

?

No Ignition

Mesoscale Deformation Mechanisms

- Crystal-Binder Interface Debonding
- Crystal Fracture
- Particle Rotation
- Others?

- Plastic Deformation
- Friction (internal cracks vs external surfaces)
- Viscoelastic Heating in Binder
- Others?

What are the heat generation sources?

Macroscale Thermo-mechanical-chemical coupling

Meshfree Conforming Reproducing Kernel Continuum Code

Handshake solve for conservation of **momentum:**

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

and **energy:**

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

Thermal conduction

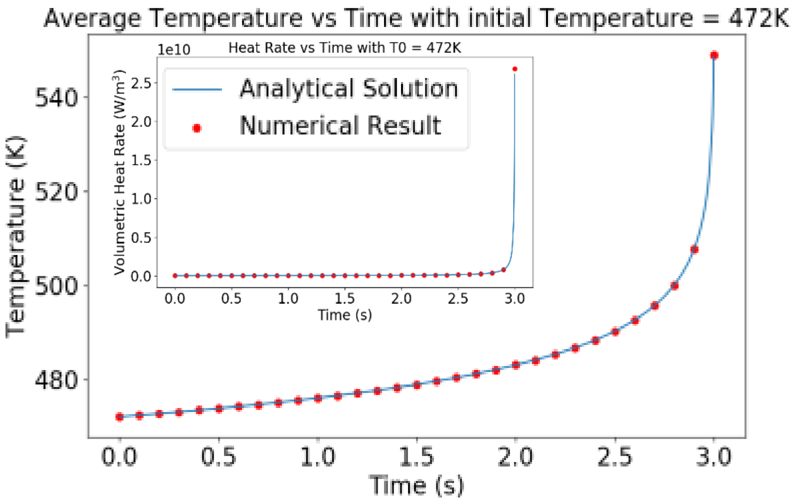
Adiabatic heating from plastic deformation

- State variable from mechanical constitutive model

Chemical heating

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

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



Thermo-chemical coupling verification

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

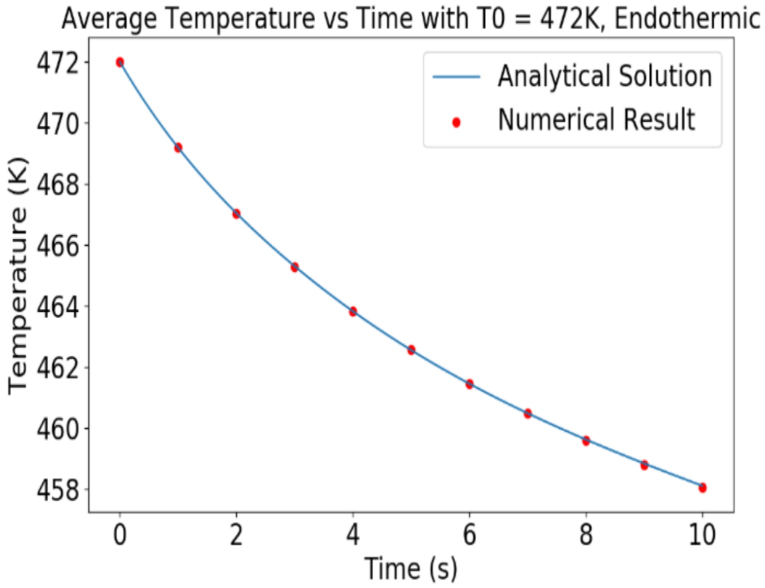
$$-\lambda\nabla^2 T + \rho C\frac{dT}{dt} = \rho\Delta H Z e^{-E_a/RT}$$

Uniform temperature change
(temporal variation only)

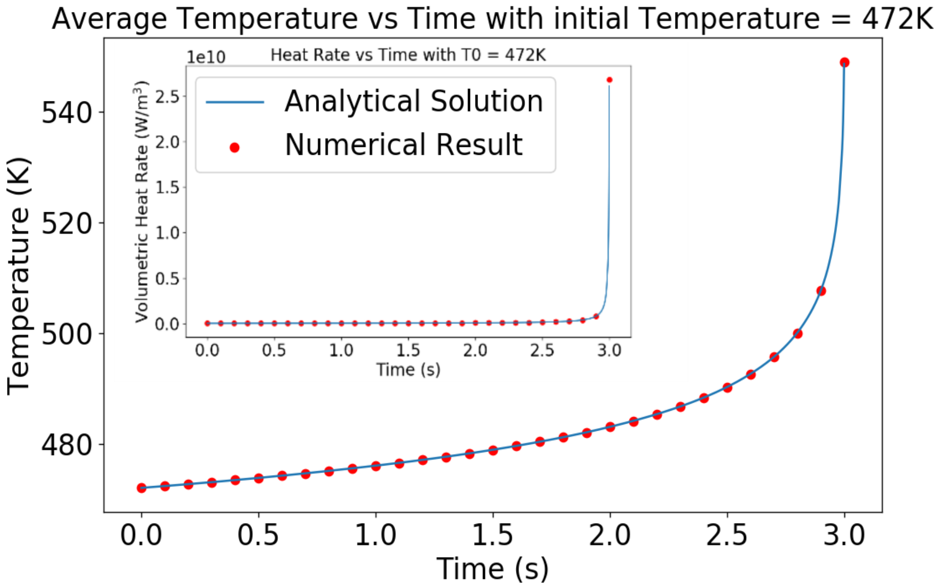
$$\xrightarrow{\hspace{3cm}}$$

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

Endothermic Process



Exothermic Process



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

Thermo-chemical coupling verification

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

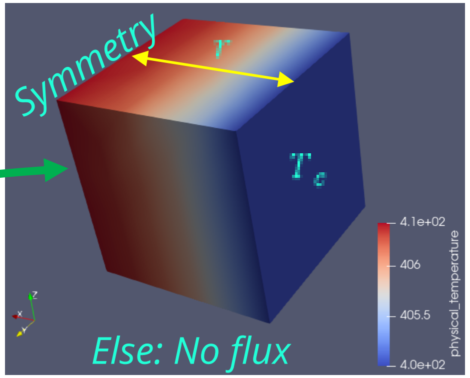
$$-\lambda\nabla^2 T + \rho C\frac{dT}{dt} = \rho\Delta H Z e^{-E_a/RT}$$

Steady state solution (spatial variation only)

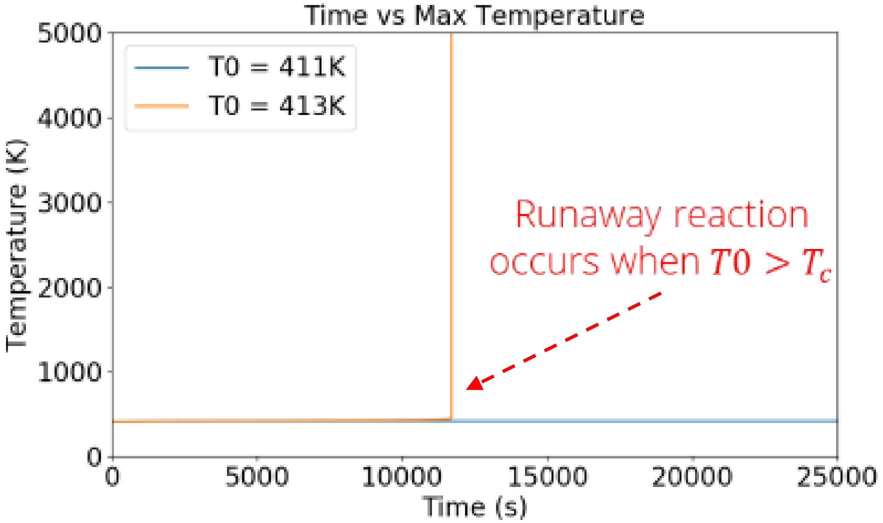
$$-\lambda\nabla^2 T = \rho\Delta H Z e^{-E_a/RT}$$

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

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



Max. Temperature at symmetry boundary



Runaway reaction occurs when $T0 > T_c$

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

Analytical Critical Temperature: ~412K

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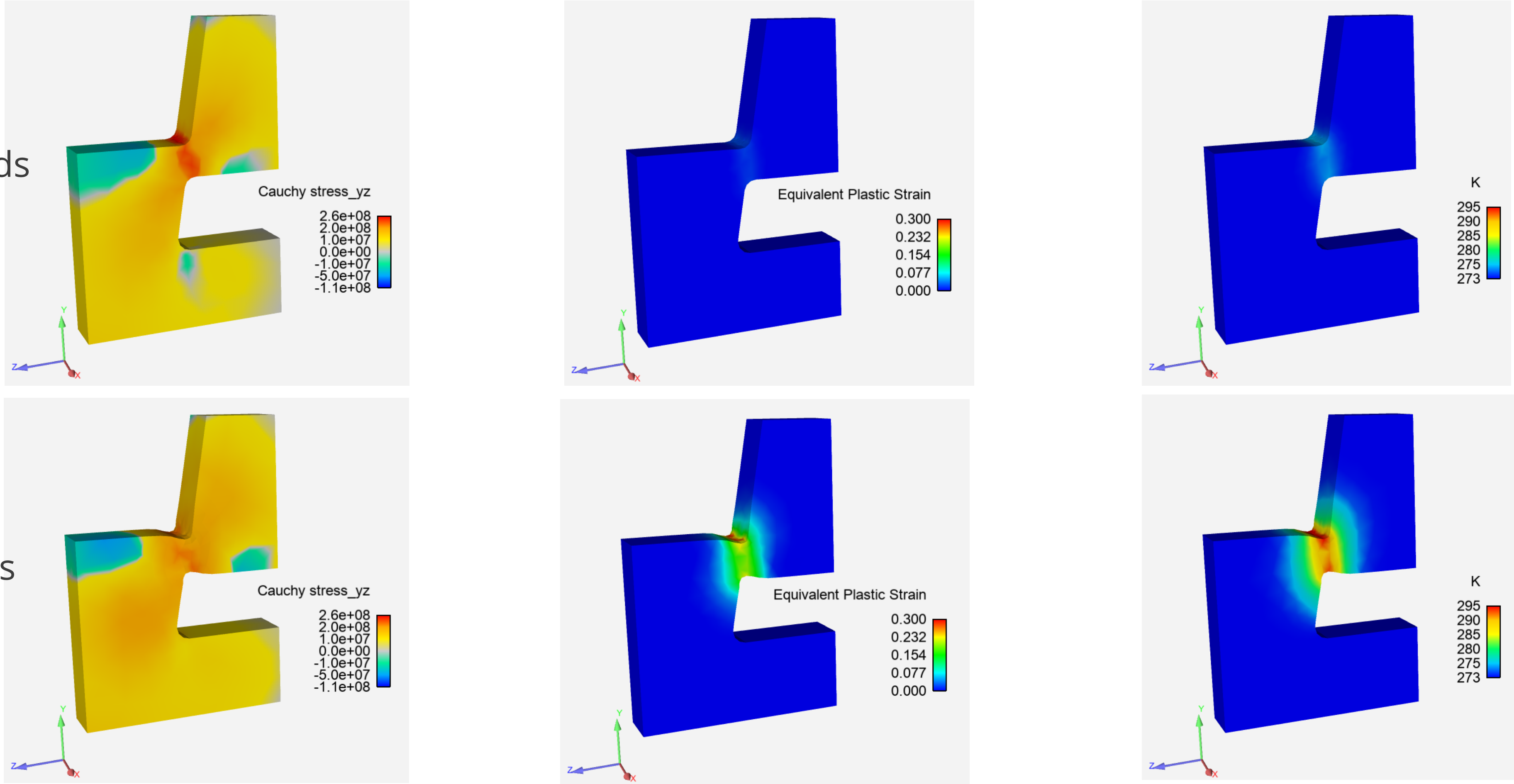
[1] Cooper, Paul W.. Explosives Engineering, John Wiley & Sons, Incorporated, 1996.

Inert Material Study: Shear-Induced Heating in Steel

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



Shear Stress

Equivalent Plastic Strain

Temperature

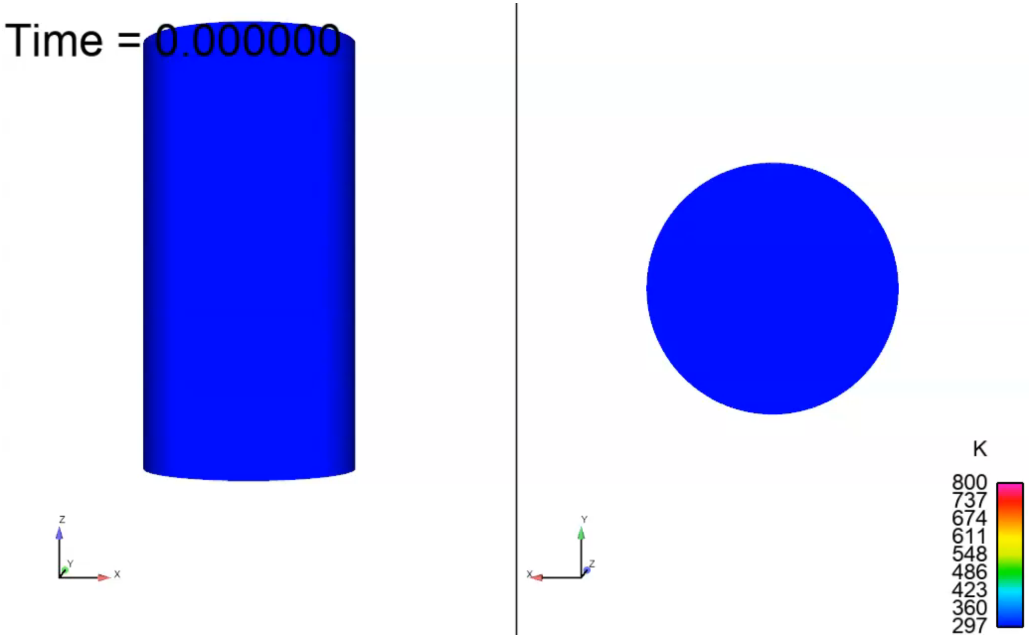
Time = 65 microseconds

Time = 250 microseconds

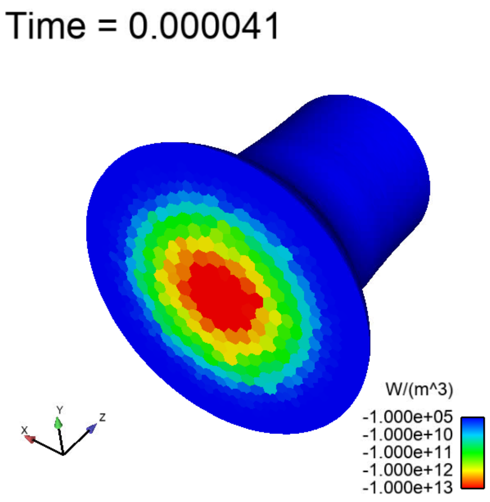
Mechanically Induced Thermal Runaway

- Taylor Bar Impact: 450 m/s
- Material properties: pure energetic crystals
- Energy dissipated due to plastic deformation raises temperature enough to start runaway chemistry

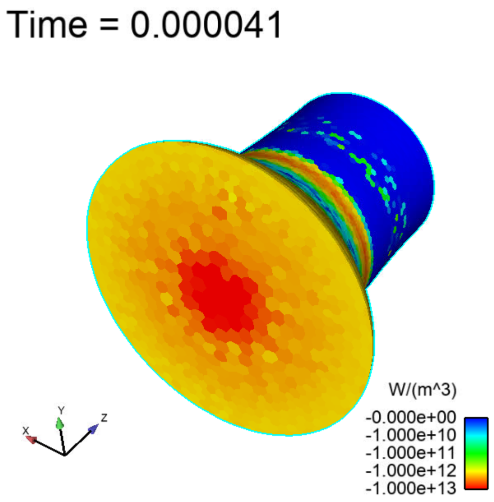
Temperature (K)



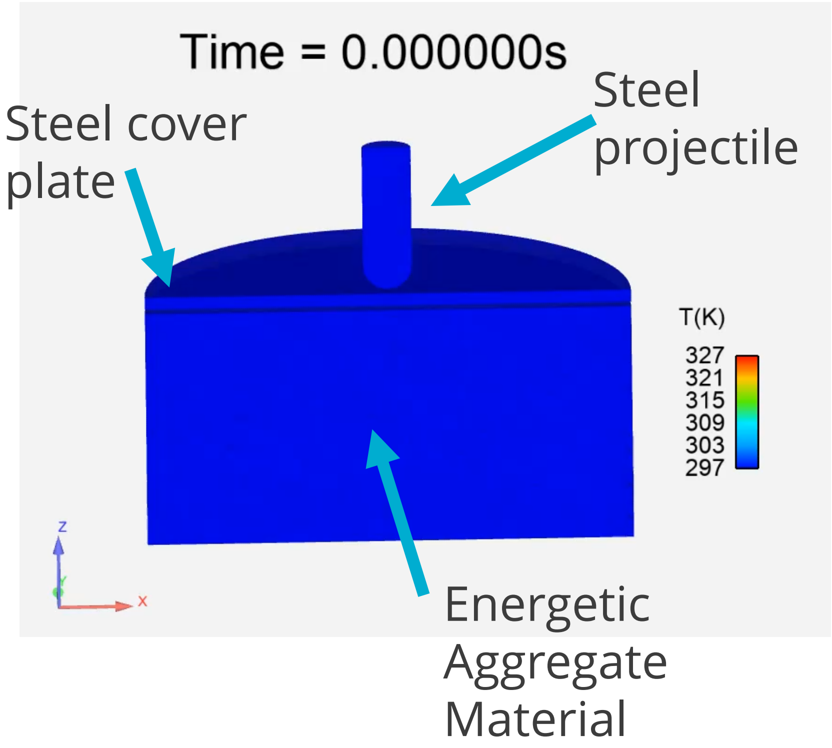
Chemistry Heating Rate



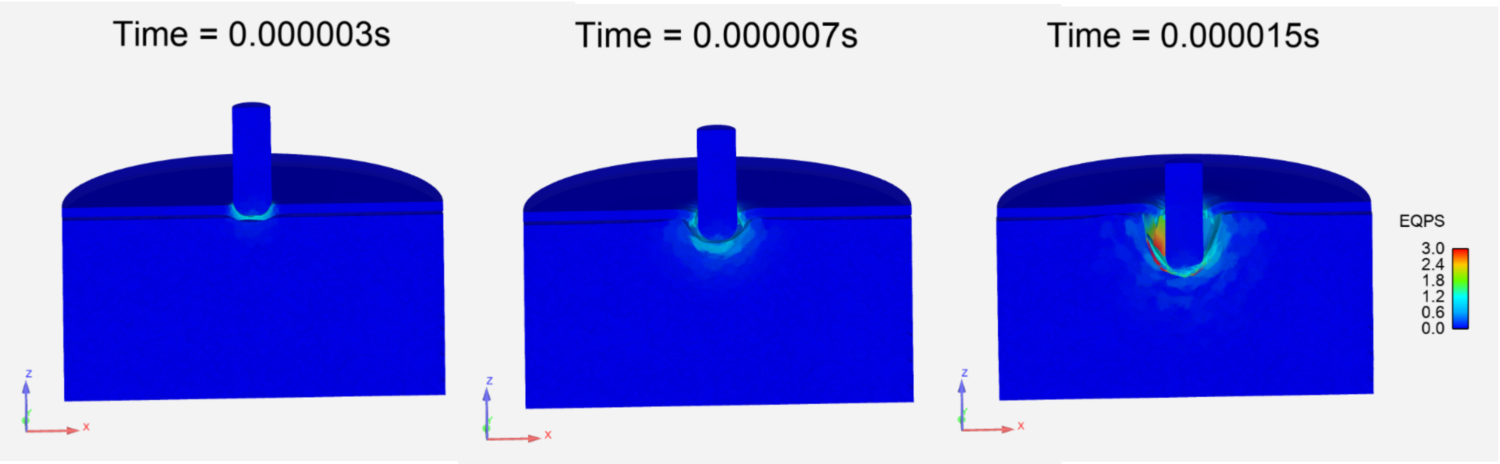
Plasticity Heating Rate



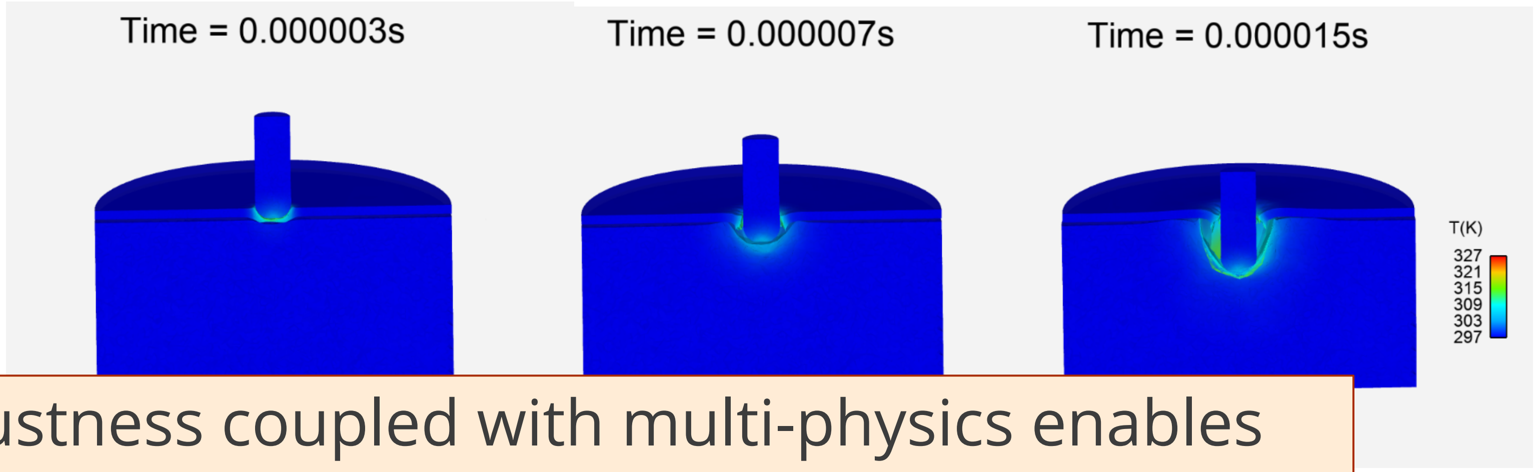
Multi-material impact example



Equivalent Plastic Strain



Temperature

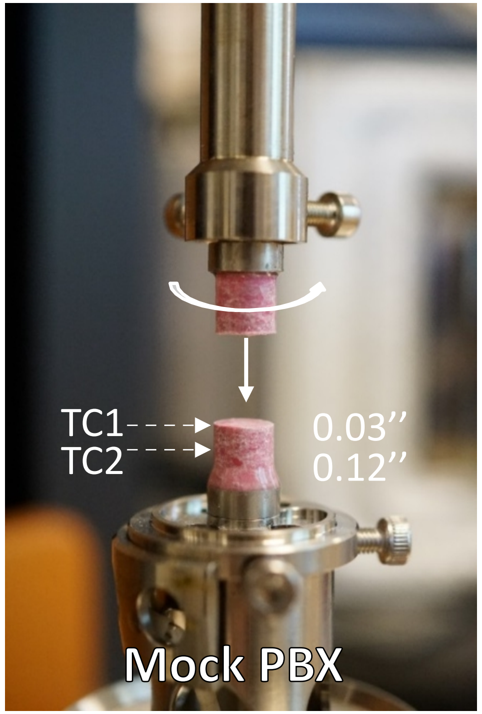


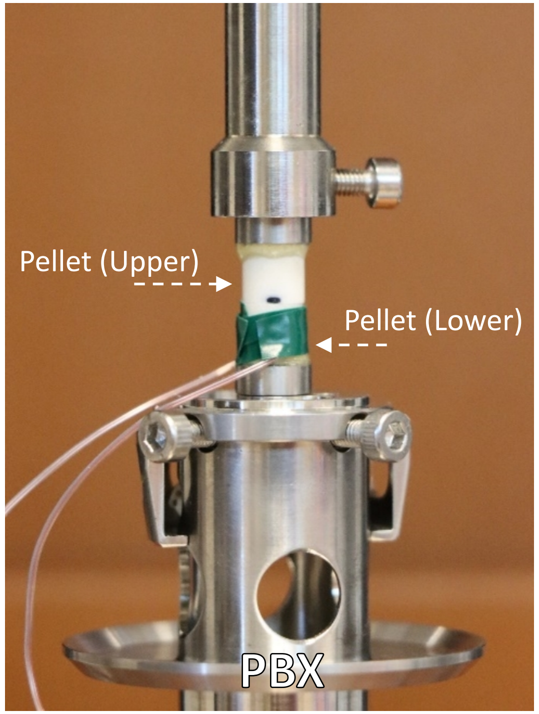
Extreme numerical robustness coupled with multi-physics enables new simulation capability

Mechanism Discovery: Frictional Heating Experiments

Objective: Isolate and measure heating due to friction

The *TA Discovery Hybrid Rheometer* was used to frictionally shear two explosive pellets at a controlled angular sliding speed and applied normal force.





Procedure

- Fix pellets to Rheometer fixtures
    - ½” dia. x ½” height pellets
- Insert into rheometer grips
- Place TC in contact with sample surface at known locations and secure with tape
- Wait for thermal equilibrium in environmental chamber
- Set axial load and run (3 rad/s, 180s)
    - 2.5N, 5N, 10N (triplicate)

Measurements

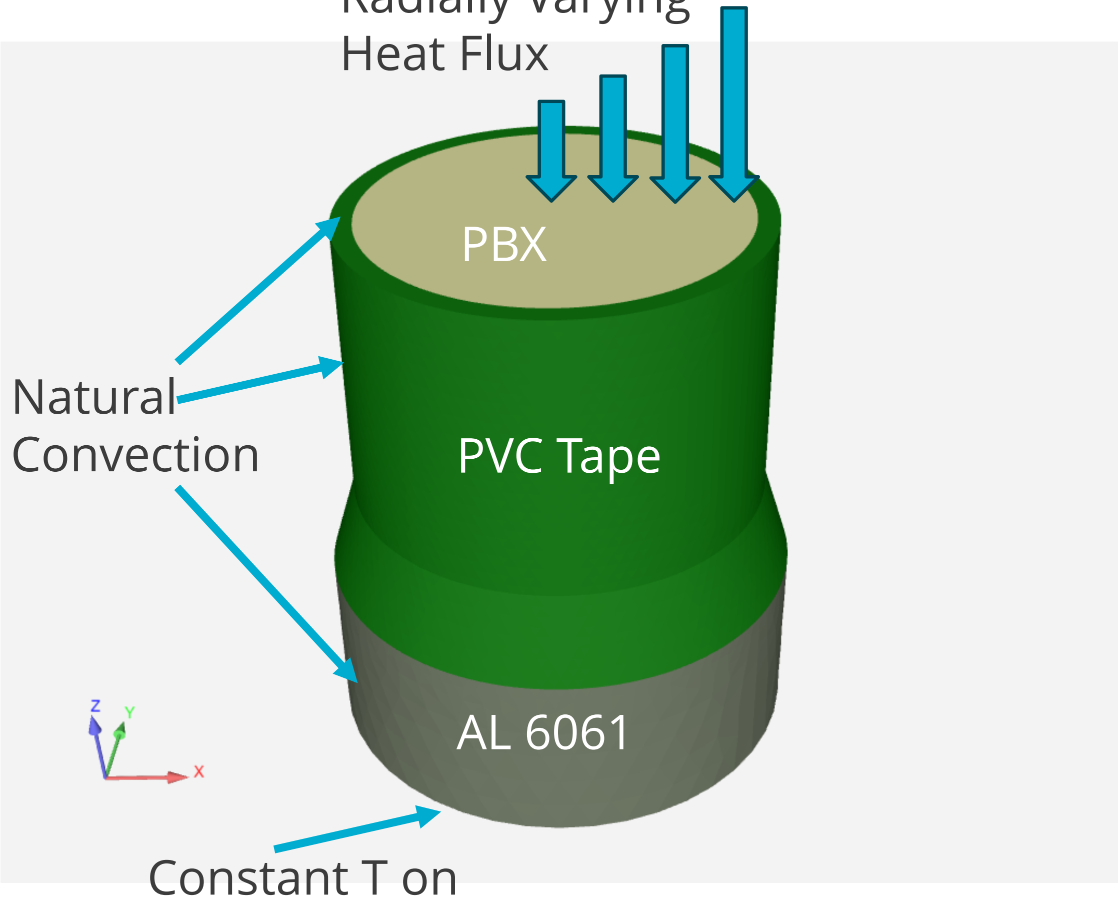
- Normal force, Torque, Chamber temperature
- Sample temperature on outer surface using T-type thermocouples (X2)

Outcome

- Temperature rise due to heat generated by friction
- Calculated coefficient of friction

Frictional Heating Model (thermal only)

$$\dot{q} = \delta_E \mu F$$



Radially Varying
Heat Flux

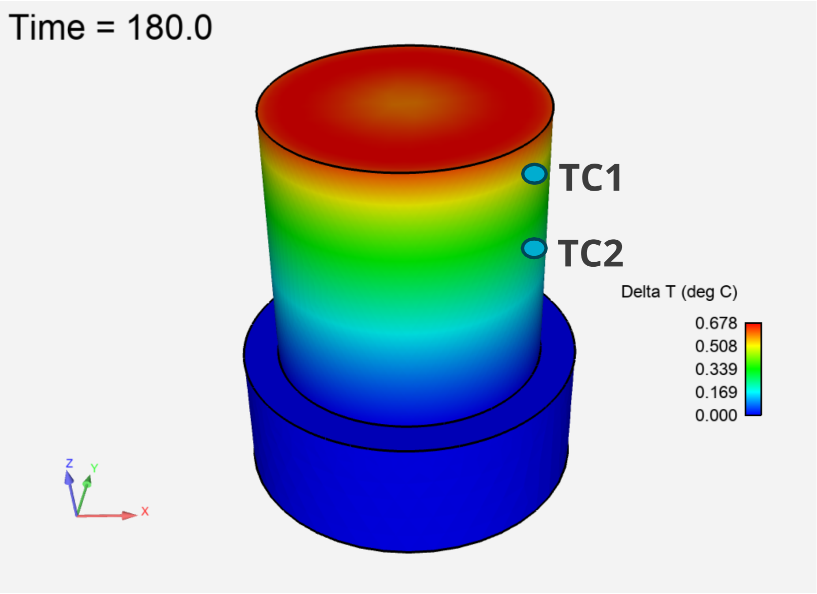
PBX

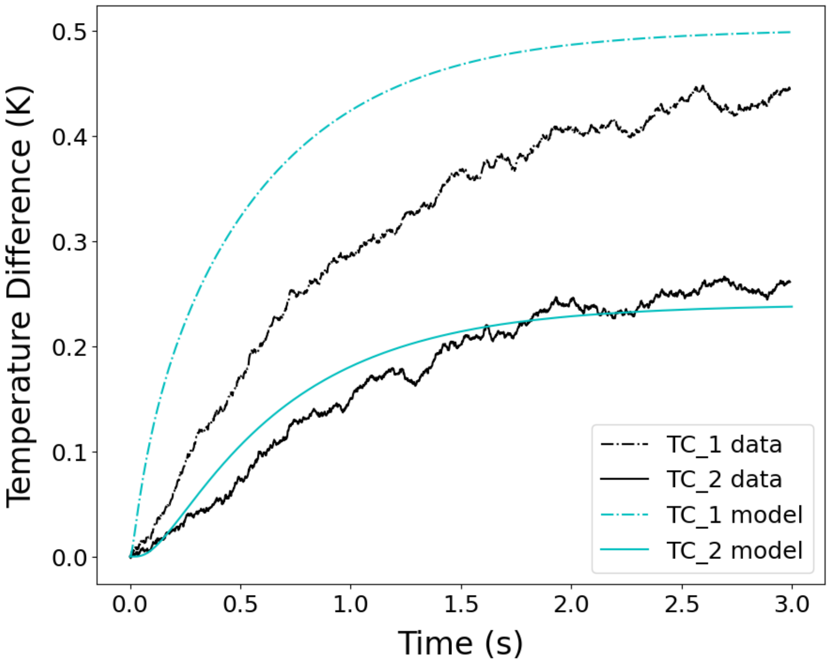
Natural
Convection

PVC Tape

AL 6061

Constant T on
bottom surface
(heat sink)

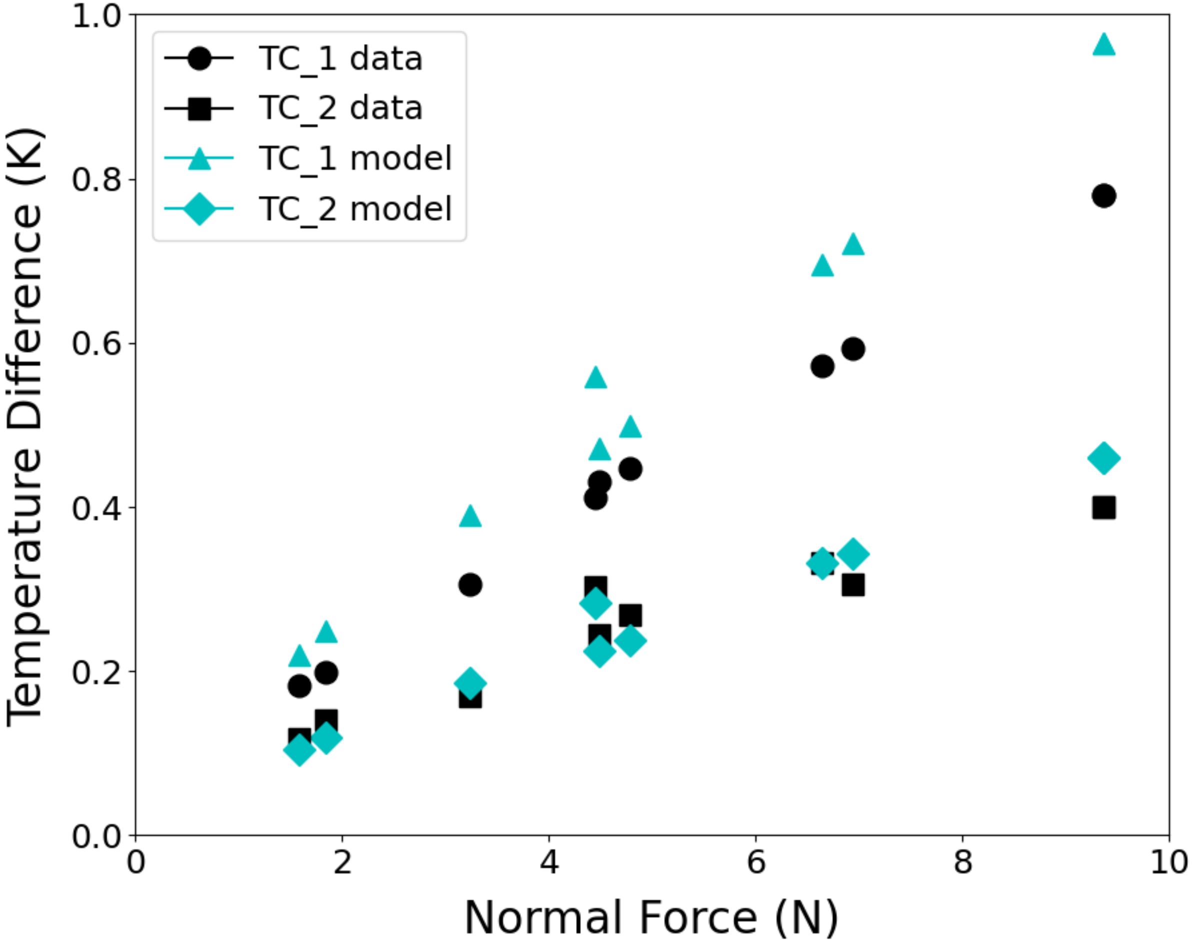


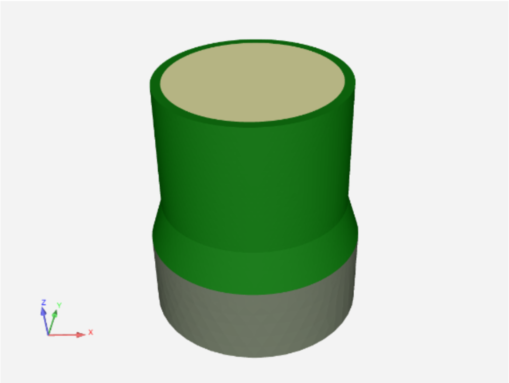


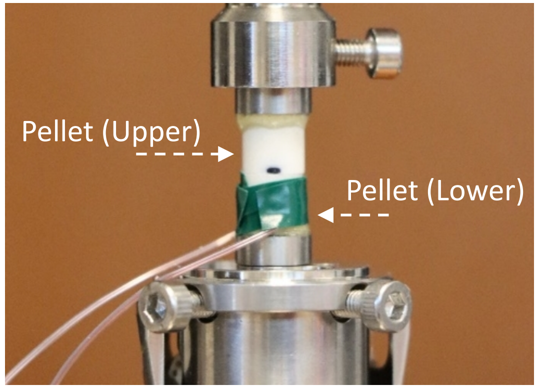
Frictional Heating Model (thermal only)

Takeaways:

- Linear global temperature rise with axial loading predicted by model
- Good match with experimental data considering the modeling uncertainties
  - E.g. properties of PVC tape, convection coefficient, small temperature rises
  - Tape geometry differences
  - Lumping of glue in with the tape







Wrap Up & Discussion Points

1. Large Deformation (Global and/or localized) and Pervasive Damage/Fracture
   - Meshfree numerical methods (continuum and mesoscale) show much promise here
     - Bonded Particle Methods enable computationally cheap, large mesoscale studies
     - Conforming Reproducing Kernel (CRK) Method as a powerful tool for *Lagrangian* continuum mechanics at massive strains and coupled physics

2. Complex mechanical behavior, requires unique constitutive models
   - Need for characterization beyond the uniaxial stress-strain curve
   - Need for flexible, efficient mesoscale models to study linkages between microscopic inelastic mechanisms and macroscale effective behaviors
     - Inform macroscale constitutive model features and balance between them (yield & failure surfaces, damage formulation, etc.)

3. Multi-physics nature of HEVR event
   - Meshfree CRK method with coupled physics shows promise for pre-ignition phase where thermo-mechanics dominates
   - Discovery experiments characterizing heat generation mechanisms still needed!

Thank You!

Some Relevant Literature

- **CRK Numerical Method:** *J. Koester, J.S. Chen, Comput. Methods Appl. Mech. Engrg. 347 (2019) 588–621*
- **Review of Mechanical Behavior of HMX and TATB-based PBX Materials:** *Plassart et al., Mech. Mat., 150 (2020) 103561.*
- **BPM Study of Pressure Dependence in Plastic Bonded Energetic Materials:** *J.T. Clemmer, K.N. Long, J.A. Brown, Mech. Mater. 184 (2023) 104693.*

ViscoPlastic-ViscoSCRAM Model Theory

- **Kinematics:**

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

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

- Viscoelasticity

$$\boxed{\dot{\boldsymbol{s}} = 2G^{\infty}\dot{\boldsymbol{e}}^{ve} + \sum_{\kappa=1}^{N}\underbrace{\left(2G^{(\kappa)}\dot{\boldsymbol{e}}^{ve} - \frac{\boldsymbol{s}^{(\kappa)}}{\tau^{(\kappa)}}\right)}_{\text{Prony series of shear moduli and relaxation times}}}$$

- SCRAM Damage

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

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

$$\underbrace{\dot{\boldsymbol{s}}^{(\kappa)} = 2G^{(\kappa)}(\dot{\boldsymbol{e}} - \dot{\boldsymbol{e}}^{p}) - \frac{\boldsymbol{s}^{(\kappa)}}{\tau^{(\kappa)}} - \frac{G^{(\kappa)}}{G_0}\left[\frac{3}{a}\left(\frac{c}{a}\right)^2\dot{c}\boldsymbol{s} + \left(\frac{c}{a}\right)^3\dot{\boldsymbol{s}}\right] \qquad D = \frac{\left(\frac{c}{a}\right)^3}{1 + \left(\frac{c}{a}\right)^3}}_{\text{M.A. Buehler, D.J. Luscher, Int. J. Num. Meth. Eng. 2014}}$$

- Drucker-Prager Plasticity

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

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

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

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