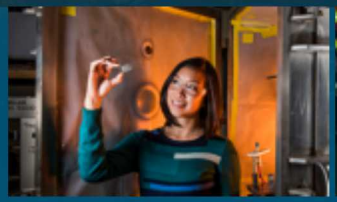
SAND2019-5736C

Sandia National Laboratories

Multiscale modeling to determine the effect of porosity distribution on shocked hexanitrostilbene



Europyro/44th International Pyrotechnics Society Seminar

Tours, France

June 3-7, 2019

PRESENTED BY

Judith Brown, David Kittell, Mitchell Wood, Aidan Thompson, Dan Bolintineanu

June 5, 2019

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.

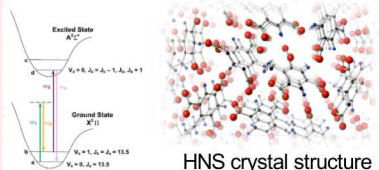
Presentation Outline

- Introduction
- Synthetic Microstructure Generation
- Continuum Hydrocode Simulations (CTH)
  - Temperature distribution statistics for many microstructures
- Molecular Dynamics Simulations (LAMMPS)
  - High-fidelity study of particular microstructures
- Conclusions & Future Work

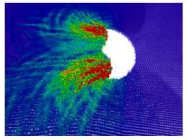
Shock Initiation of Explosives at Sandia

❖Generate a high fidelity baseline

Quantum / MD Large Scalable Codes

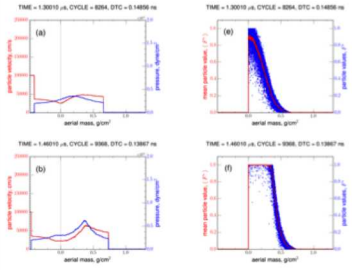


HNS crystal structure



LAMMPS + Kokkos

New Continuum Codes



Stochastic reactive shock waves

Formation Modeling

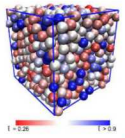
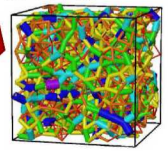


Image stack, or simulated μstructure

-poured
-pressed
-deposited
-AM of EM



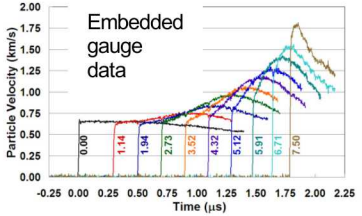
Graph of contact network

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

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

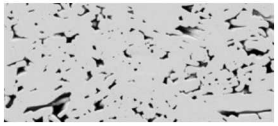
Tests and Experiments

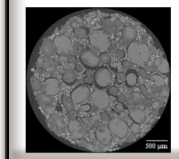
- Performance
- Sensitivity
- Threshold and UQ



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

Microstructural Analysis

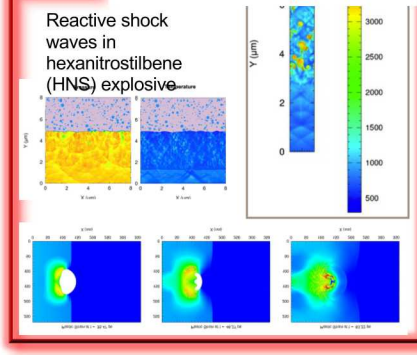




X-section of HNS pellet (top) and CT scan courtesy of Andres Chavez (left)

Mesoscale Simulations

Reactive shock waves in hexanitrostilbene (HNS) explosive

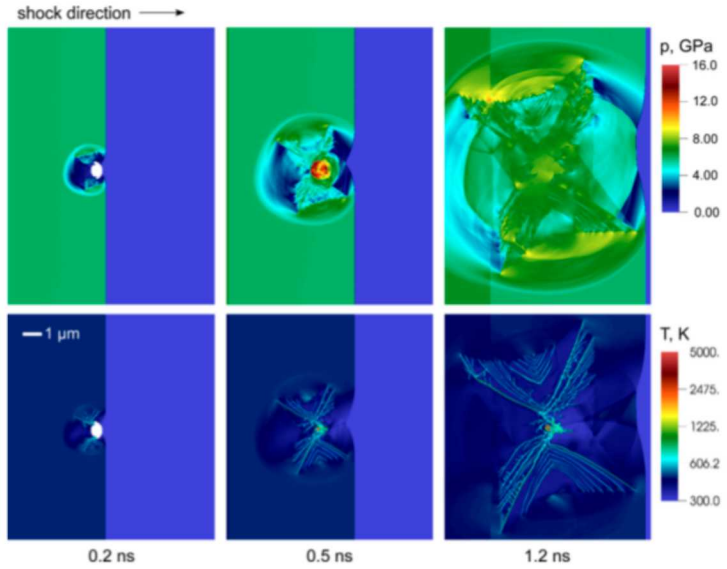


Adapt/remove approximations to agree with MD

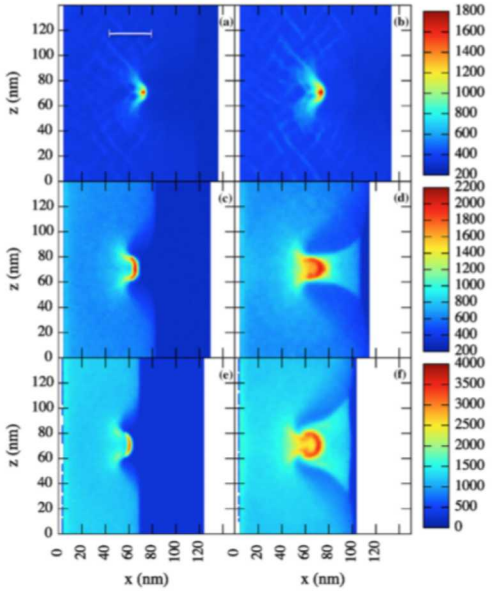
Role of Porosity in Shock Initiation

- 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



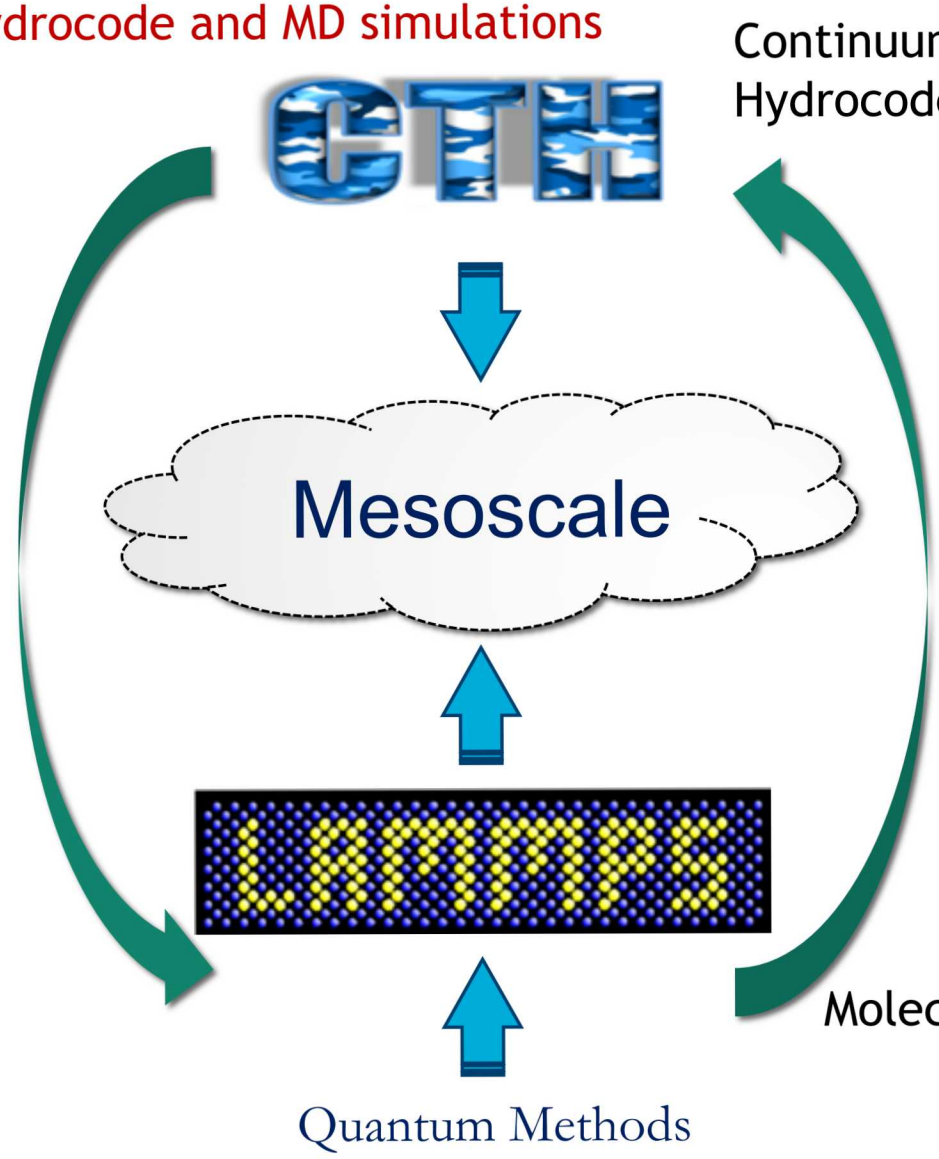
Eason and Sewell, J. Dynamic Behavior Mater. 1 (2015), 423-438

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:

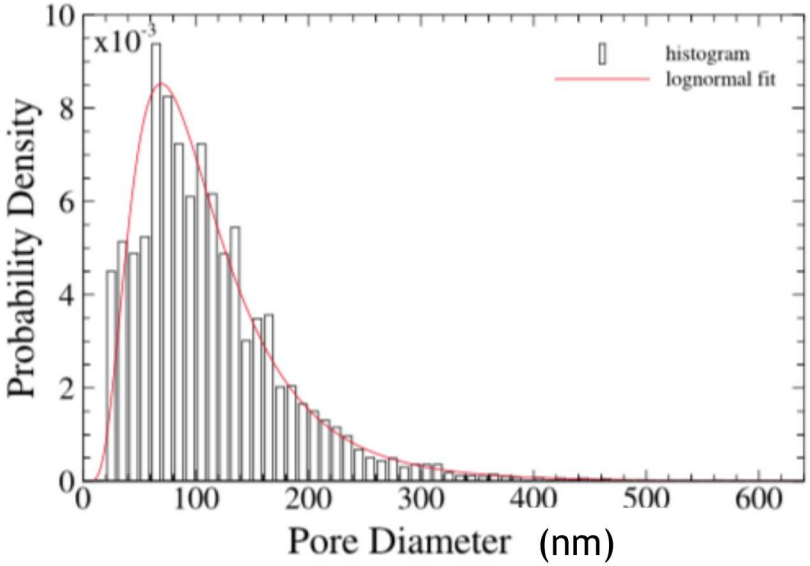
- 'Critical' local microstructure features
- Evaluate measures of sensitivity
- Integration with new experimental diagnostics

Atomistic Properties Propagated Up:

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

Microstructure of Pressed Hexanitrostilbene

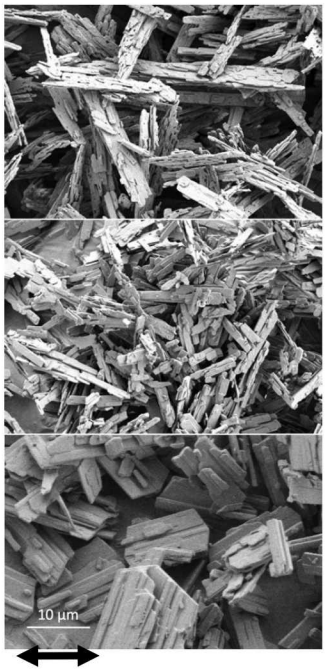
- HNS-IV powder pressed to 72 – 92% TMD



HNS-IV Lot 1

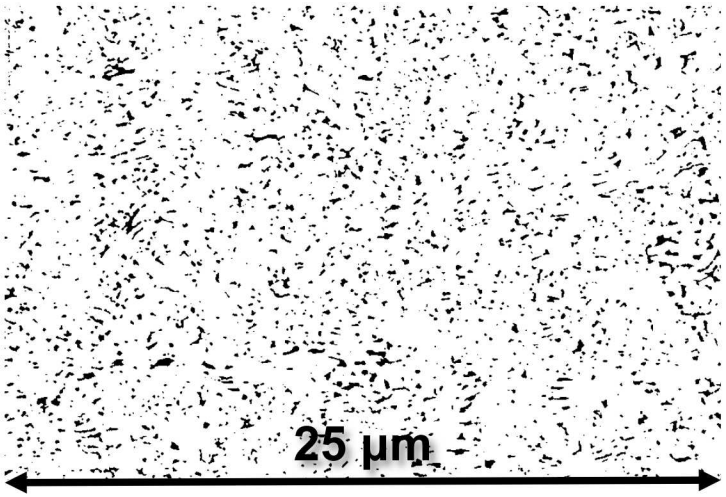
HNS-IV Lot 2

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

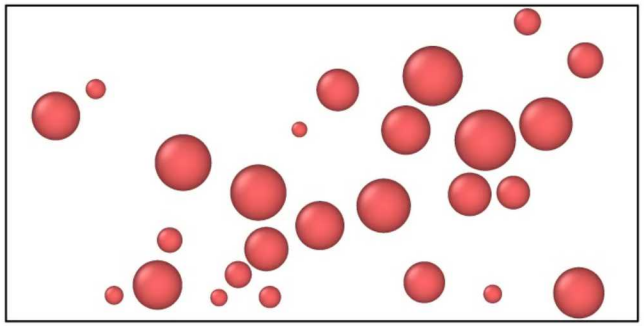
Synthetic Microstructure Generation

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

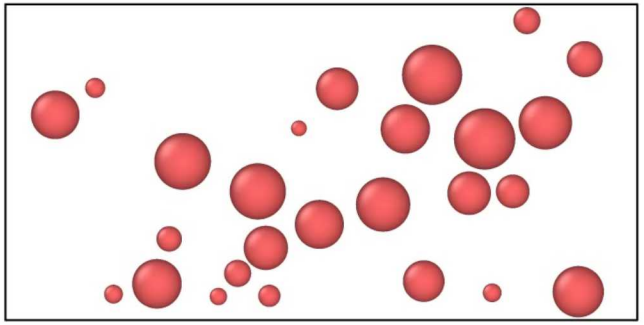
Initial state: spheres placed at random in 250 X 500 nm domain, no overlaps

Langevin dynamics with range of contact cohesion values:

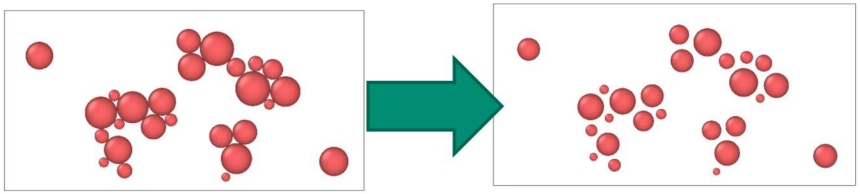
Low cohesion



High cohesion

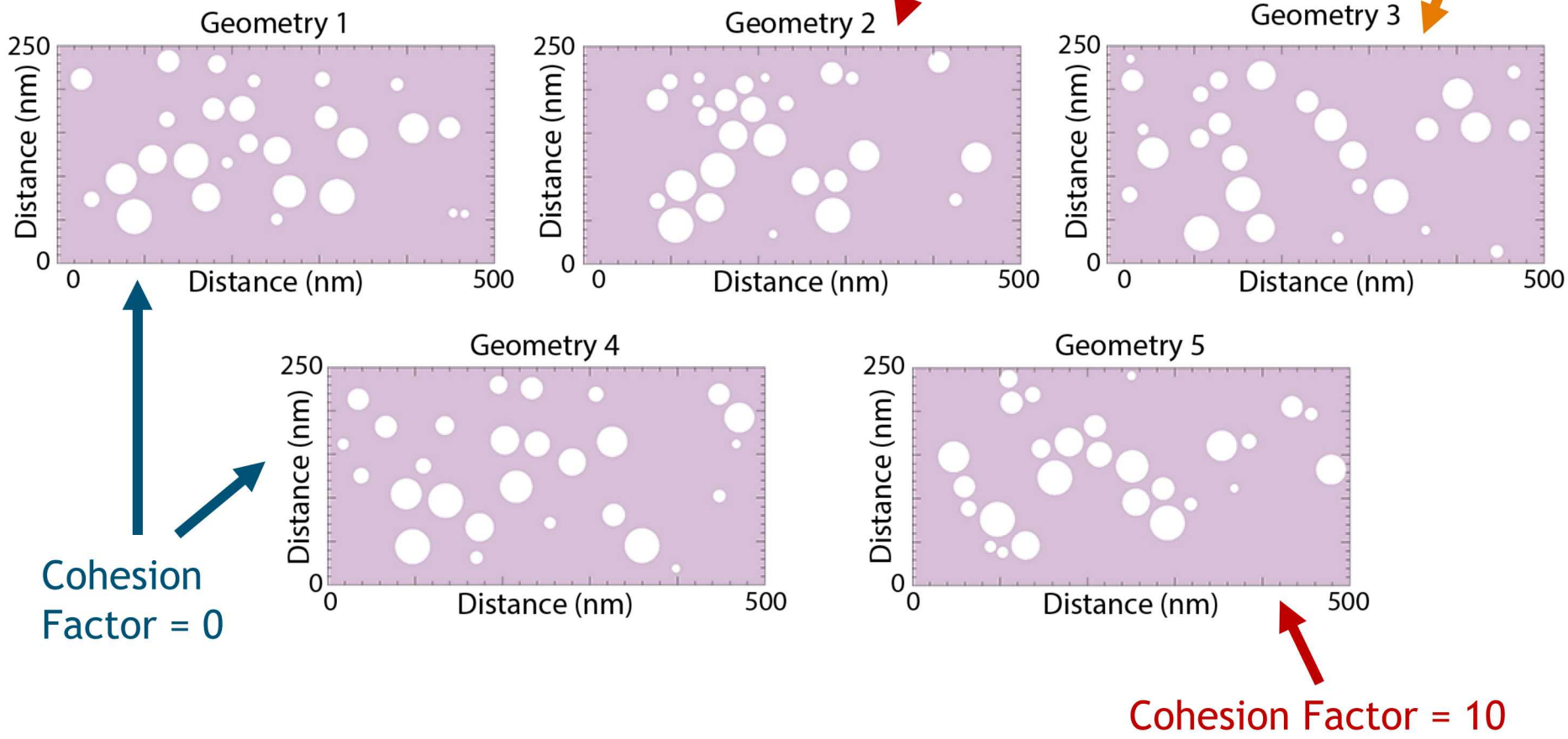


Final step: shrink particles uniformly to generate final configuration



Variations: Particle size distribution, TMD, cohesion, friction, random seed

Example Synthetic Microstructures



Continuum Hydrocode Simulations—CTH

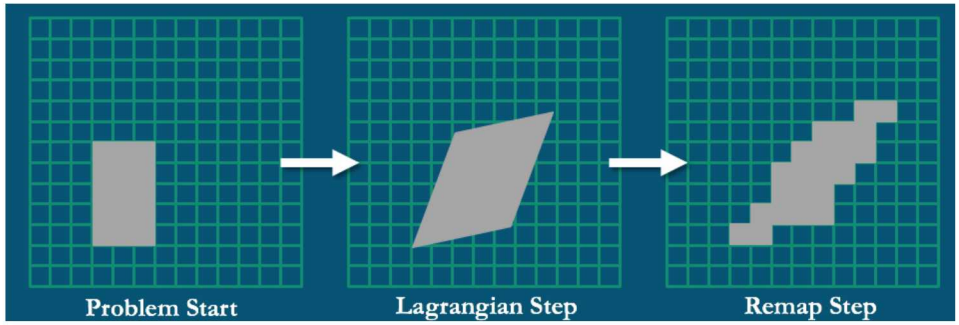
- CTH—3D, large deformation, multi-material shock physics hydrocode developed at Sandia National Laboratories

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

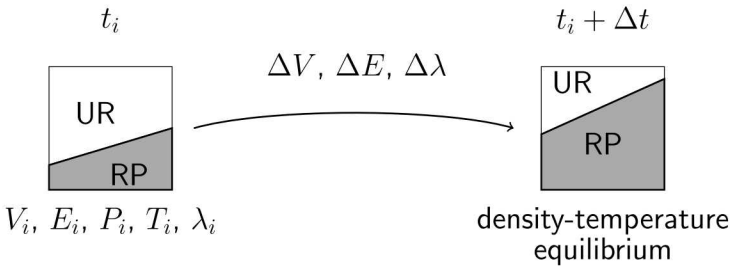
Momentum $$\rho \frac{d\vec{V}}{dt} = -\nabla P - \nabla \bullet \left[\boldsymbol{\sigma} + \mathbf{Q}\left(\vec{V}, c_s\right)\right]$$

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

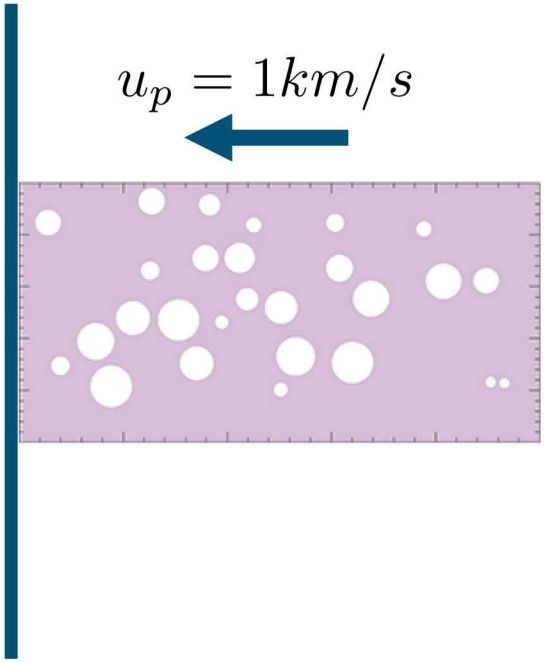


McGlaun, J. M., Thompson, S. L., and Elrick, M. G., *Int. J. Impact Engng.*, 10 (1990) 351-360.

Continuum Hydrocode Simulations—CTH

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

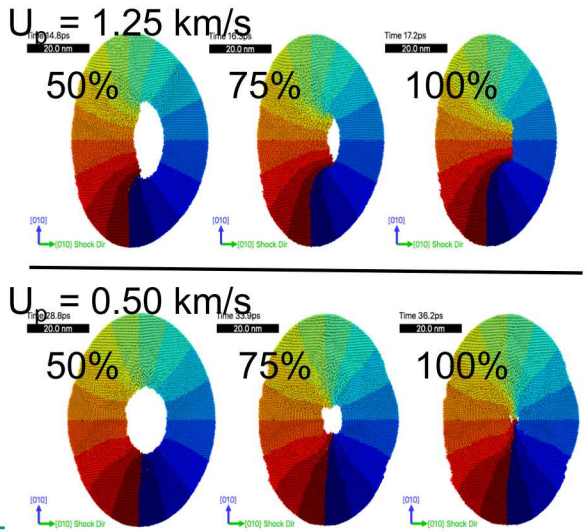
Symmetric impact



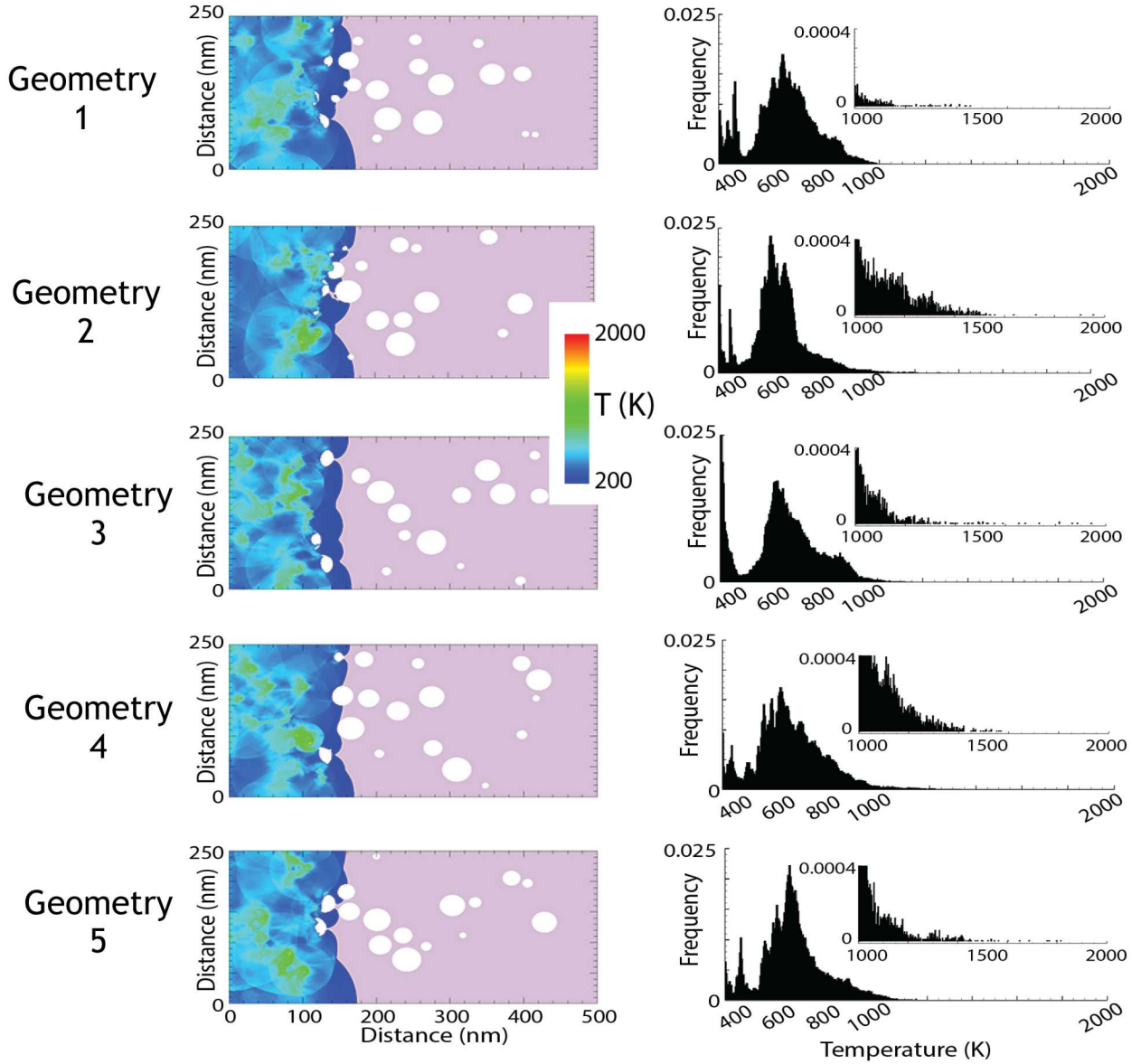
Material Models

- Pores treated as void
- HNS matrix:
  - Mie-Grüneisen equation of state
  - Stienberg-Guinan-Lund viscoplastic strength model

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



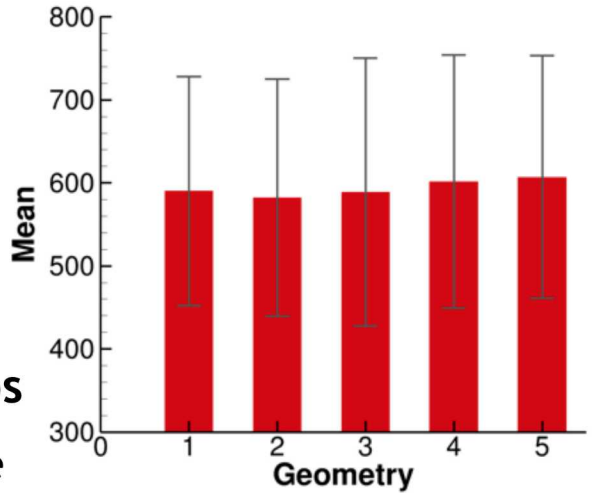
Temperature Distributions for Unique Microstructures

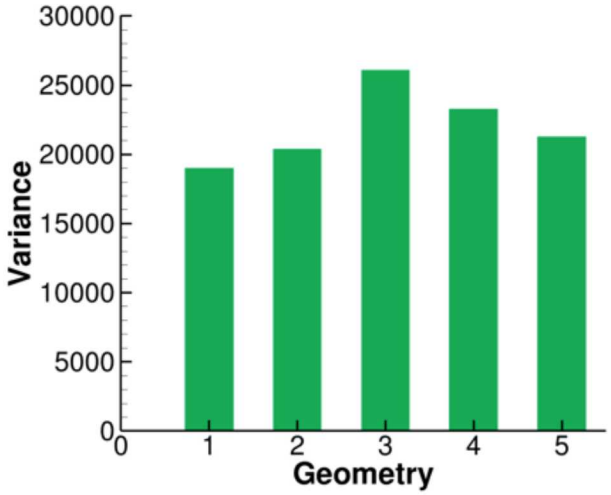


Time = 50 ps

- Non-planar shock front due to multiple pore interactions
- Temperature histogram for each microstructure provides unique "fingerprint" at a given instant in time
- Most common temperature close to T_H =581 K
- Outlier temperatures > 1000K

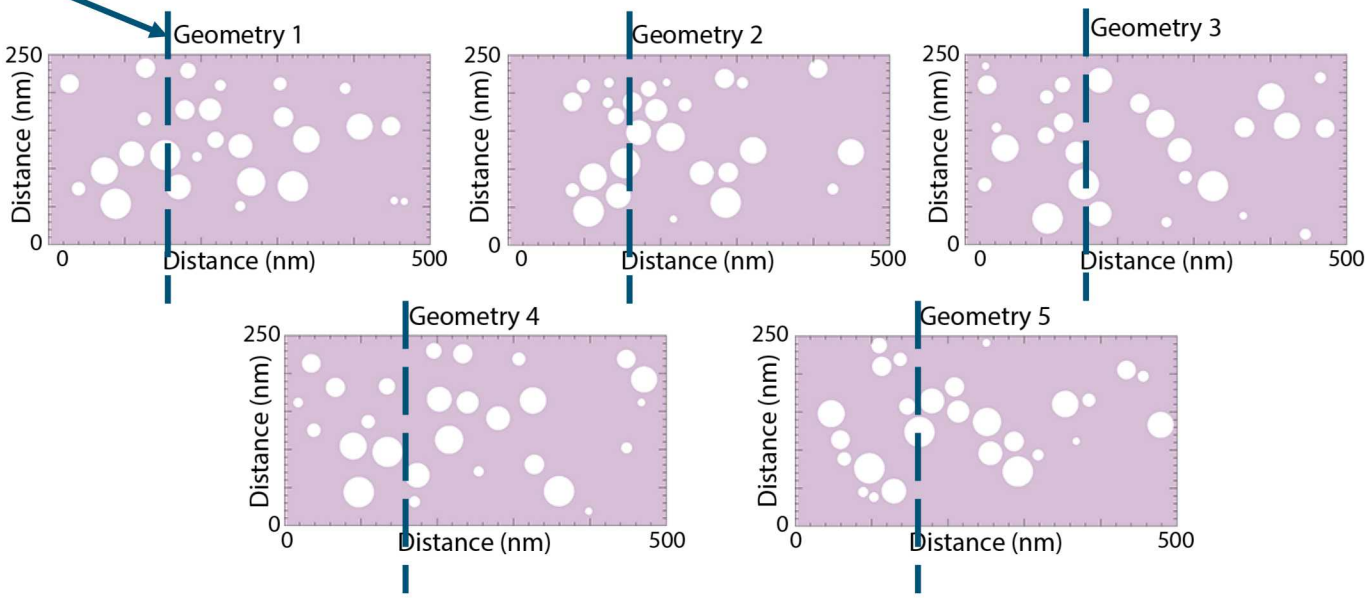
Mean Temperatures Independent of Geometry



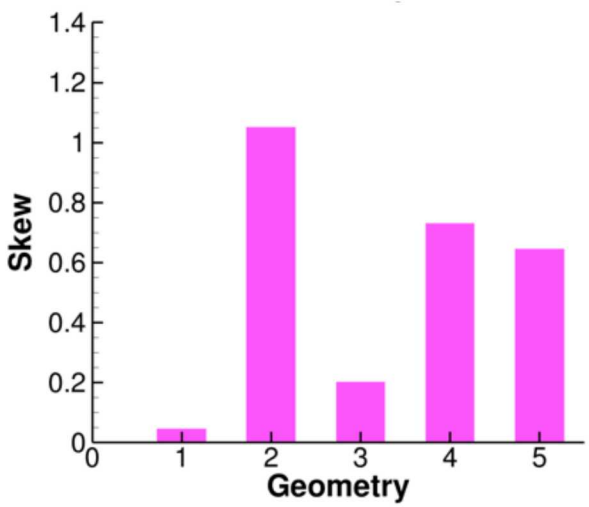


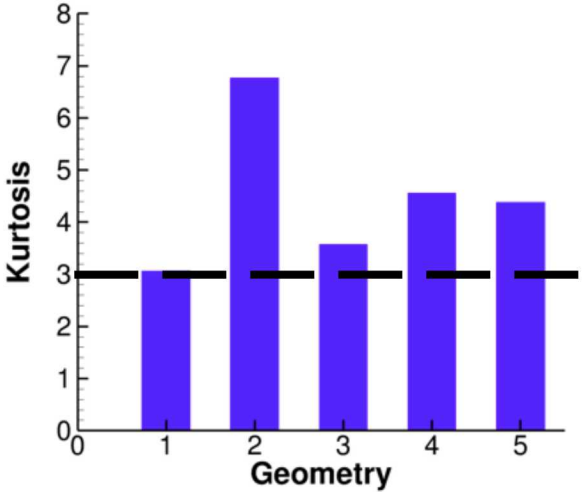
Time = 50 ps

Approximate shock wave position



Hot Spots Related to Temperature Outliers

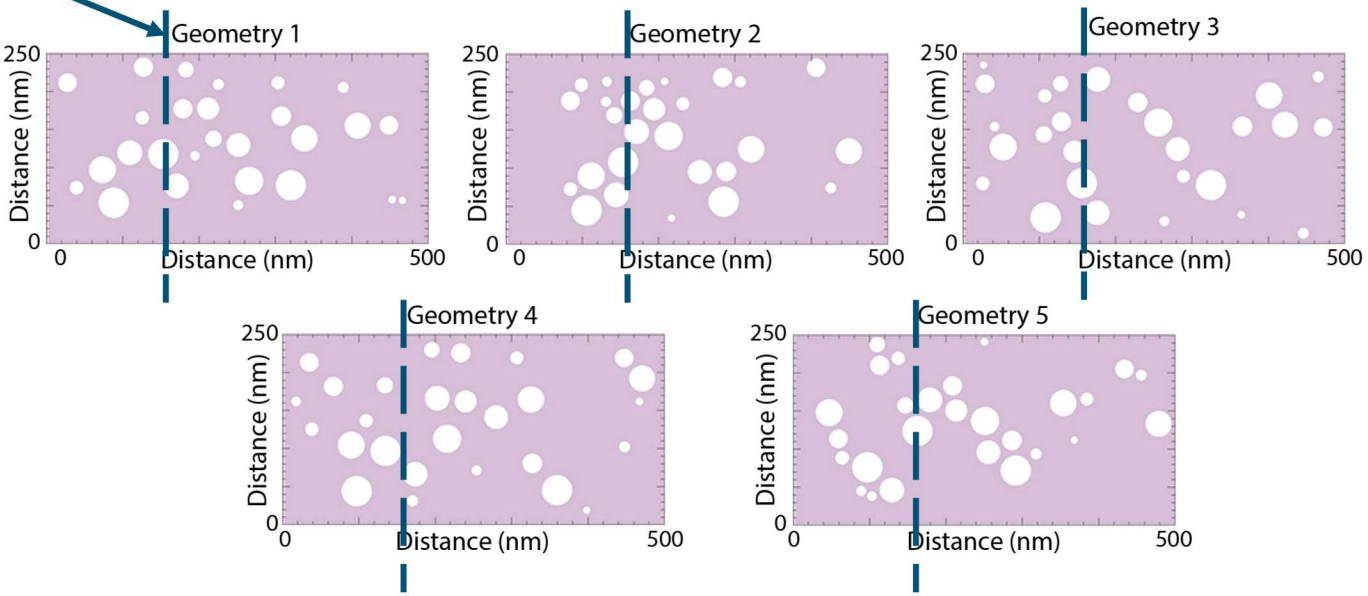




Gaussian Distribution Kurtosis = 3

Time = 50 ps

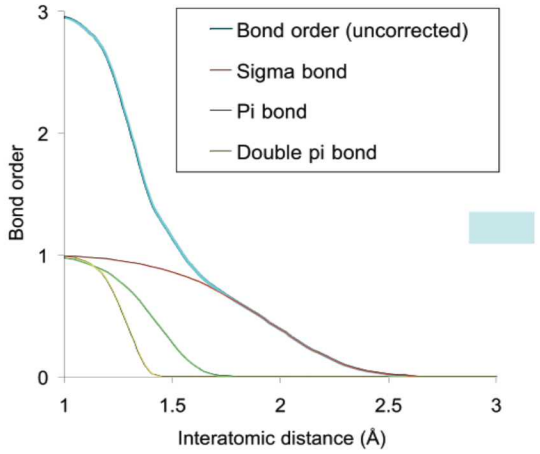
Approximate shock wave position

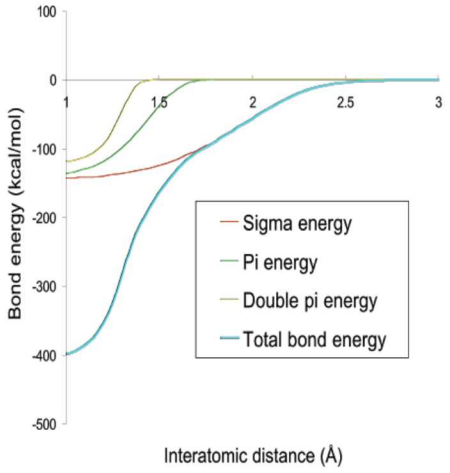


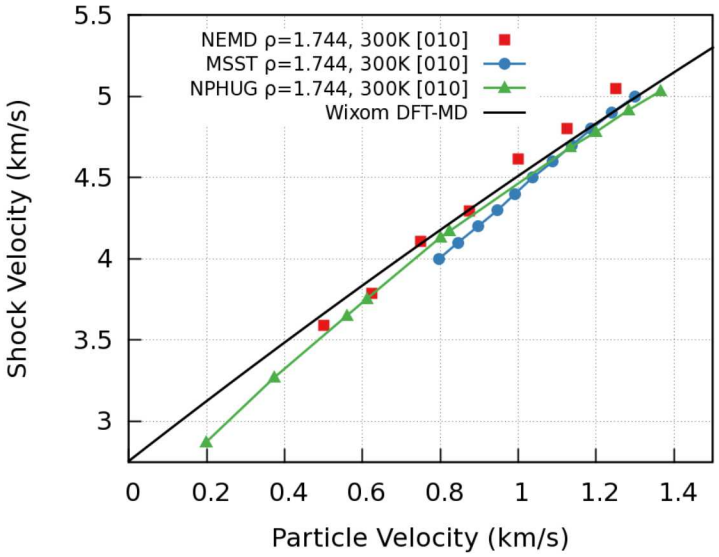
Molecular Dynamics Simulations

- 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



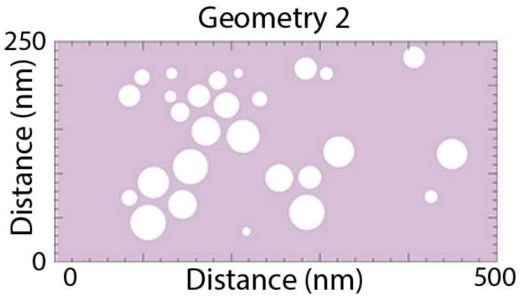




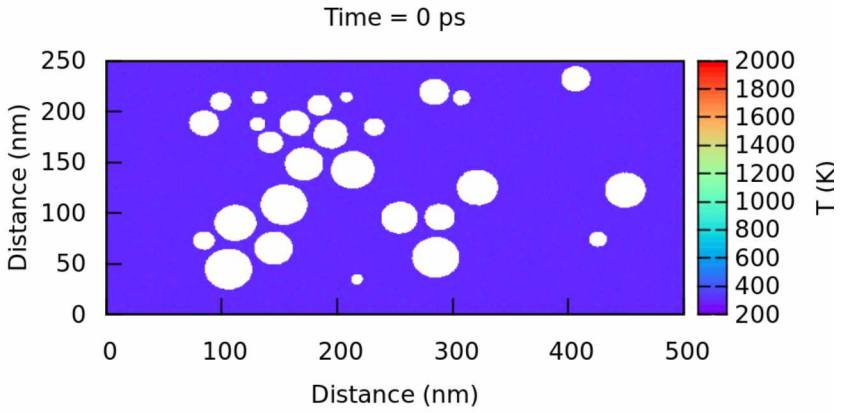
Chenoweth, van Duin and Goddard, J. Phys. Chem. A, 112, 1040-1053 (2008)
Strachan *et al.* J. Chem. Phys. 122, 054502 (2005)
Castro-Marcano *et al.* Combustion and Flame 159(3) 1272-1285 (2012)
Wood, van Duin, Strachan , J. Chem .Phys. A 118, 885 (2014)
Rappe and Goddard, J. Phys. Chem 1991, 95, 3358-3363

MD Simulation of Clustered Porosity

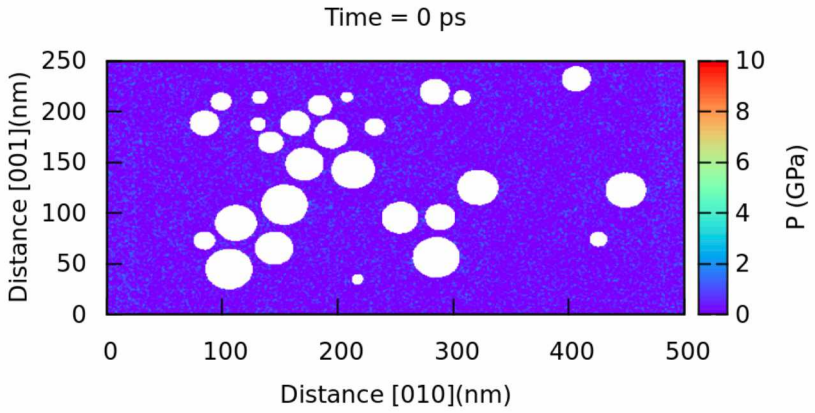
- Geometry 2:
  - Large pore cluster between 100-200 nm
  - Temperature distribution with high skew and kurtosis



Temperature (K)



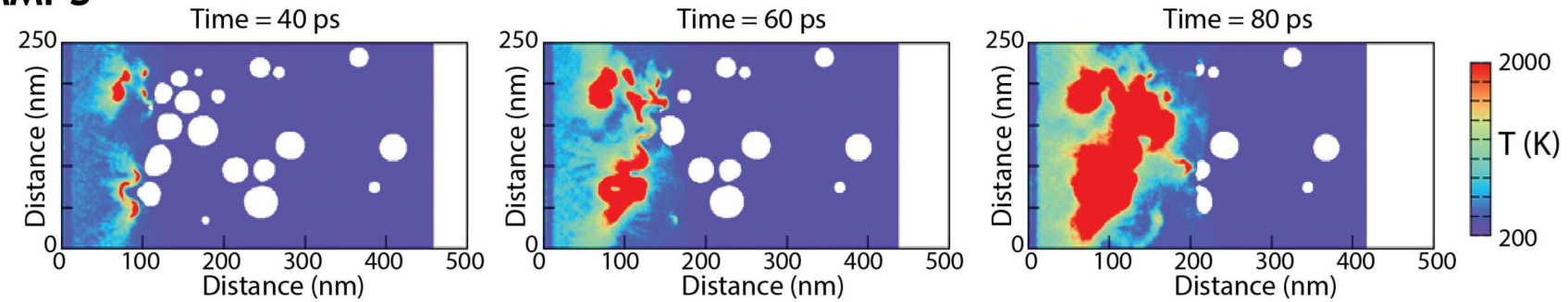
Pressure (GPa)



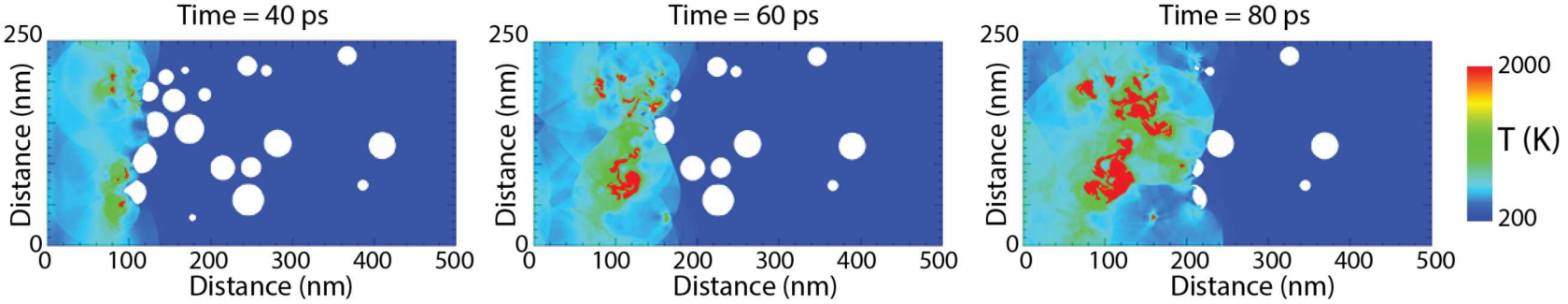
Comparison of MD vs CTH with reaction

- Good qualitative agreement in spatial temperature fields
- Shock wave front well resolved in both codes
- Temperature magnitude in reacting areas higher in MD

LAMMPS



CTH



Conclusions

- Skew and kurtosis of instantaneous temperature distribution provide information of how many high temperature outliers are present
  - May be good indicator for hot spots
- Pore clustering seems to be a driver for more high temperature outlier events
- Evolution of temperature distribution with time is a complex function of chemistry and microstructure features

Future Work

- Characterize evolution of statistical metrics over time
- Better quantitative match of temperature predictions between MD and CTH

Thank You!

Time-Evolution of Temperature Distributions

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

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

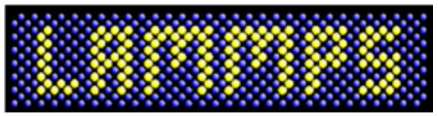
Energy

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

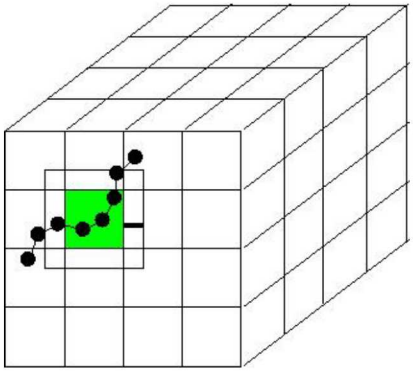
$$-\boldsymbol{S} = P\boldsymbol{I} + \boldsymbol{\sigma} + \boldsymbol{Q}(\vec{V}, c_s)$$

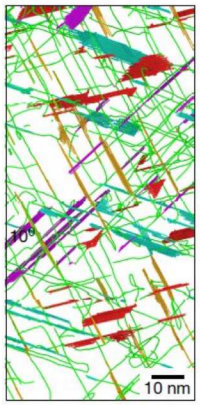
Stress Tensor — Spherical Part — Deviatoric Part — Artificial Viscosity

What is LAMMPS?



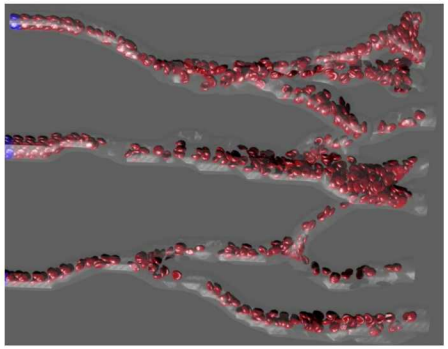
- Large-scale Atomic/Molecular Massively Parallel Simulator
  http://lammps.sandia.gov
- Open source, highly portable C++, free under GPL license
- Well documented with many examples, easily extendable for user specific needs
- Variety of boundary conditions, constraints, ensemble sampling methods etc.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



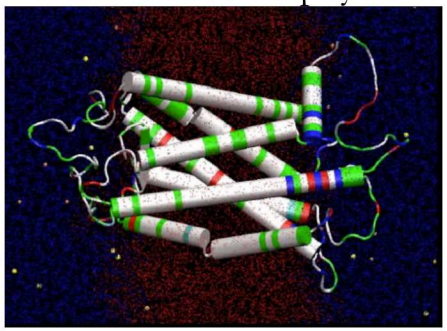


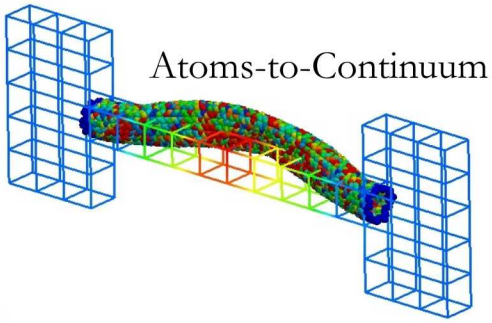
Dislocations in Materials

Blood Flow



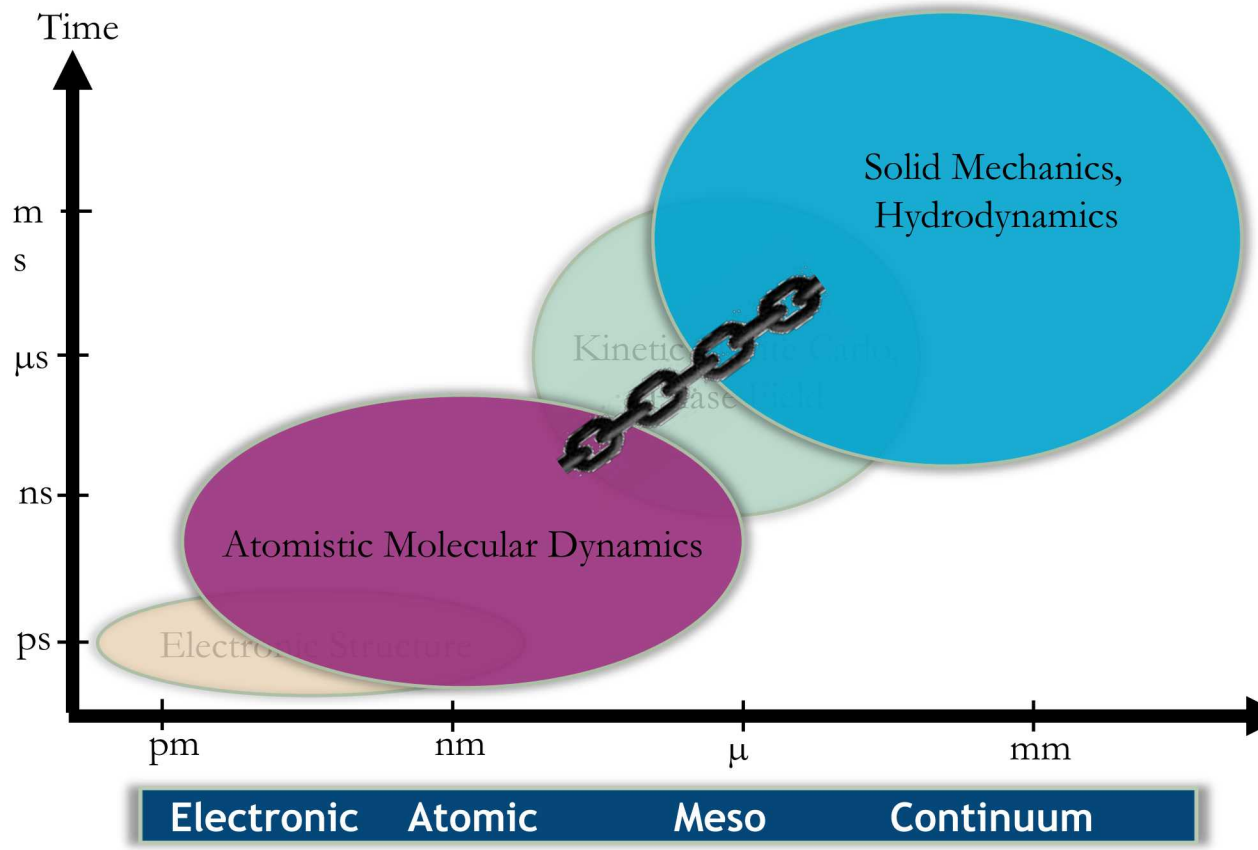
Proteins and Biophysics





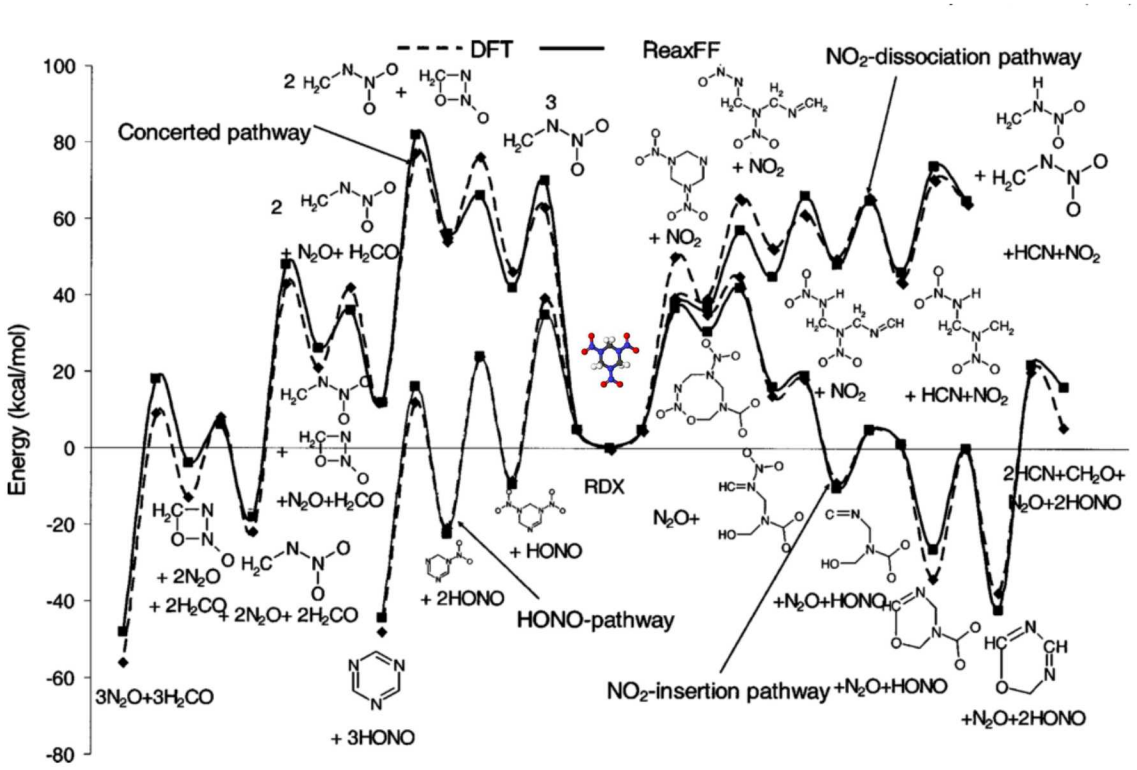
Atoms-to-Continuum

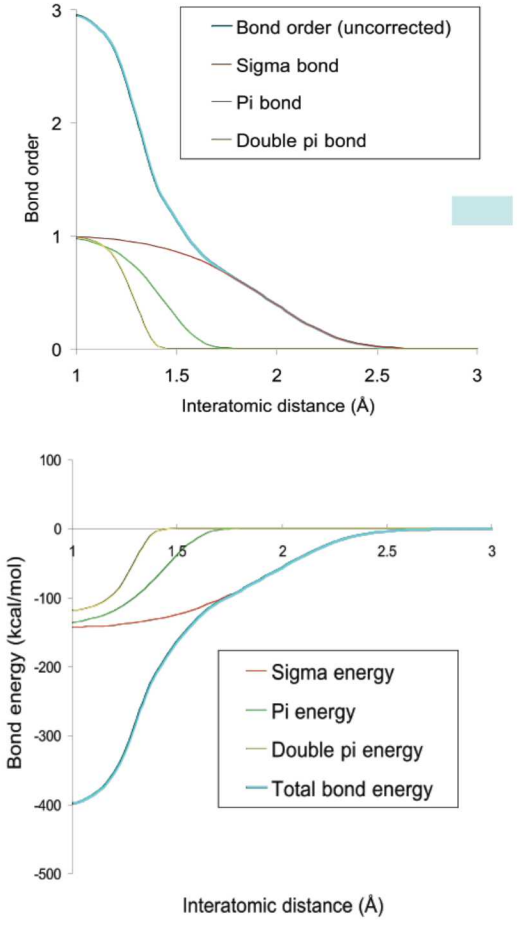
Useful, Co-dependent Models



- 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

Reactive Potentials in MD (the approximation)

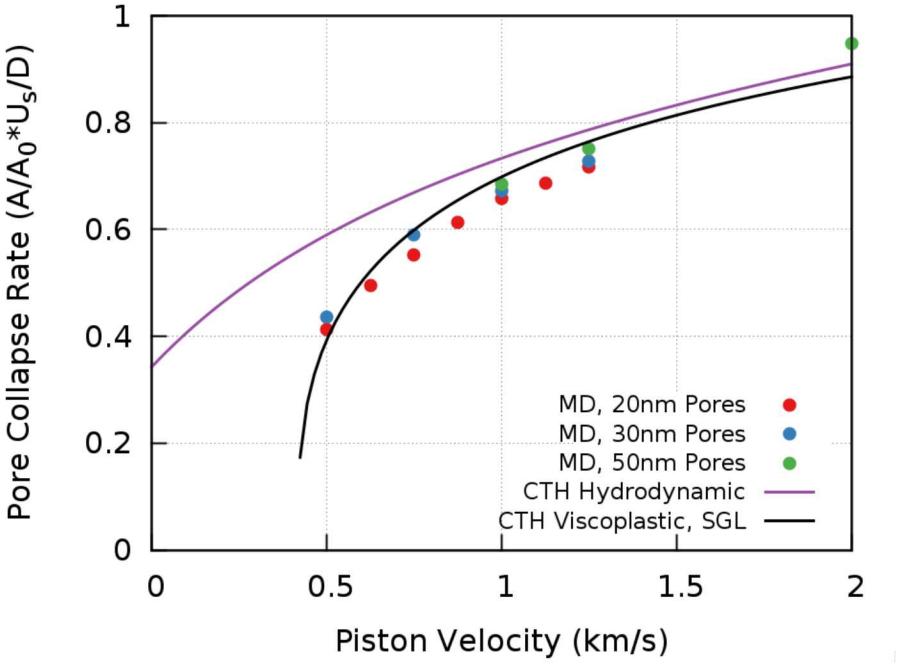


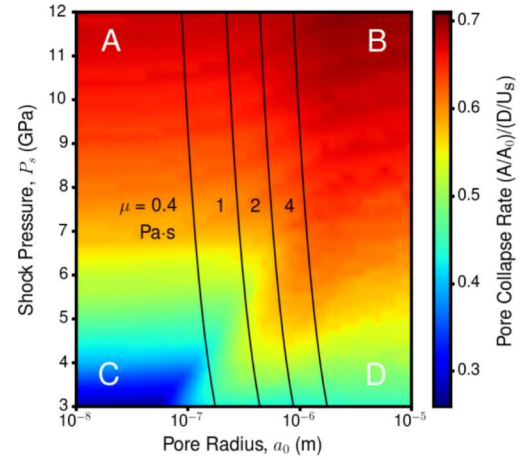


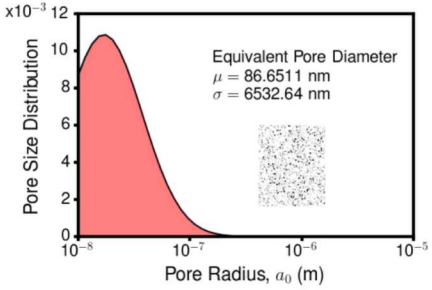
Chenoweth, van Duin and Goddard, J. Phys. Chem. A, 112, 1040-1053 (2008)
Castro-Marcano *et al.* Combustion and Flame 159(3) 1272-1285 (2012)
Rappe and Goddard, J. Phys. Chem 1991, 95, 3358-3363

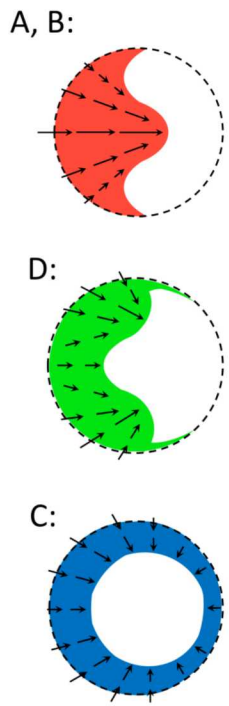
Strachan *et al.* J. Chem. Phys. 122, 054502 (2005)
Wood, van Duin, Strachan , J. Chem .Phys. A 118, 885 (2014)

SGL Strength Model Calibrated from MD



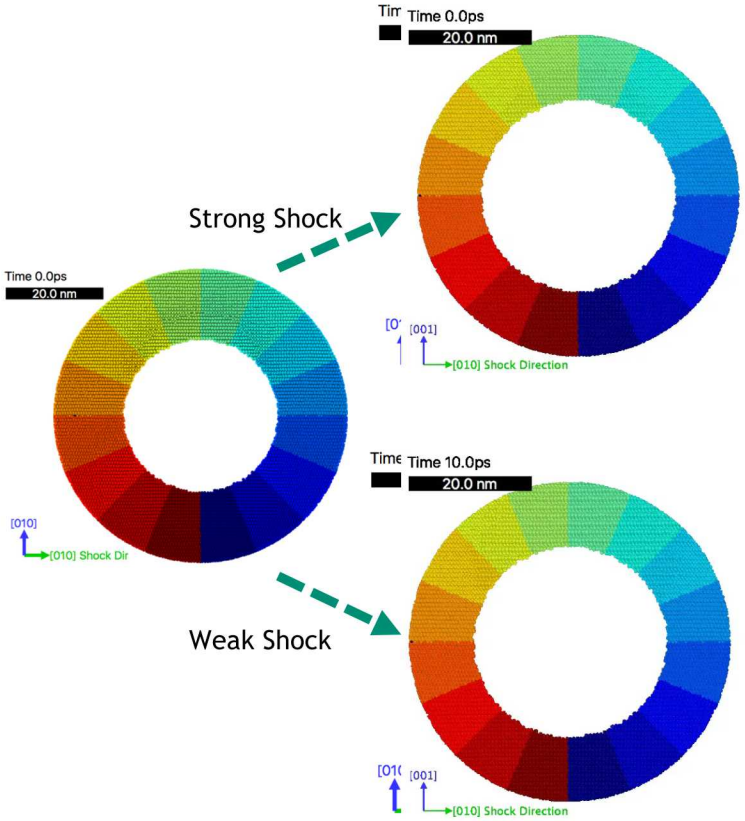




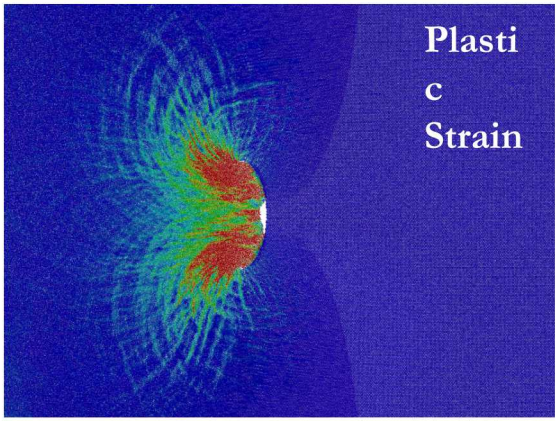


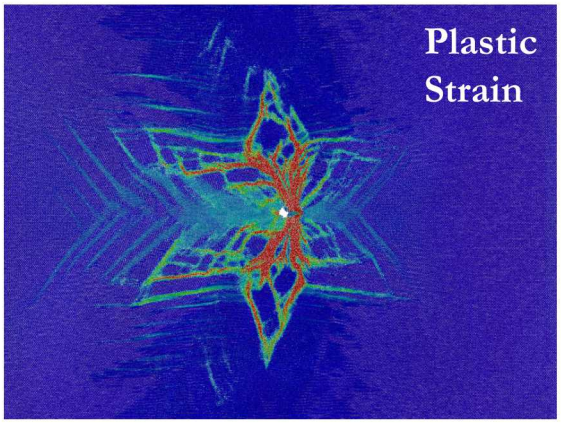
- Training data of collapsing pores from MD sent to CTH for strength model parameterization

Is the MD Model Useful?



OVITO : A. Stukowski, Modelling Simul. Mater. Sci. Eng. 18 (2010), 015012

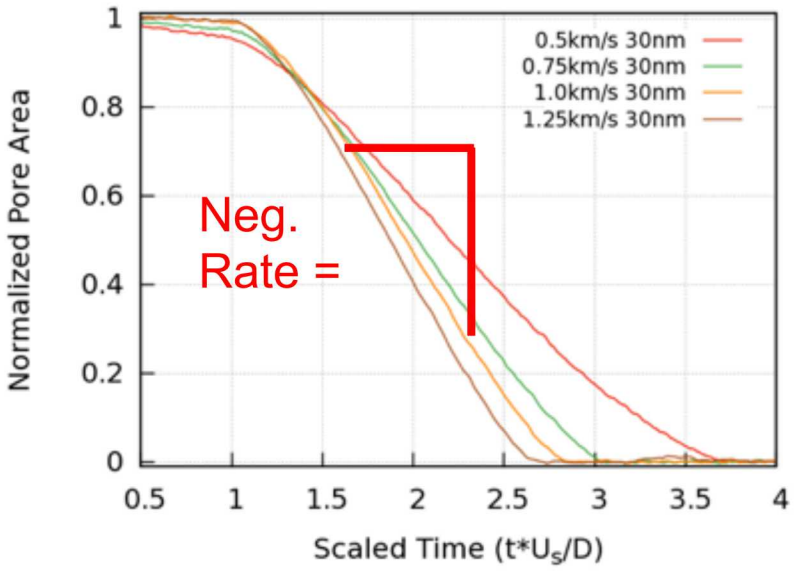




Metrics Passed from MD to CTH

Training Metric

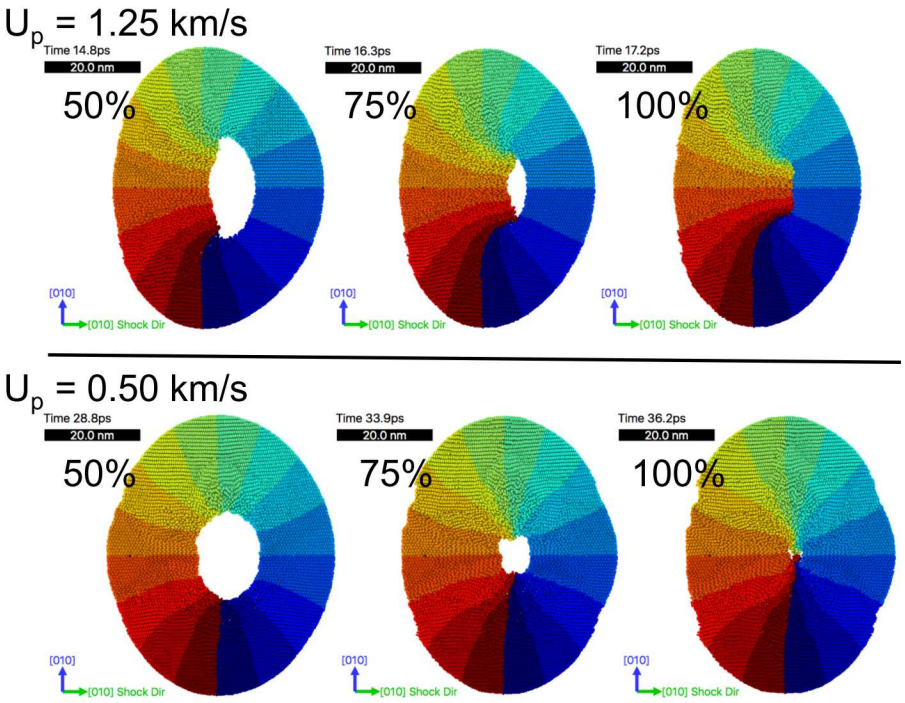
- Collapse rate is used to calibrate strength models in CTH



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

Comparison Metrics

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

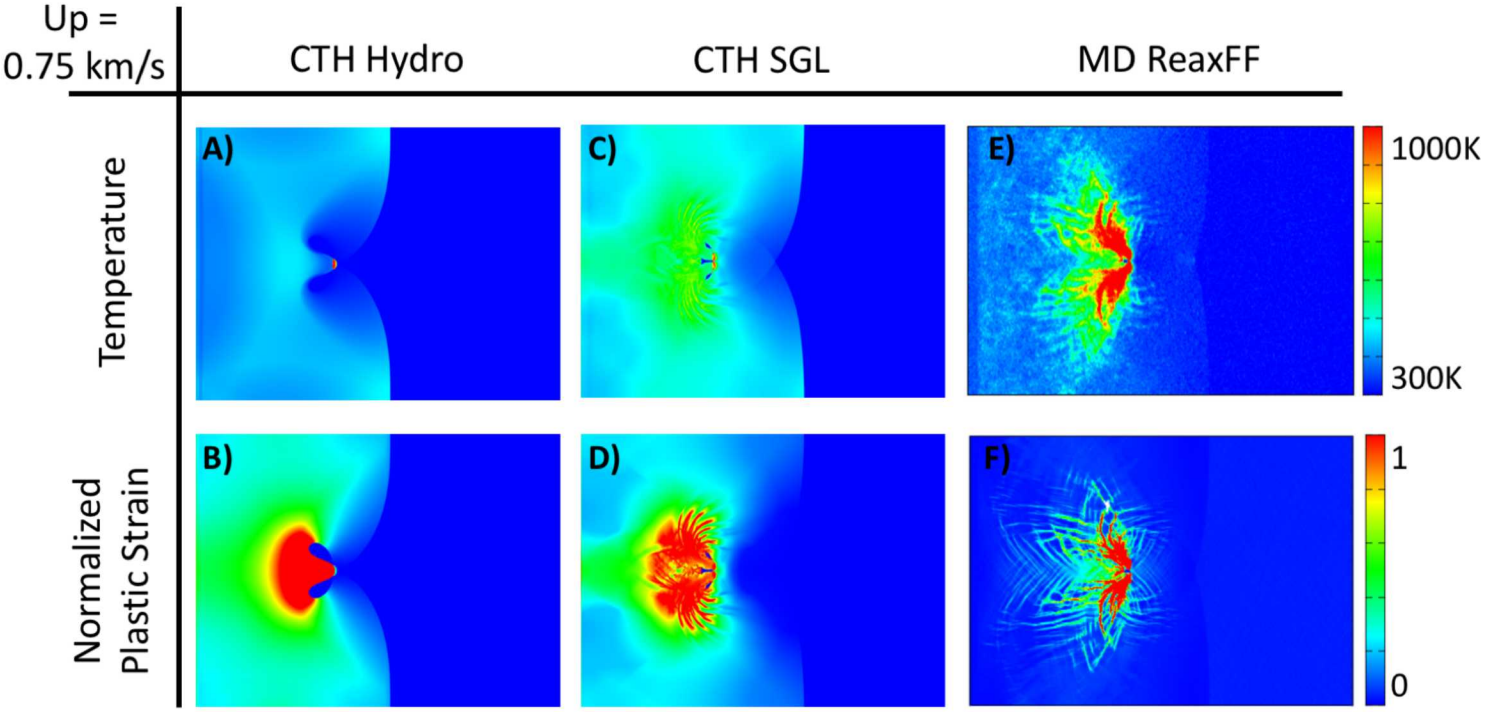


CTH Strain Rate Dependent Model – Steinberg, Guinan and Lund (1988)

- 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:	$\gamma = \gamma_0/(1+\mu)$	

Much Better Mechanical Agreement



CTH now predicts:

- A much more detailed strain field, viscoplastic deformation
- Correlation between temperature and regions of high strain