SAND2020-2374C

Multiscale modeling to study effects of microstructure in shocked hexanitrostilbene

TMS 2020 Annual Meeting and Exhibition

San Diego, CA

February 23-27, 2020

PRESENTED BY

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February 24, 2019

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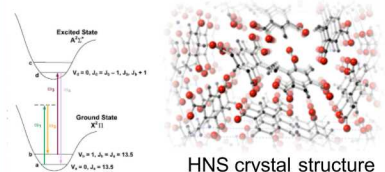
Presentation Outline

- Introduction
- Synthetic Microstructure Generation
- Continuum Hydrocode Simulations (CTH)
- Temperature distribution statistics for many microstructures
  - Can we mine these for sensitivity metrics and correlate these to microstructure?
- Outlook & Perspective

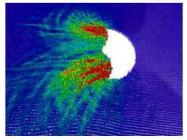
Shock Initiation of Explosives at Sandia

❖Generate a high fidelity baseline

Quantum / MD Large Scalable Codes

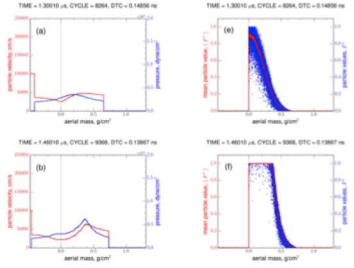


HNS crystal structure



LAMMPS + Kokkos

New Continuum Codes



Stochastic reactive shock waves

Formation Modeling

-poured
-pressed
-deposited
-AM of EM

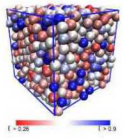
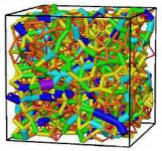


Image stack, or simulated μstructure



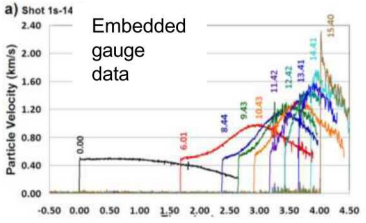
Graph of contact network

Images from SAND2018-4593PE (J. Lechman and D. Bolintineanu)

Objective: Science-based engineering and design of new explosive components

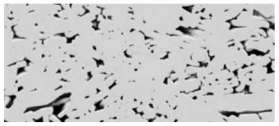
Tests and Experiments

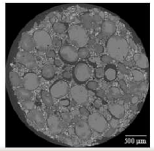
- Performance
- Sensitivity
- Threshold and UQ



Burns *et al.* J. Appl. Phys. (2012)

Microstructural Analysis

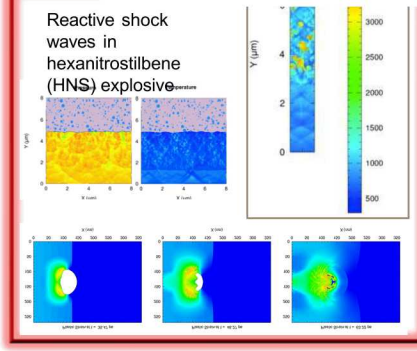




X-section of HNS pellet (top) and CT scan courtesy of Andres Chavez (left)

Mesoscale Simulations

Reactive shock waves in hexanitrostilbene (HNS) explosive

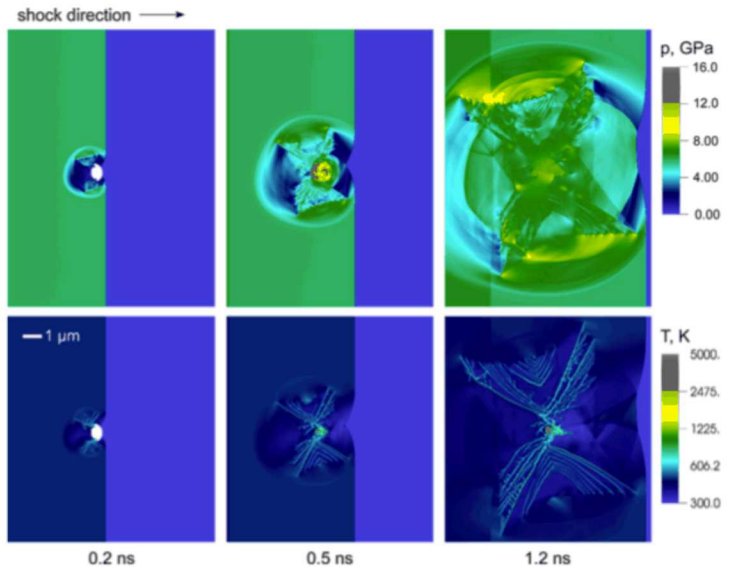


Adapt/remove approximations

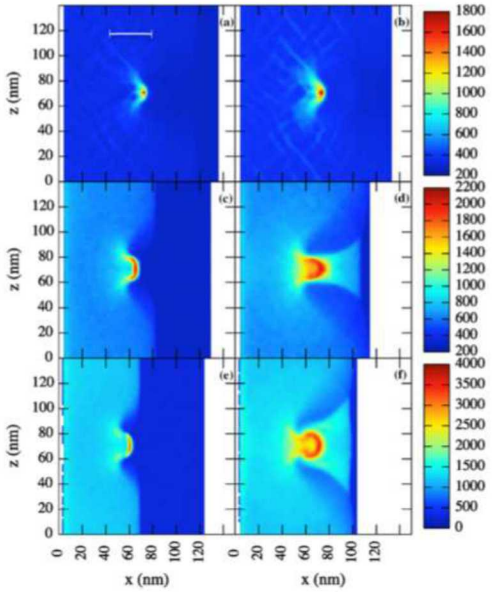
Role of Porosity in Shock Initiation

- Some degree of porosity present in almost all energetic materials
- Pore collapse can be key mechanism for hot spot formation

Many Single-Pore Collapse Studies



Austin et. al, J. App. Phys. 117 (2015), 185902



Eason and Sewell, J. Dynamic Behavior Mater. 1 (2015), 423-438

What about pore interactions?

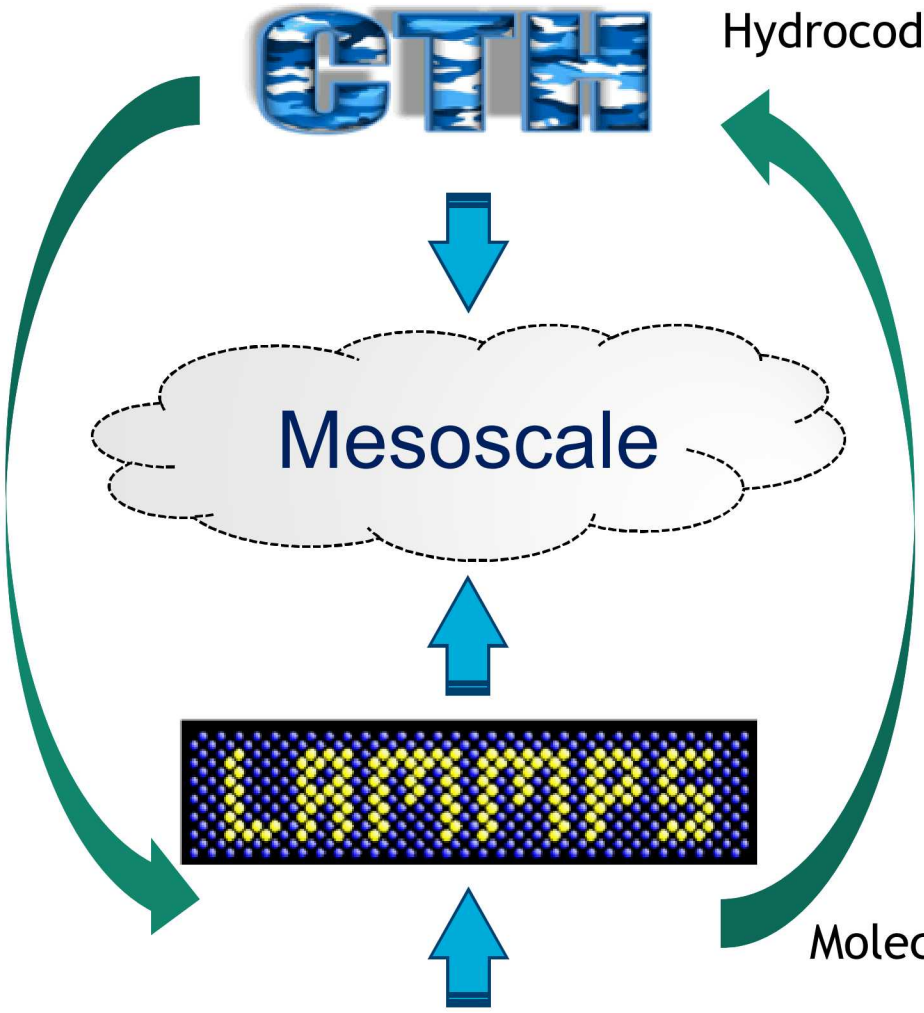
- Can we link particular porosity configurations/geometries with some metric of likelihood for hot spot formation??
  - Use Multiscale approach with both continuum hydrocode and MD simulations to explore this

Multiscale Approach

Both continuum hydrocode and MD simulations

Continuum Properties Propagated Down:

- 'Critical' local microstructure features
- Evaluate measures of sensitivity
- Integration with new experimental diagnostics

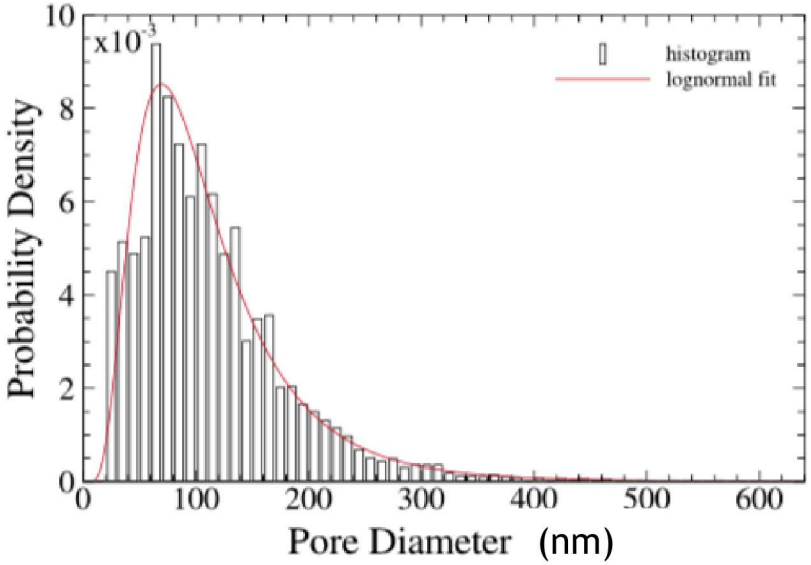


Atomistic Properties Propagated Up:

- Global reaction kinetics
- Improved strength models
- Effects of anisotropy in strength, EOS

Microstructure of Pressed Hexanitrostilbene

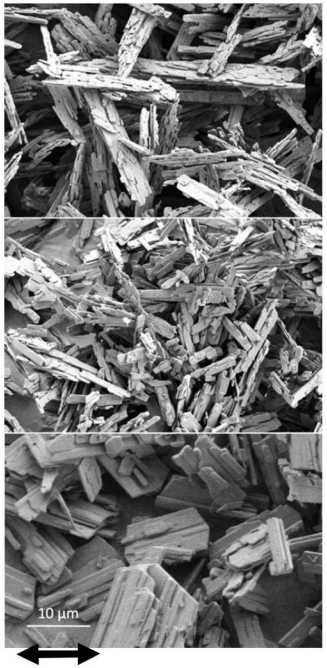
- HNS-IV powder pressed to 72 – 92% TMD



HNS-IV Lot 1

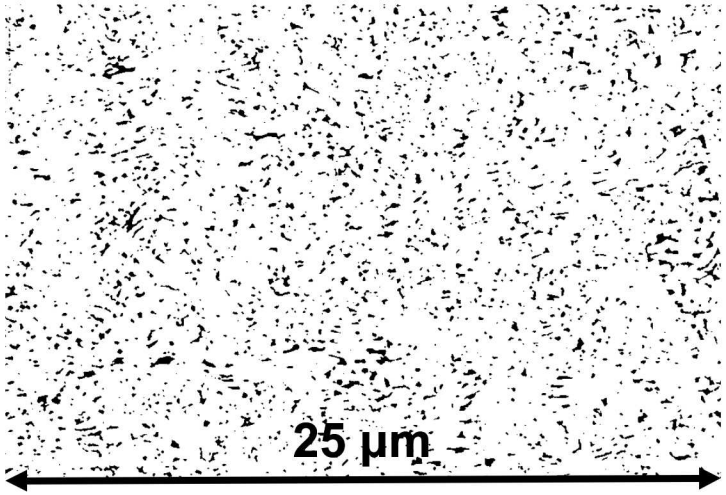
HNS-IV Lot 2

HNS-I



10 µm

Thresholded SEM image of pressed microstructure



C.D. Yarrington, R.R. Wixom, D.L. Damm, J. App. Phys. 123 (2018) 105901

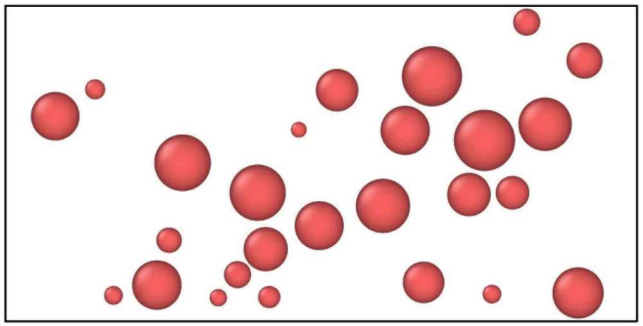
Synthetic Microstructure Generation

- 2D Discrete Element Method (DEM) simulations used to generate many microstructures with different porosity configurations

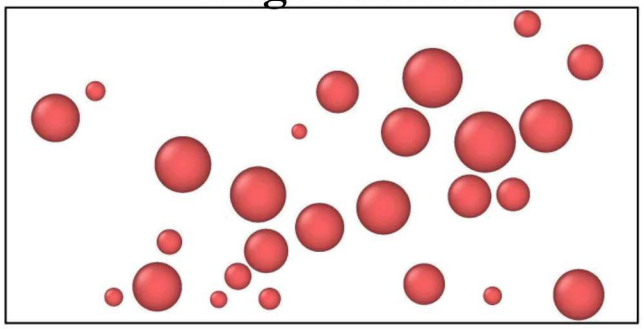
Initial state: spheres placed at random in 250 X 500 nm domain, no overlaps

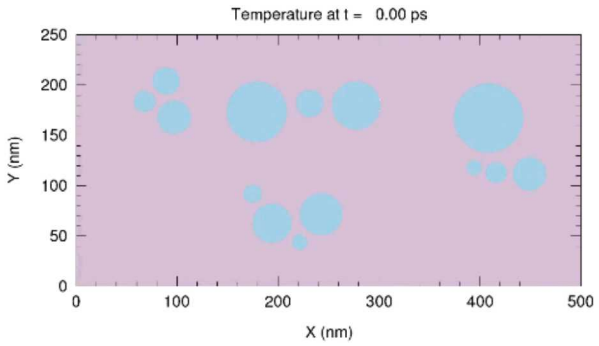
Langevin dynamics with range of contact cohesion values:

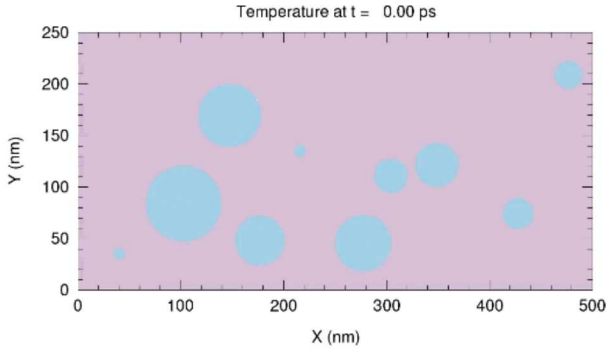
Low cohesion

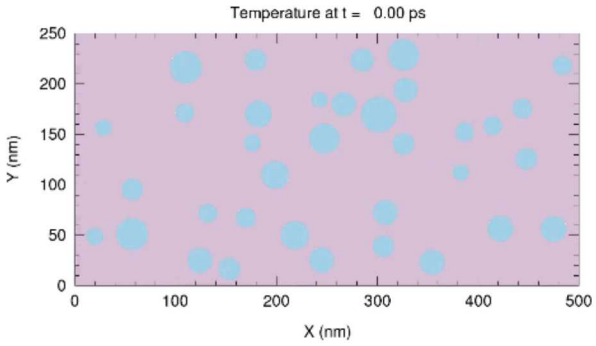


High cohesion



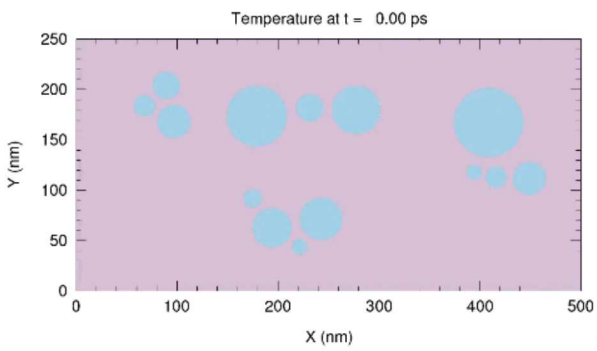


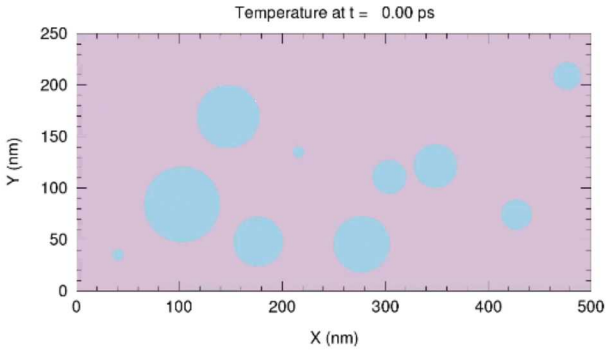


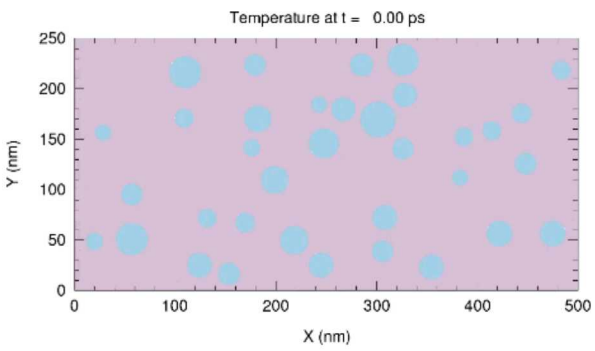


Example Synthetic Microstructures

180 different microstructures generated, 88% TMD







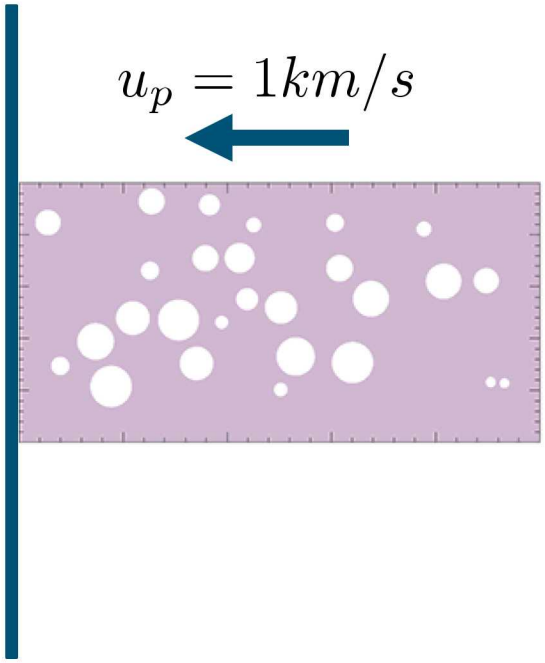
Microstructure Geometry Metrics:

- Specific Surface Area
- Fraction of 2-body connected pores
- Fraction of 3-body connected pores
- Compact 3-body fraction

Continuum Hydrocode Simulations—CTH

- Reverse ballistic impact calculation
- Evaluate many microstructures to elucidate geometries that show higher propensity for hot spot formation

Symmetric impact



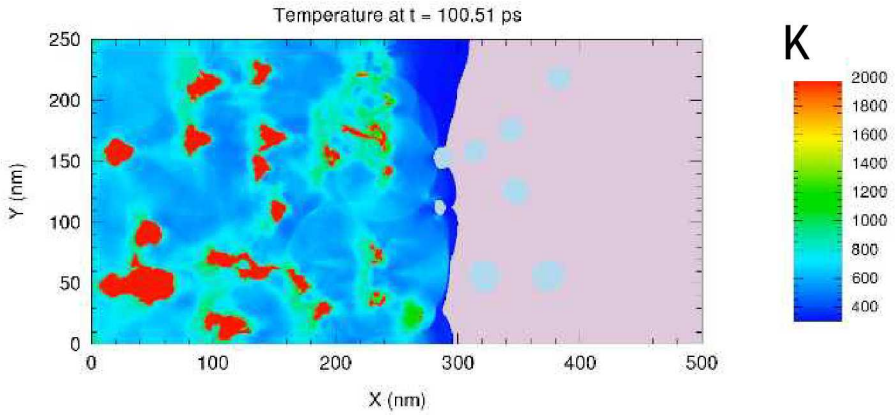
Material Models

- Pores filled with air
- HNS matrix:
  - Mie-Grüneisen equation of state
  - Stienberg-Guinan-Lund viscoplastic strength model
  - Arrhenius burn model

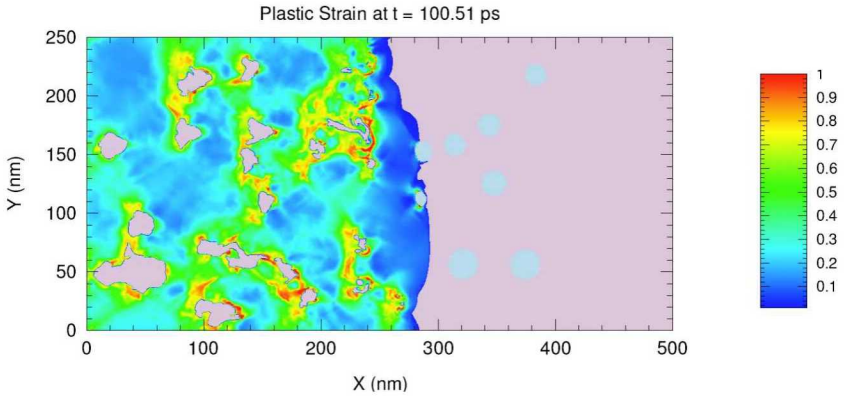
Single-pore collapse rate was used to calibrate SGL model from MD simulations

Each Simulation Provides Rich Numerical Dataset

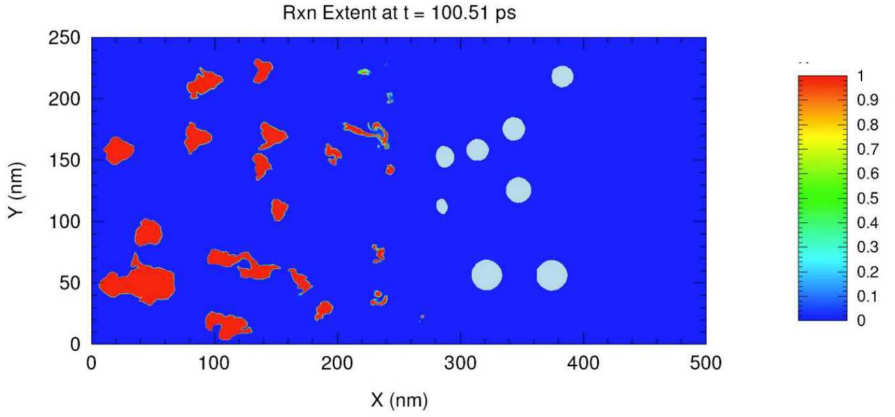
Temperature



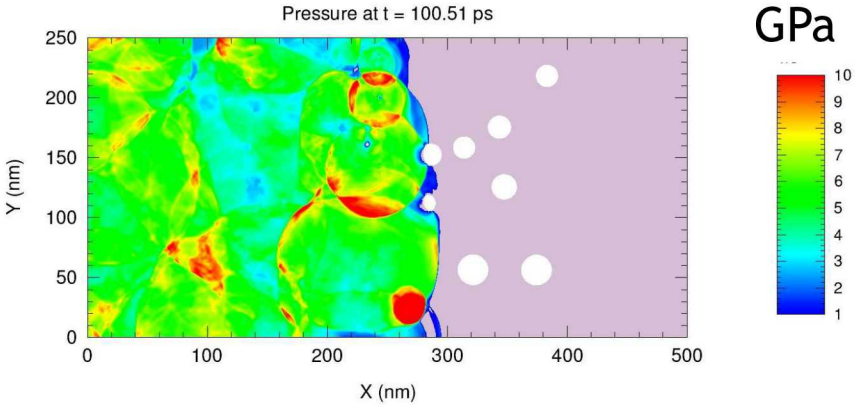
Plastic Strain



Extent of Reaction

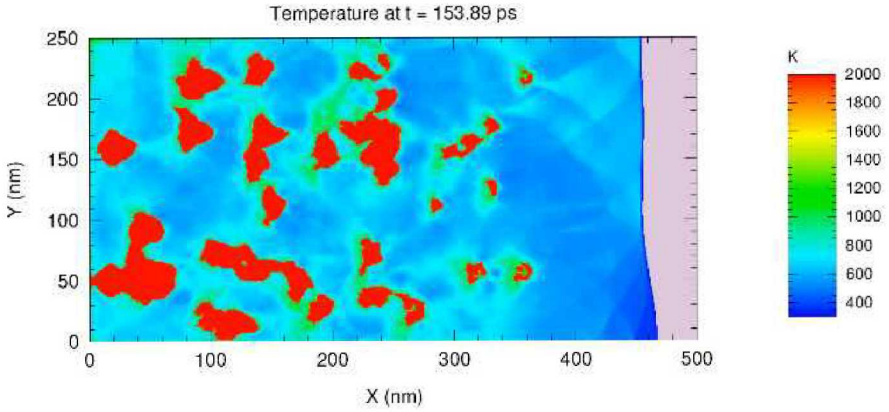


Pressure

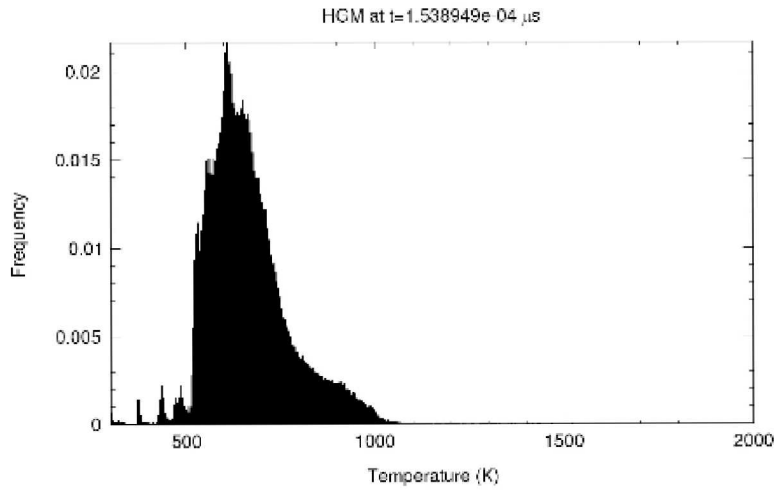


Mine Temperature Field Data for Sensitivity Indicators

- Temperature Field Data



- Histogram

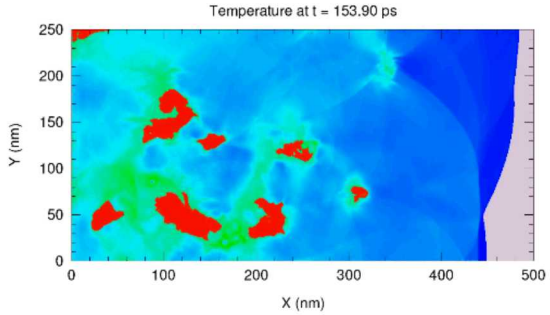


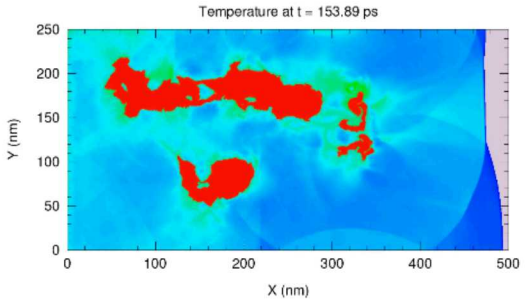
- Statistical Moments of Temperature Distribution
  - Mean
  - Variance
  - Skew
  - Kurtosis
- Area Fraction of Reacted Material

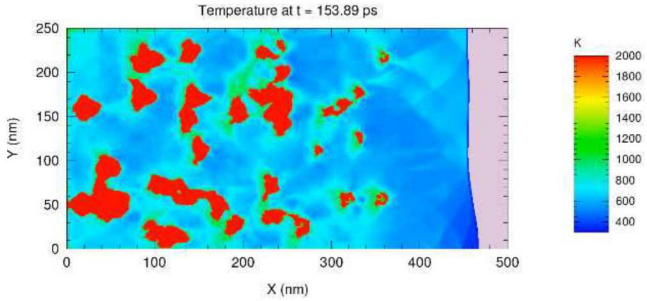
$$F_r = \frac{\Sigma area(\lambda > 0)}{totalarea}$$

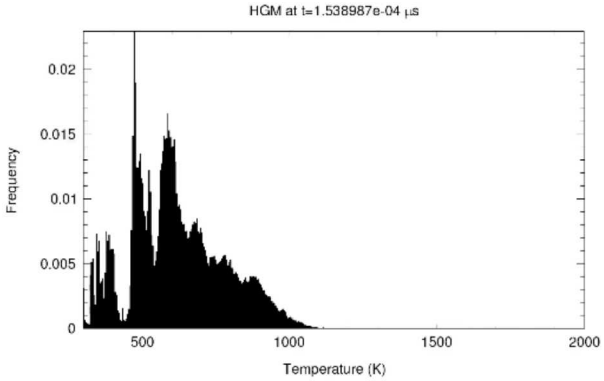
Mine Temperature Field Data for Sensitivity Indicators

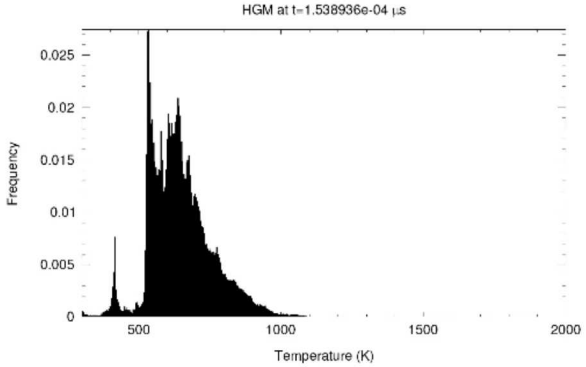
- Temperature histograms provide fingerprint for each microstructure and its hot-spot evolution---note these change over time and include both ignition and growth information

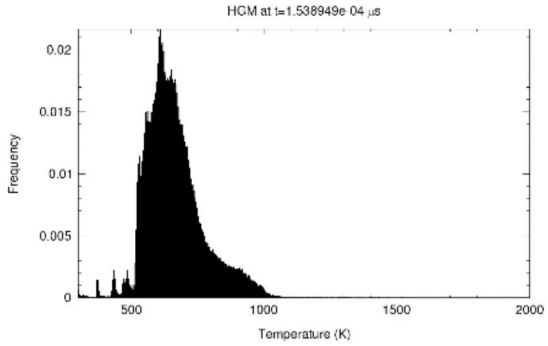








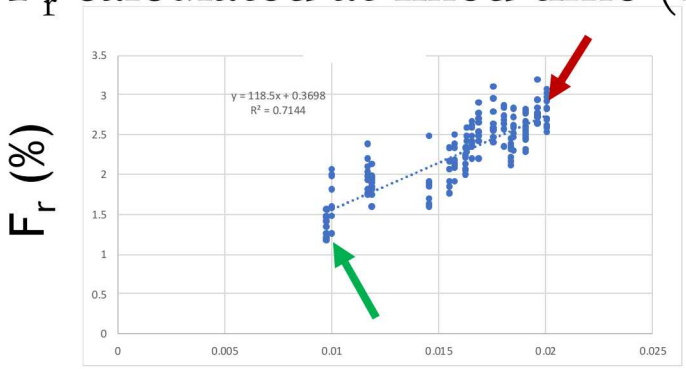




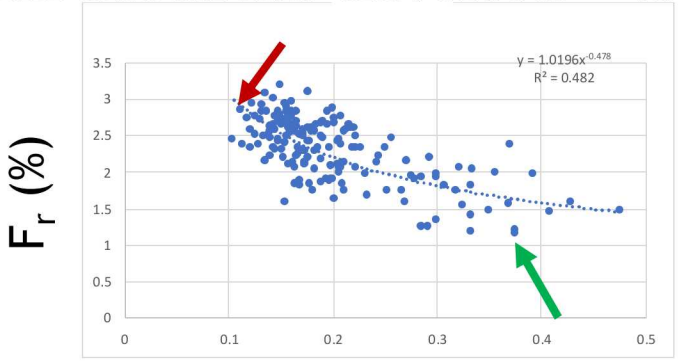
- Area fraction of reacted material, F_r provides information about reaction growth

Area Fraction of Reacted Material Across Many Different Microstructures

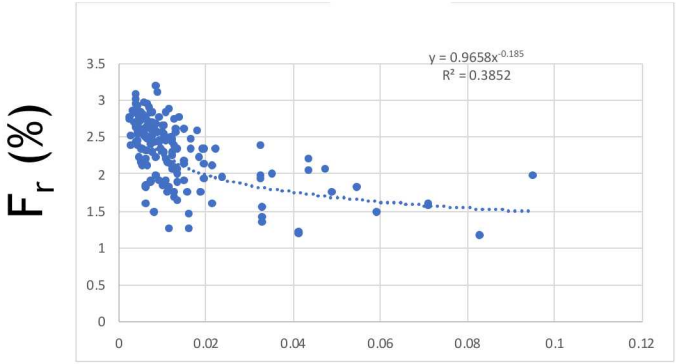
- F_r calculated at fixed time (150ps) when shock has traversed ~450 nm



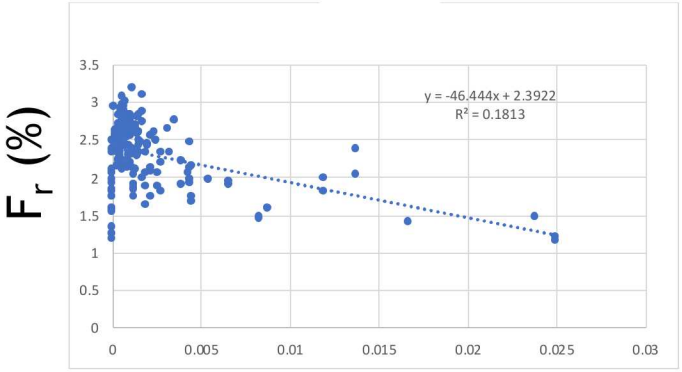
Specific Surface Area



2-Body Fraction



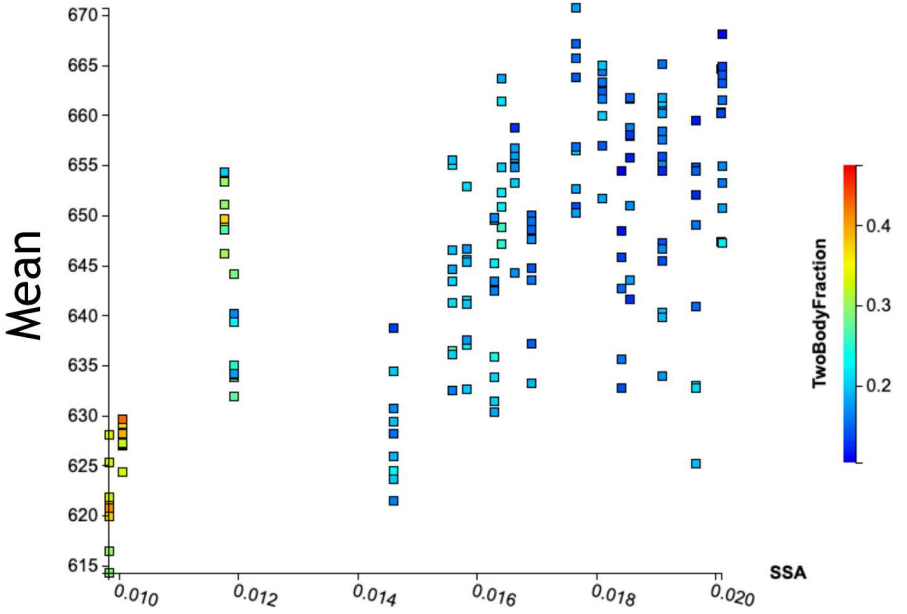
3-Body Fraction



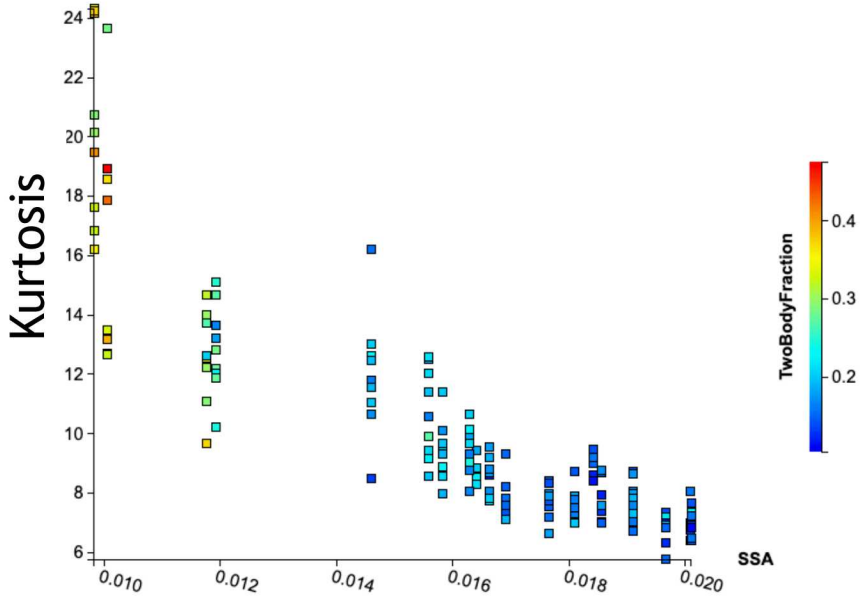
Compact 3-Body Fraction

Temperature Field Statistics Across Many Different Microstructures

- Statistics taken at fixed time (150ps) when shock has traversed ~450 nm



Specific Surface Area

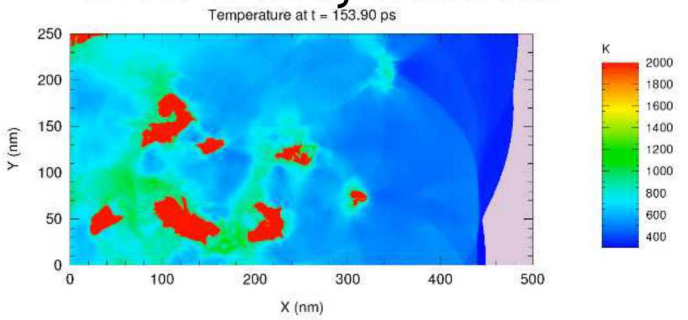


Specific Surface Area

Length Scales, Time History, and Appropriate RVE size

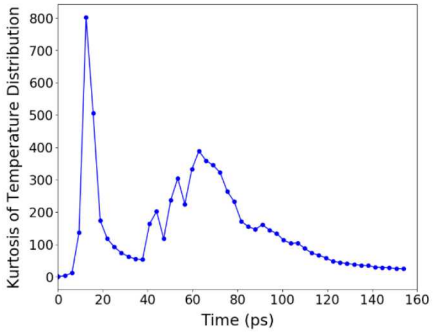
- Some run distance required to reach steady-state kurtosis in temperature distribution

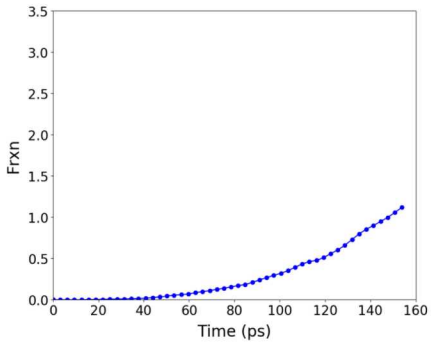
Larger pores, lower SSA, lower 2-body fractions



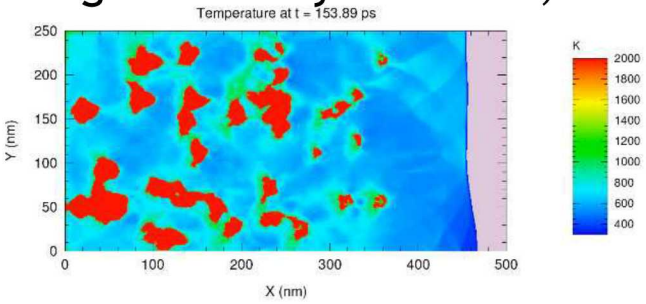
Lower initial peak

Longer time to steady state

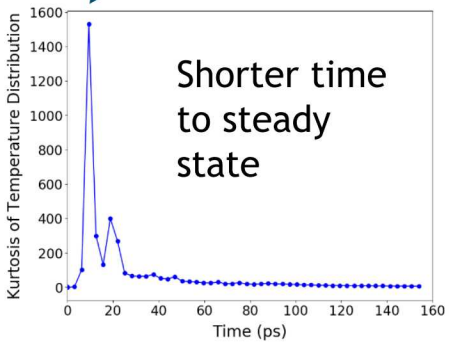




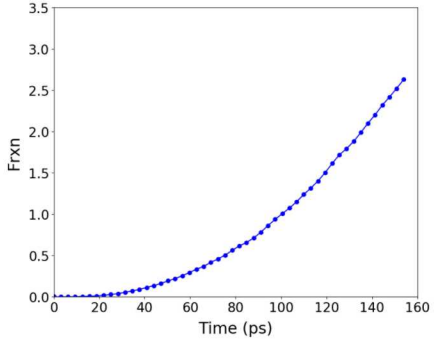
Smaller pores, lower SSA, higher 2-body fractions,



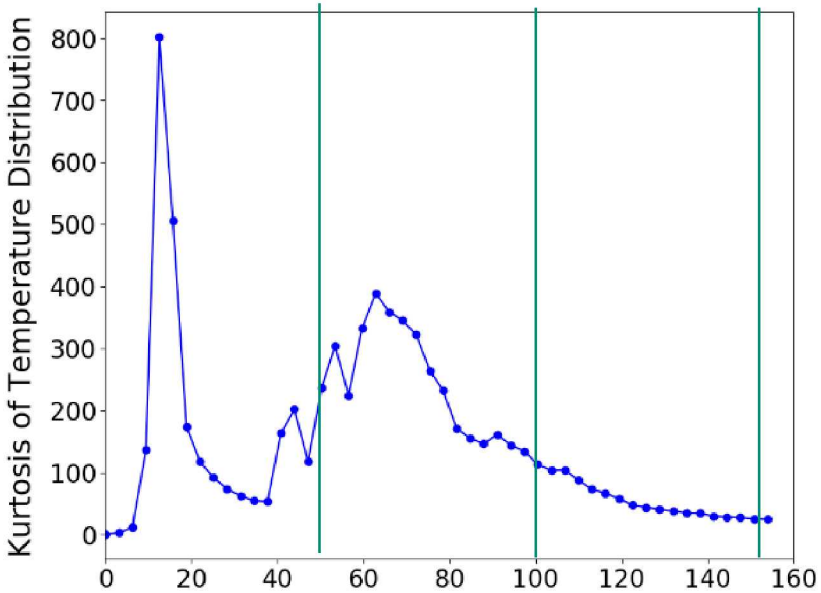
Higher initial peak

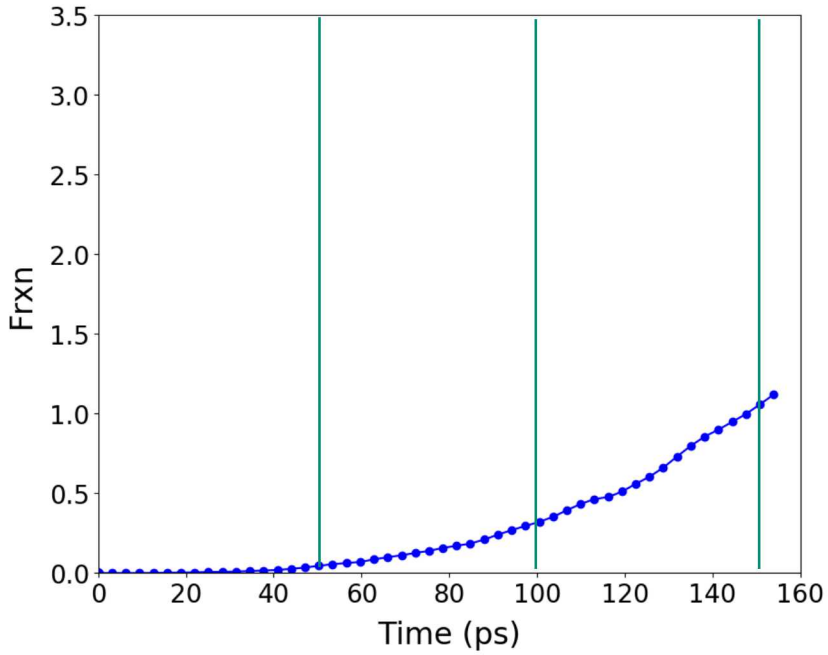


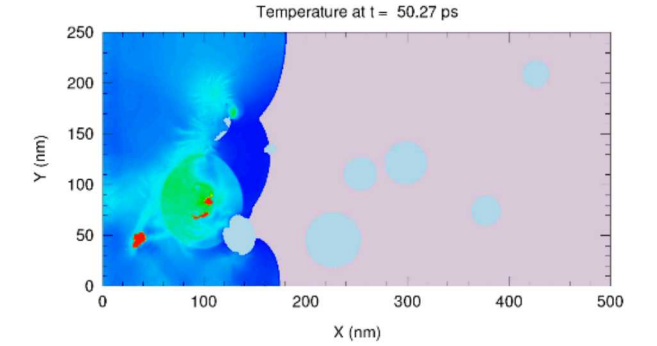
Shorter time to steady state

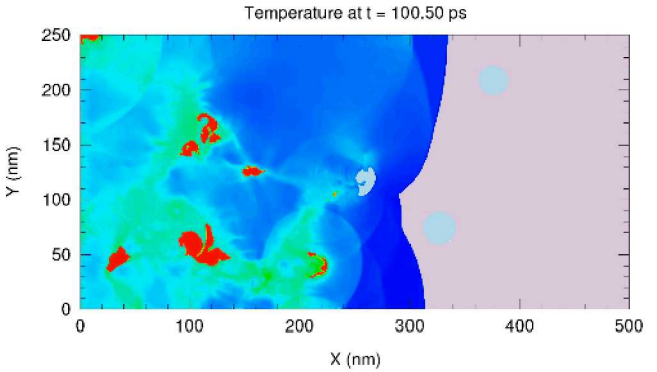


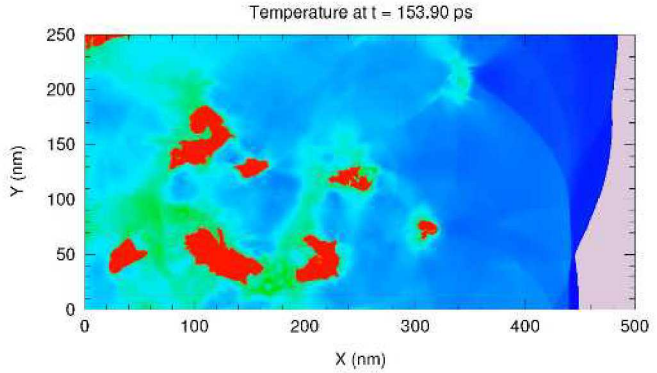
Temperature Metrics Over Time: Low SSA



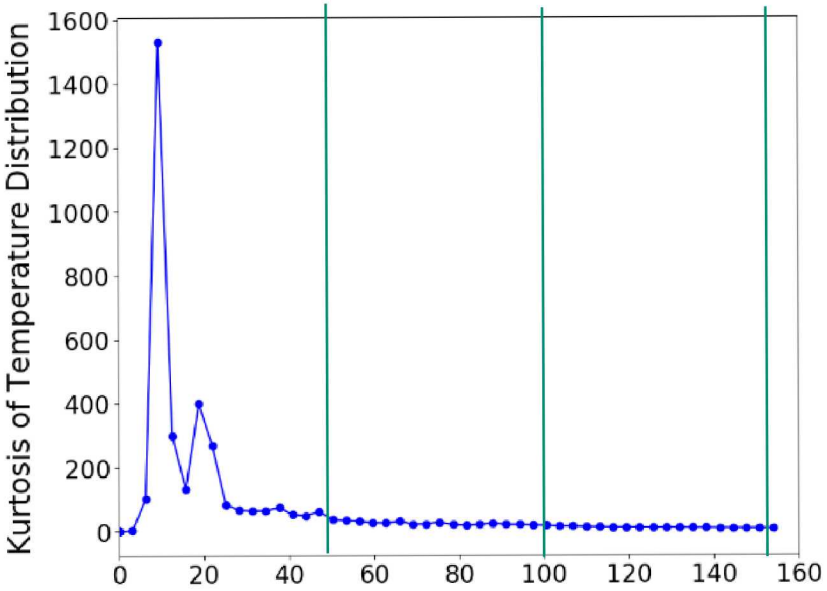


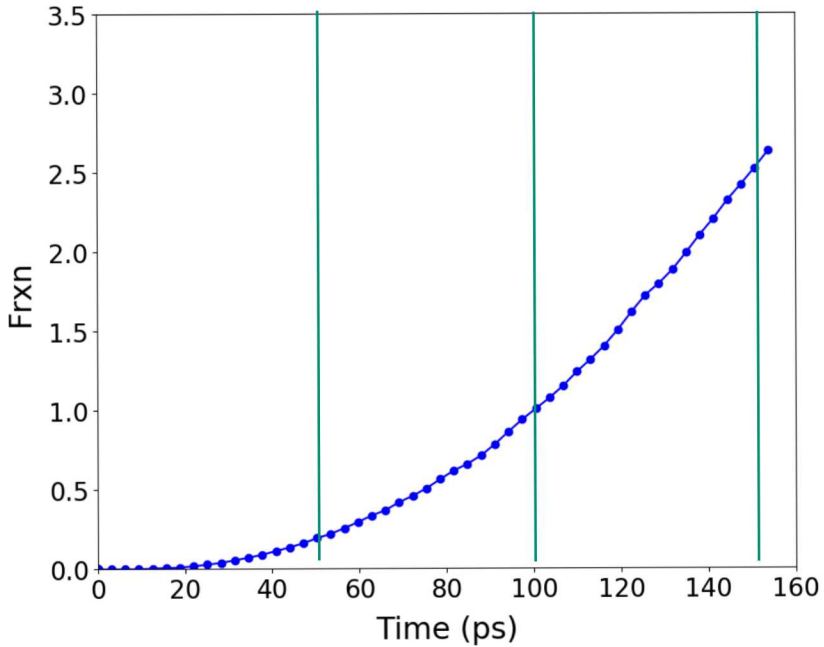


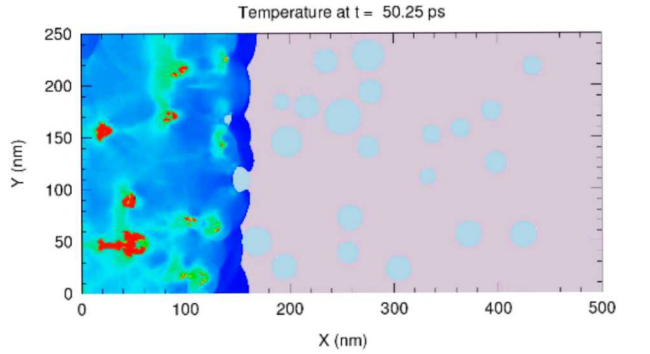


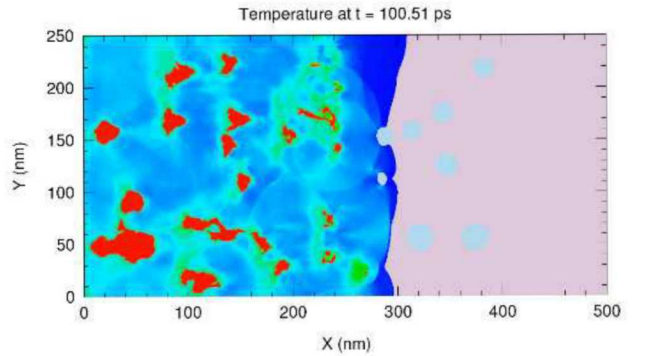


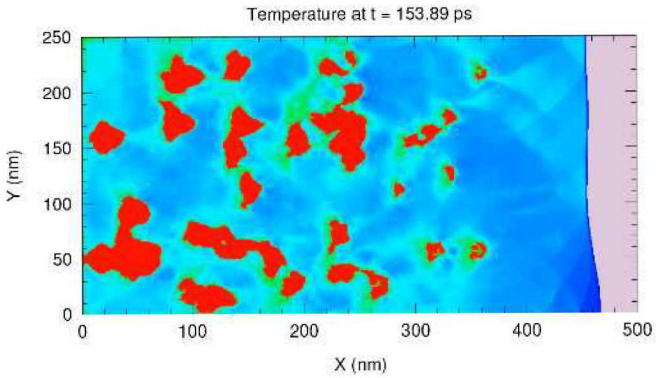
Temperature Metrics Over Time: High SSA





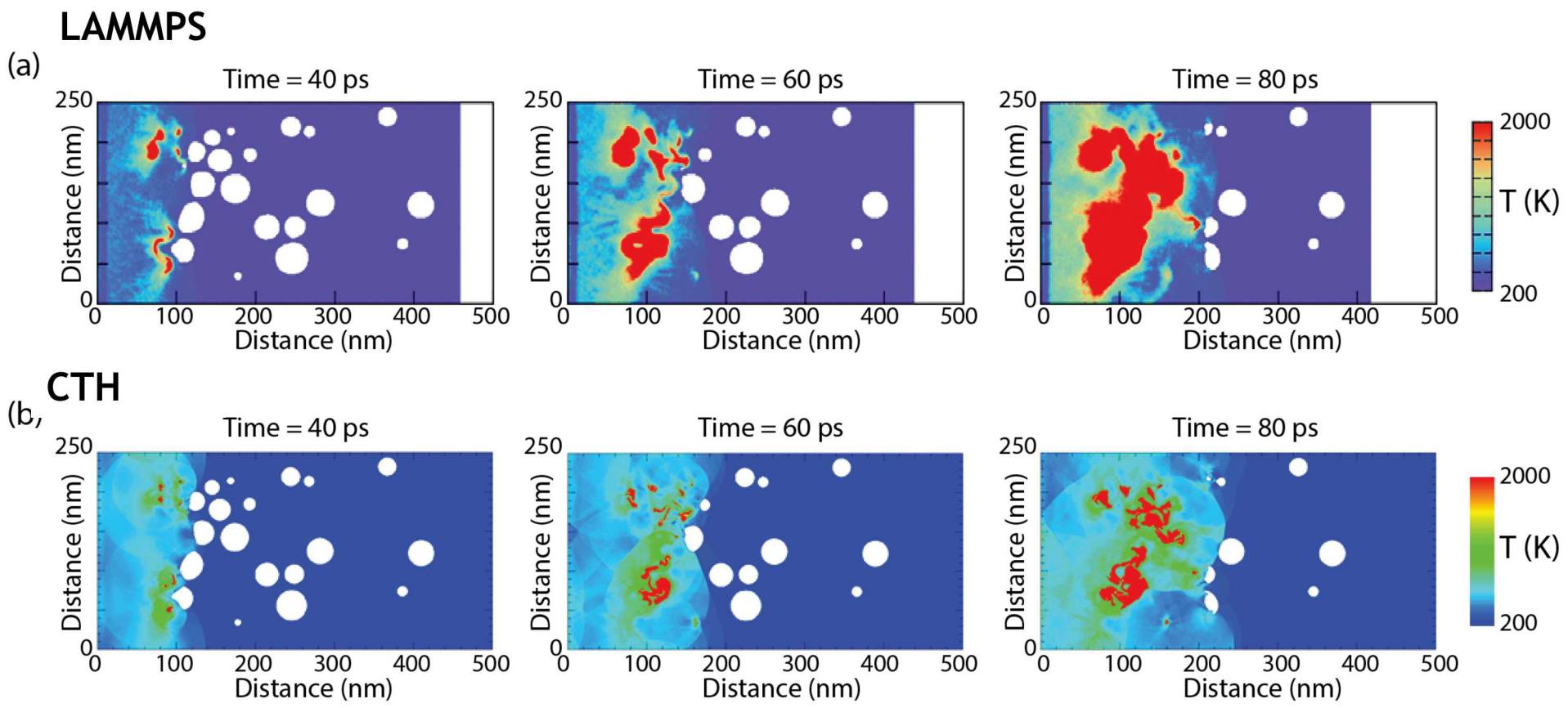






Comparison of MD vs CTH

- Good qualitative agreement in spatial temperature fields
- Shock wave front well resolved in both codes



Outlook & Perspective

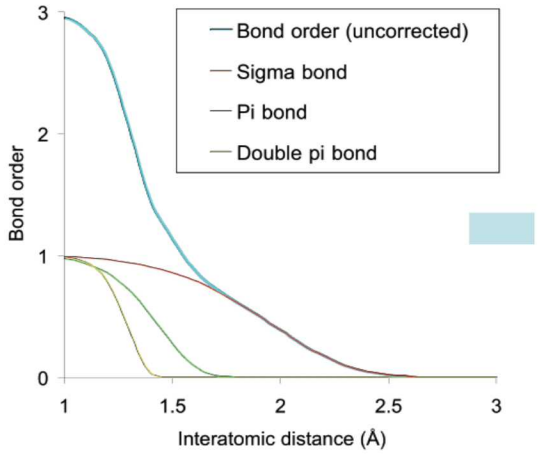
- Sensitivity metrics for hot spot formation are distinct and unique from growth metrics
  - shock propagation & chemical reactions introduce different length and time scales
- How to define RVE?
  - Physical and chemical response should define RVE
- Evolution of temperature distribution with time and shock run distance is a complex function of chemistry and microstructure features
  - Kurtosis initially peaks and evolves to steady-state value over time
  - Run distance required for steady-state kurtosis related to spatial features of porosity
  - Magnitude of initial kurtosis peak provides indicator for number of reaction sites
- specific surface area and 2-body fraction are leading geometric indicators of sensitivity

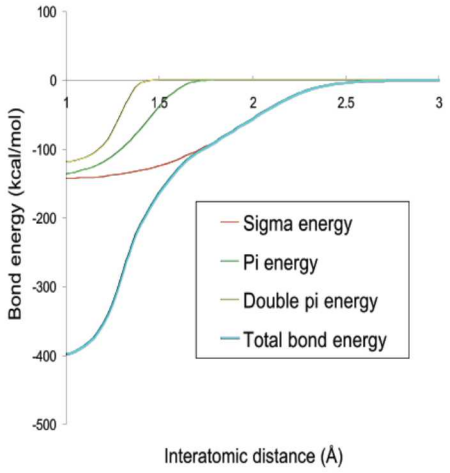
Thank You!

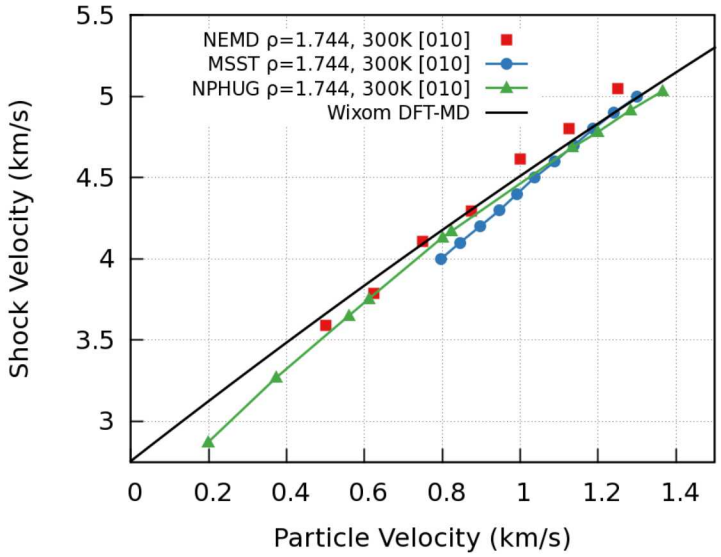
Molecular Dynamics Simulations

- Use MD simulation to gain more physical insight into highly clustered microstructure configurations

ReaxFF Interatomic Potential → Detailed chemistry is incorporated in these MD potentials, hot spot evolution is captured naturally





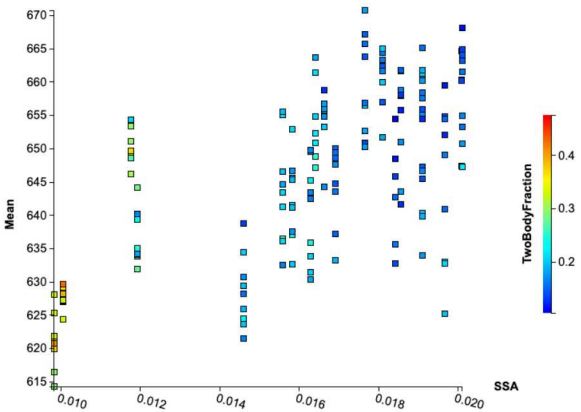


Chenoweth, van Duin and Goddard, J. Phys. Chem. A, 112, 1040-1053 (2008)
Strachan *et al.* J. Chem. Phys. 122, 054502 (2005)
Castro-Marcano *et al.* Combustion and Flame 159(3) 1272-1285 (2012)
Wood, van Duin, Strachan , J. Chem .Phys. A 118, 885 (2014)
Rappe and Goddard, J. Phys. Chem 1991, 95, 3358-3363

Temperature Field Statistics Across Many Different Microstructures

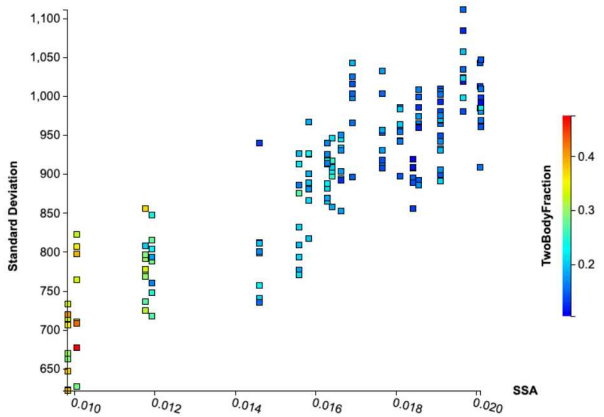
- Statistics taken at fixed time (150ps) when shock has traversed ~450 nm

Mean



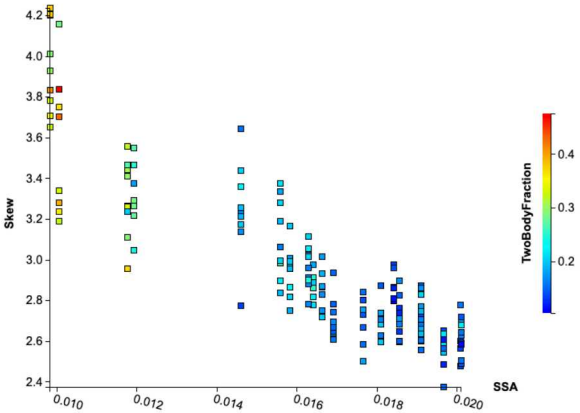
Specific Surface Area

Standard Deviation



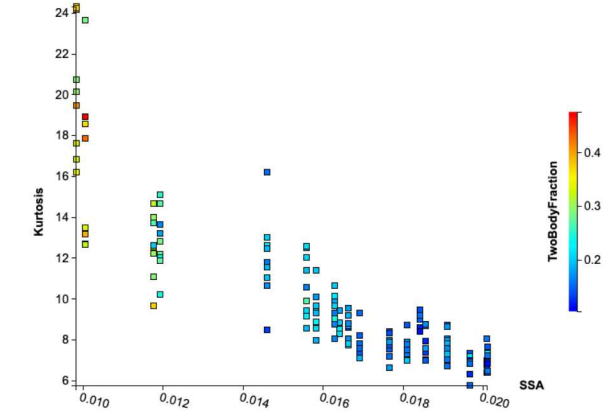
Specific Surface Area

Skew



Specific Surface Area

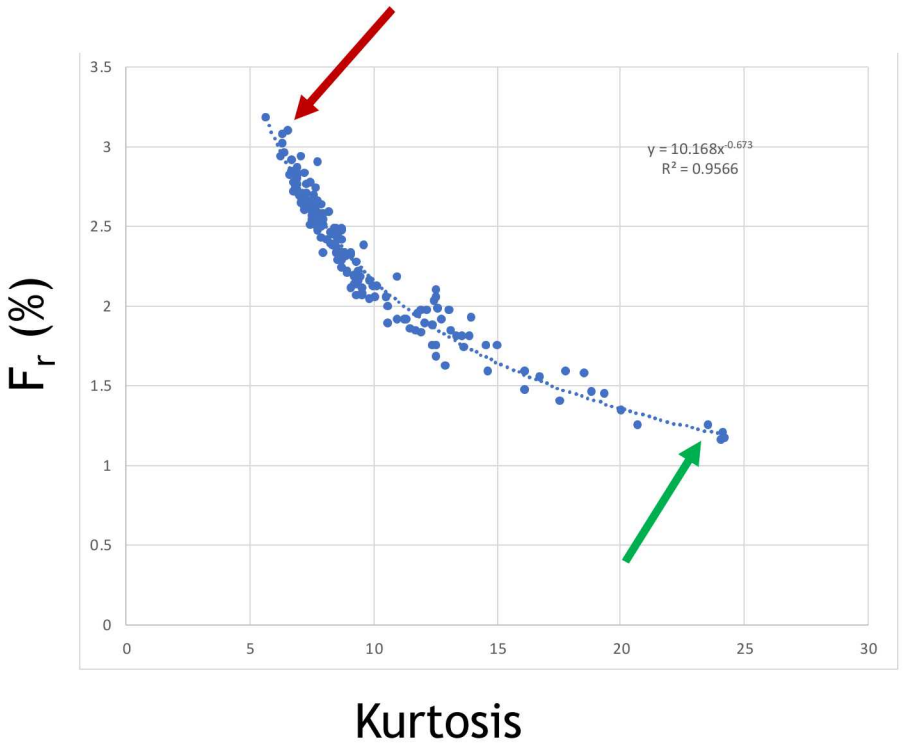
Kurtosis

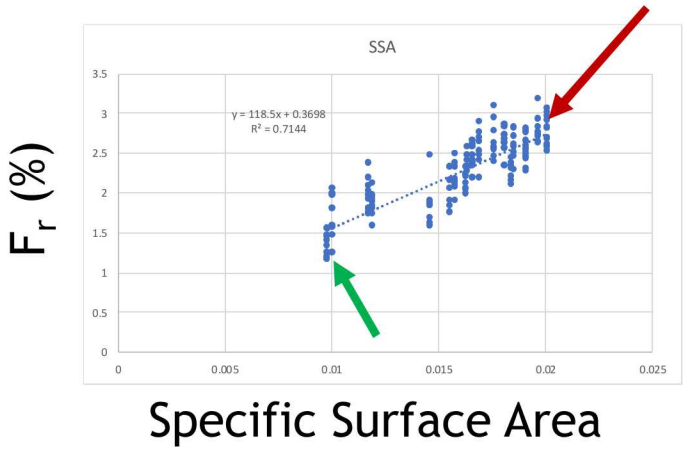


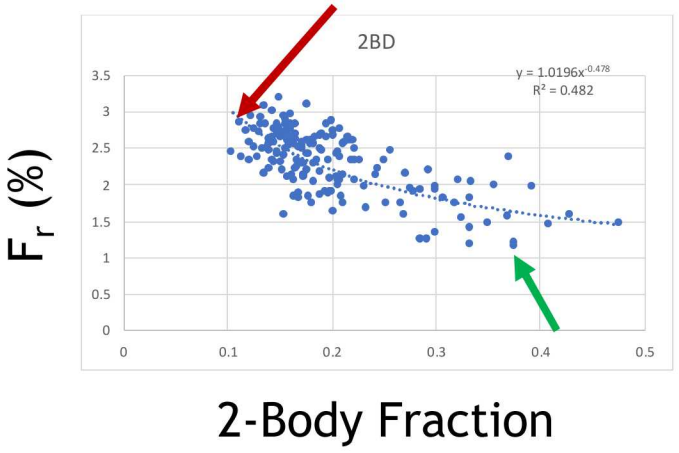
Specific Surface Area

Area Fraction of Reacted Material Across Many Different Microstructures

- Is kurtosis of temperature distribution a good indicator for sensitivity to reaction?

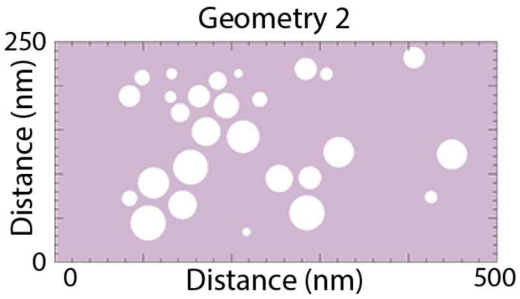




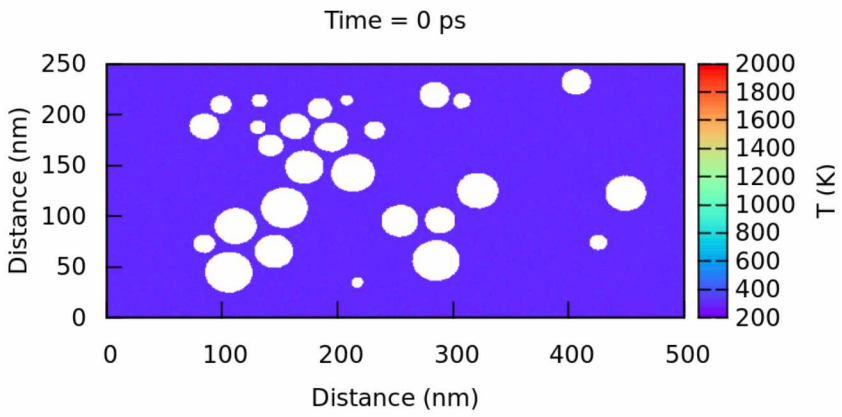


MD Simulation of Clustered Porosity

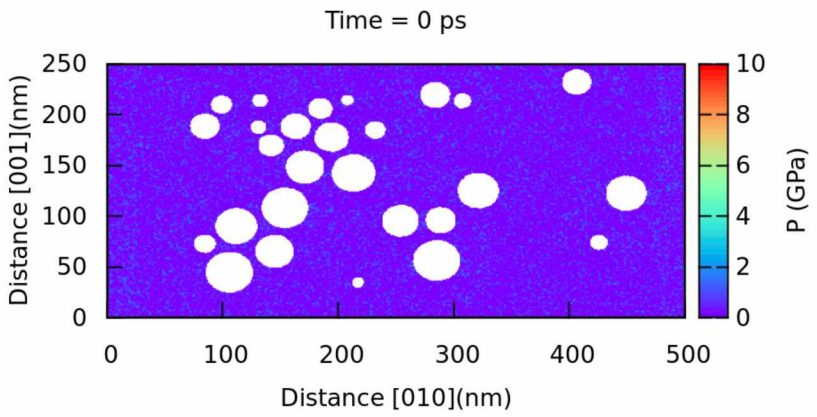
- Geometry 2:
  - Large pore cluster between 100-200 nm
  - Temperature distribution with high skew and kurtosis



Temperature (K)



Pressure (GPa)



CTH Conservation Equations

- Real material behavior comes from an **accurate equation-of-state (EOS)** plus a **constitutive model** with parameters fit to the appropriate, dynamic regime.
  - spherical part is the equation of state $P = f(\rho, E)$
  - deviatoric part is the constitutive model $\boldsymbol{\sigma} = f(\text{strain}, \ldots)$
  - numerical part is the artificial viscous stress $\boldsymbol{Q} = f(\text{velocity and } c_s)$

Mass $$\frac{d\rho}{dt} = -\rho \nabla \bullet \vec{V}$$

Momentum $$\rho \frac{d\vec{V}}{dt} = -\nabla P - \nabla \bullet \left[\boldsymbol{\sigma} + \mathbf{Q}\left(\vec{V}, c_s\right)\right]$$

Energy $$\rho \frac{dE}{dt} = -P \nabla \bullet \vec{V} - \left[\boldsymbol{\sigma} + \mathbf{Q}\left(\vec{V}, c_s\right)\right] \bullet \nabla \vec{V}$$

$$-\boldsymbol{S} = P\boldsymbol{I} + \boldsymbol{\sigma} + \boldsymbol{Q}\left(\vec{V}, c_s\right)$$

Stress Tensor | Spherical Part | Deviatoric Part | Artificial Viscosity

Continuum Hydrocode Simulations—CTH

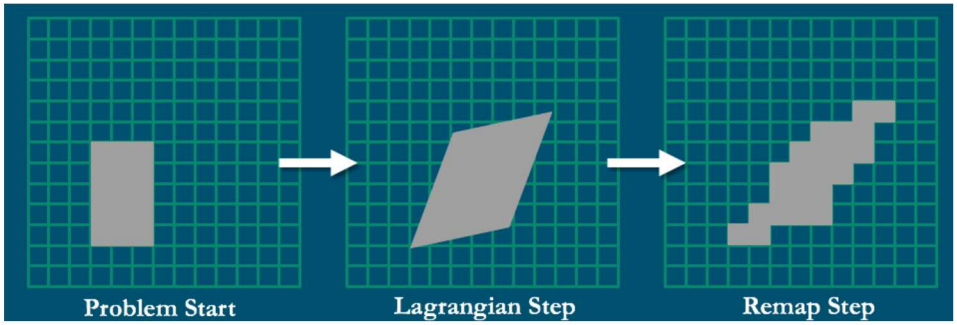
- CTH—3D, large deformation, multi-material shock physics hydrocode developed at Sandia National Laboratories

Mass
$$\frac{d\rho}{dt} = -\rho \nabla \bullet \vec{V}$$

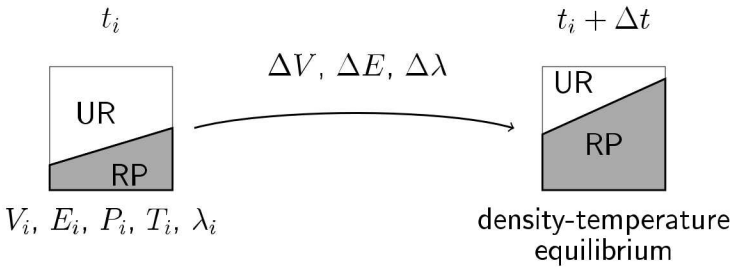
Momentum
$$\rho \frac{d\vec{V}}{dt} = -\nabla P - \nabla \bullet \left[\boldsymbol{\sigma} + \mathbf{Q}\left(\vec{V}, c_s\right)\right]$$

Energy
$$\rho \frac{dE}{dt} = -P \nabla \bullet \vec{V} - \left[\boldsymbol{\sigma} + \mathbf{Q}\left(\vec{V}, c_s\right)\right] \bullet \nabla \vec{V}$$

Lagrangian and remap solution steps as they appear in CTH

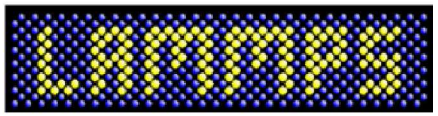


Density-temperature equilibrium for reactive burn models

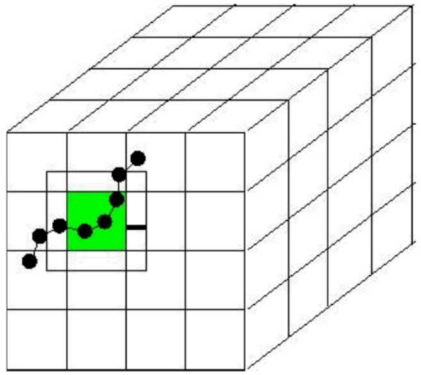


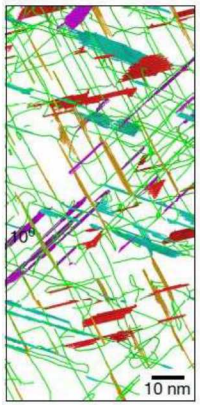
McGlaun, J. M., Thompson, S. L., and Elrick, M. G., *Int. J. Impact Engng.*, 10 (1990) 351-360.

What is LAMMPS?



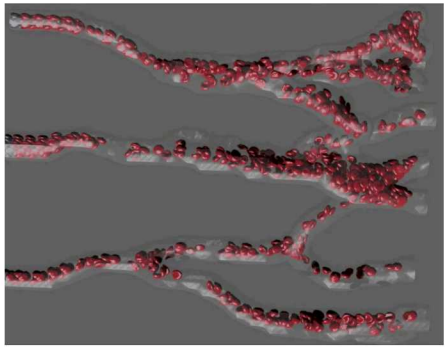
- Large-scale Atomic/Molecular Massively Parallel Simulator
  http://lammps.sandia.gov
- Open source, highly portable C++, free under GPL license
- Well documented with many examples, easily extendable for user specific needs
- Variety of boundary conditions, constraints, ensemble sampling methods etc.
- Parallelism through spatial decomposition of simulation domain
- Short and long ranged interactions allowed/included
- CPU cost is (N/P) and communication is $(N/P)^{2/3}$



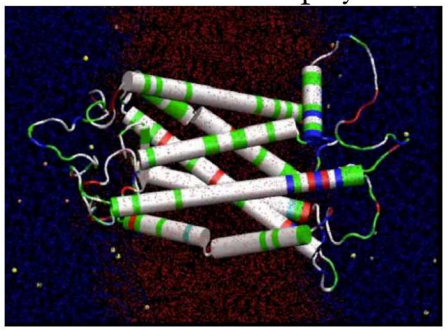


Dislocations in Materials

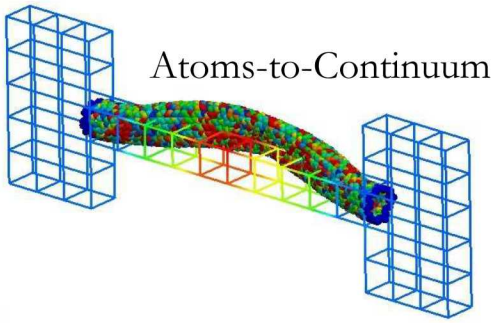
Blood Flow



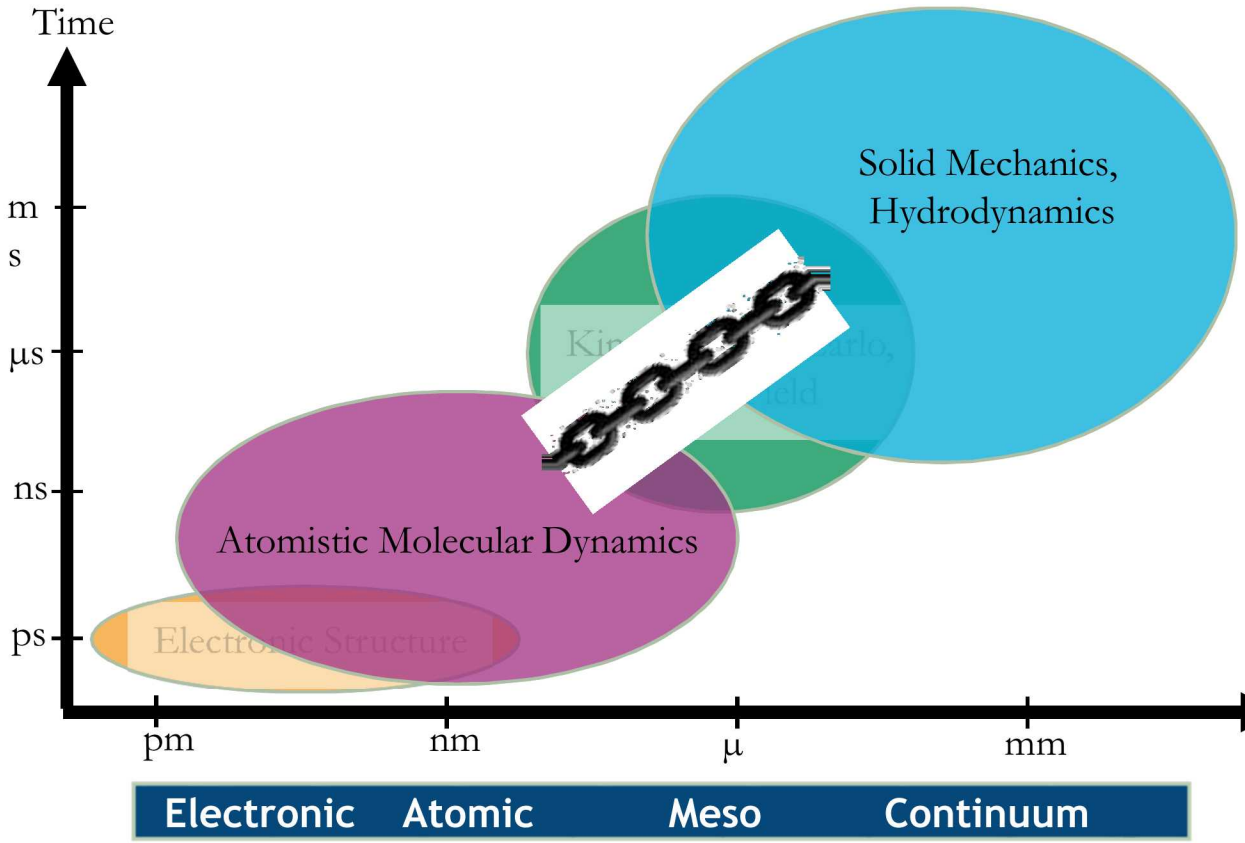
Proteins and Biophysics



Atoms-to-Continuum

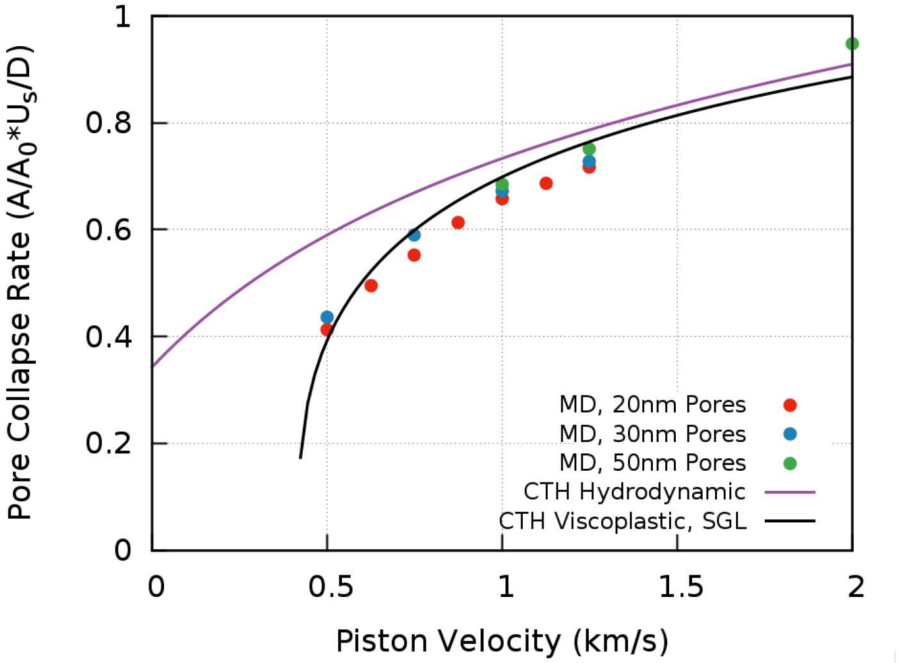


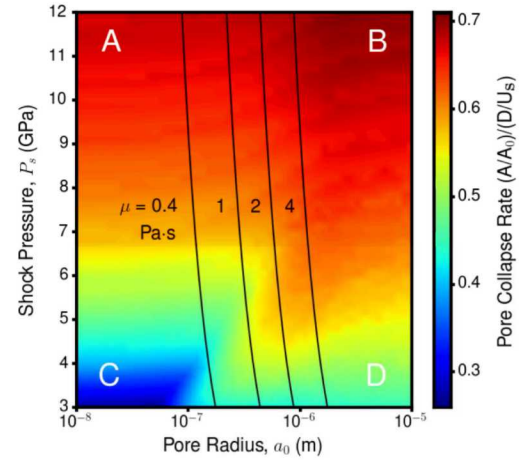
Useful, Co-dependent Models

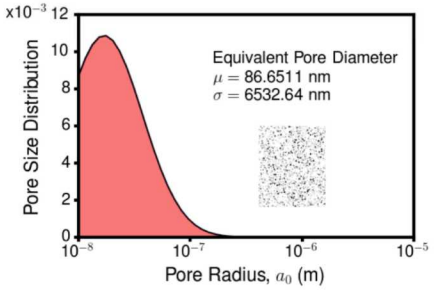


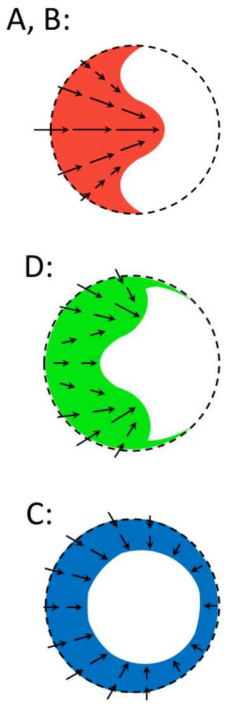
- Predictions at the mesoscale now share approximations of either model
- Sacrificed some ability to extrapolate, but have built a sandbox reality where much can be learned
- Actively looking for experimental integration as validation

SGL Strength Model Calibrated from MD







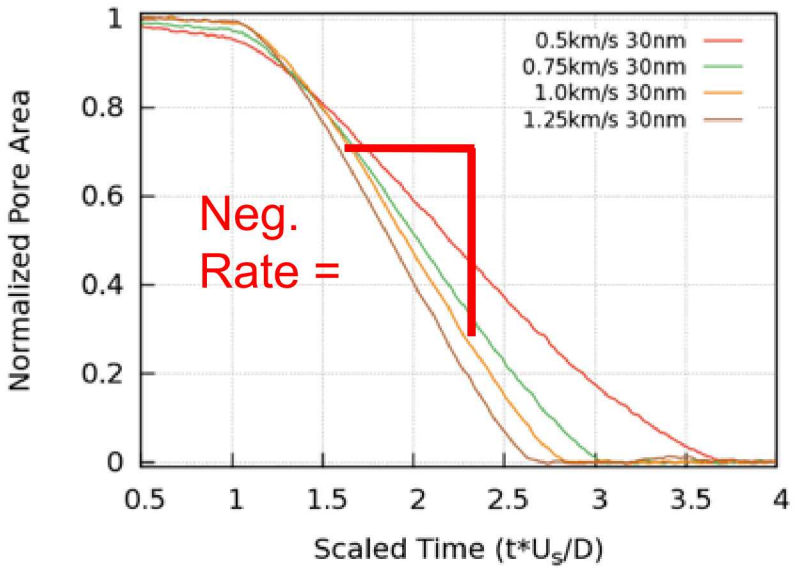


- Training data of collapsing pores from MD sent to CTH for strength model parameterization

Metrics Passed from MD to CTH

Training Metric

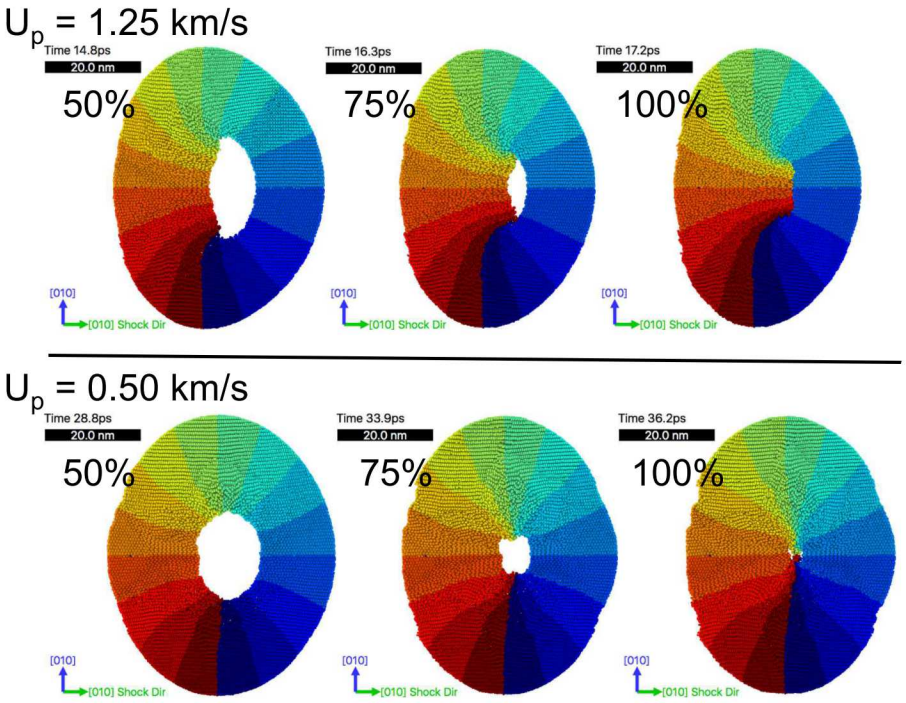
- Collapse rate is used to calibrate strength models in CTH



Quantitative post-processing was done using the OVITO code [10]

Comparison Metrics

- Radial distribution of plastic strain
- Temperature histograms
- Etc.



CTH Strain Rate Dependent Model – Steinberg, Guinan and Lund (1988)

- We believe that only a strain rate-dependent model can match MD results for viscoplastic pore collapse; EPPVM and Johnson-Cook are not up to the task.
  - Assume a constant shear modulus
  - Neglect work hardening
  - Assume linear variation of the Grüneisen parameter

Yield Strength:	$Y = \{Y_T(\dot{\varepsilon}_p, T) + Y_A f(\varepsilon_p)\}$	
Shear Modulus:	$G(P,T) = G_0$	
Thermal Activation: (Implicit Equation)	$\dot{\varepsilon}_p = \left\{\frac{1}{C_1} exp\left[\frac{2U_K}{kT}\left(1-\frac{Y_T}{Y_P}\right)^2\right] + \frac{C_2}{Y_T}\right\}^{-1}$	$Y_T \leq Y_P$
Melting Curve: ($Y = 0$ when $T \geq T_m$)	$T_m = T_{m0} exp\{2a(1-1/\eta)\}\eta^{2(\gamma_0 - a - 1/3)}$	
Grüneisen parameter:	$\gamma = \gamma_0/(1+\mu)$	