Exceptional service in the national interest

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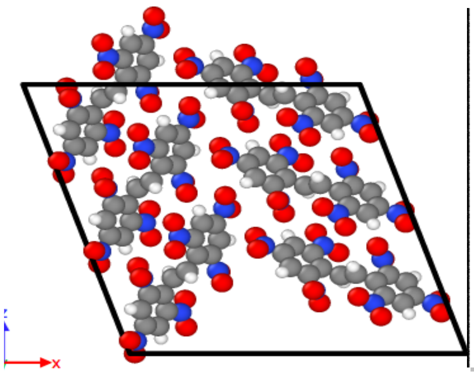

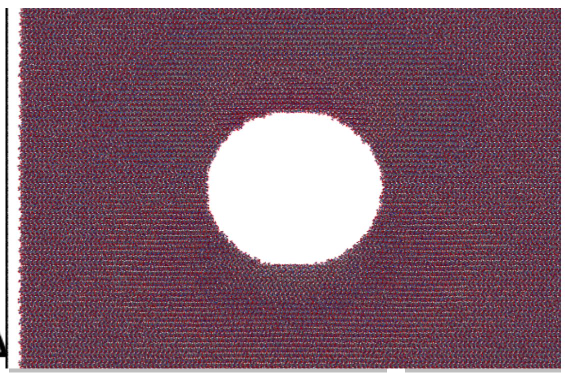

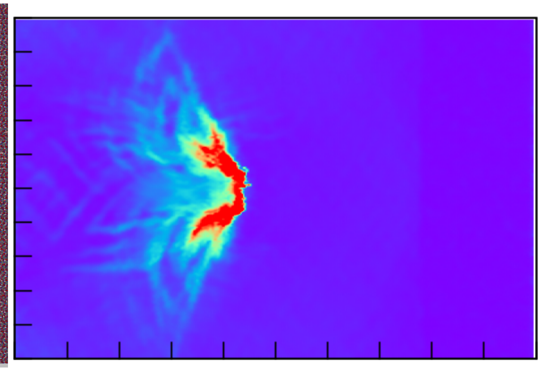

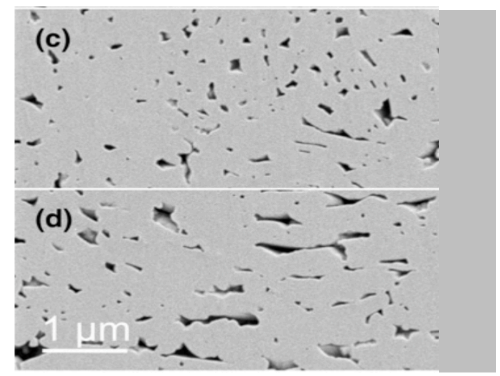

Large-Scale Reactive Simulations of Energetic Materials

Aidan Thompson

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Collaborators: Mitch Wood, Ray Shan, Stan Moore
Cole Yarrington, David Kittell

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

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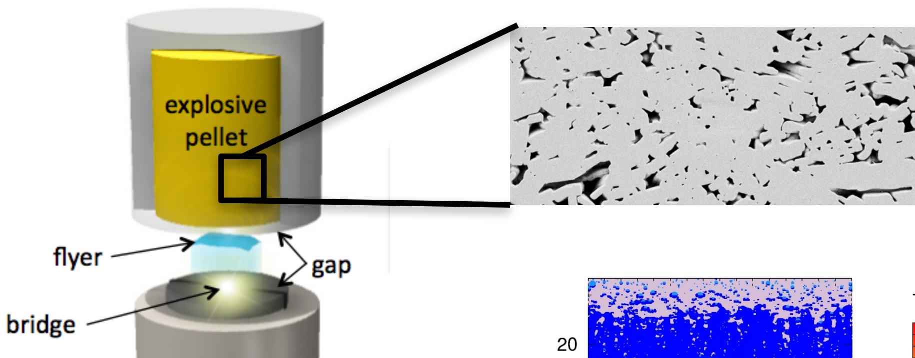
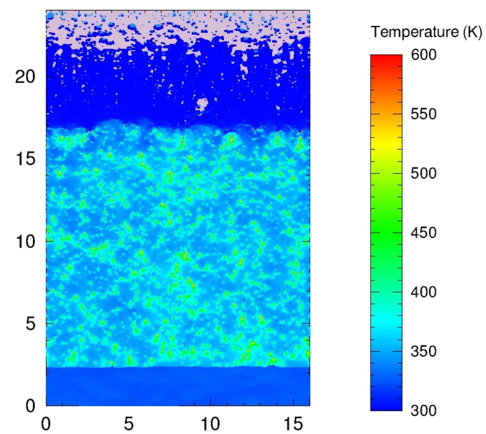
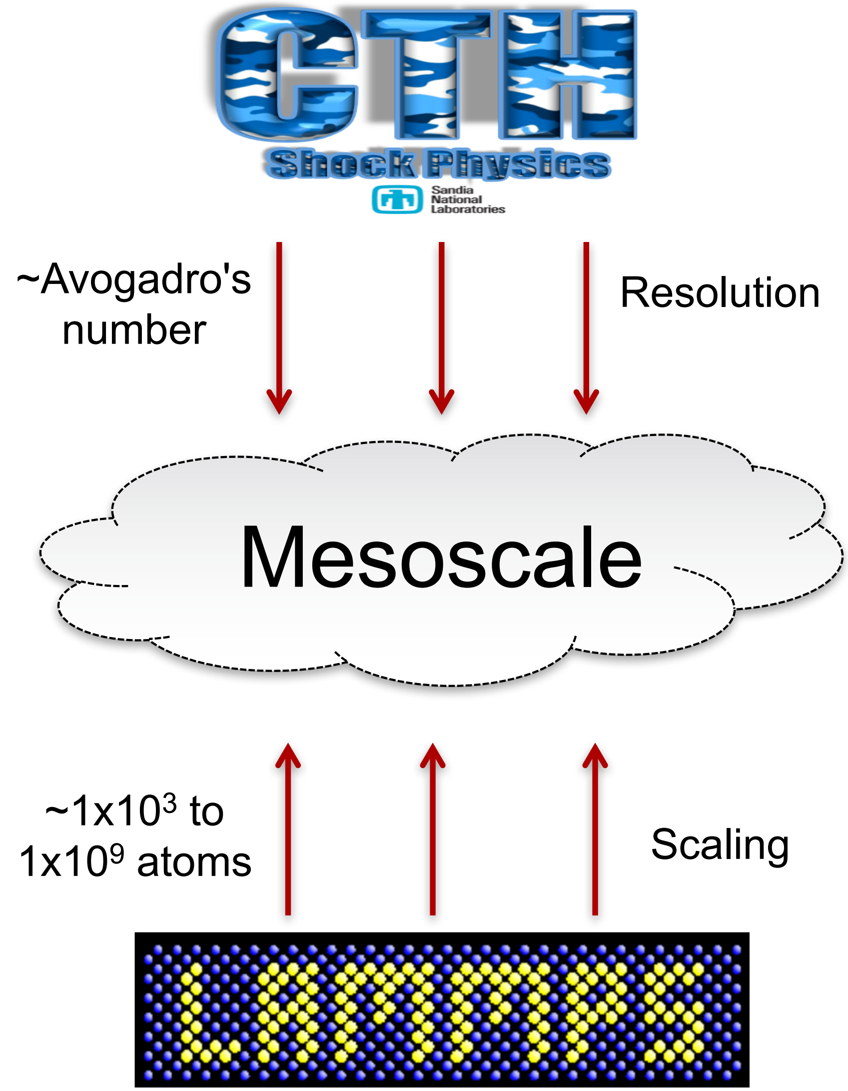
Understanding Initiation Energetic Materials





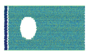


- Microstructural features and heterogeneities known to strongly affect sensitivity
- Generally challenging problems involving physics at many length/time scales
- Shock to detonation transition in energetics fits the bill of being truly "mesoscale"

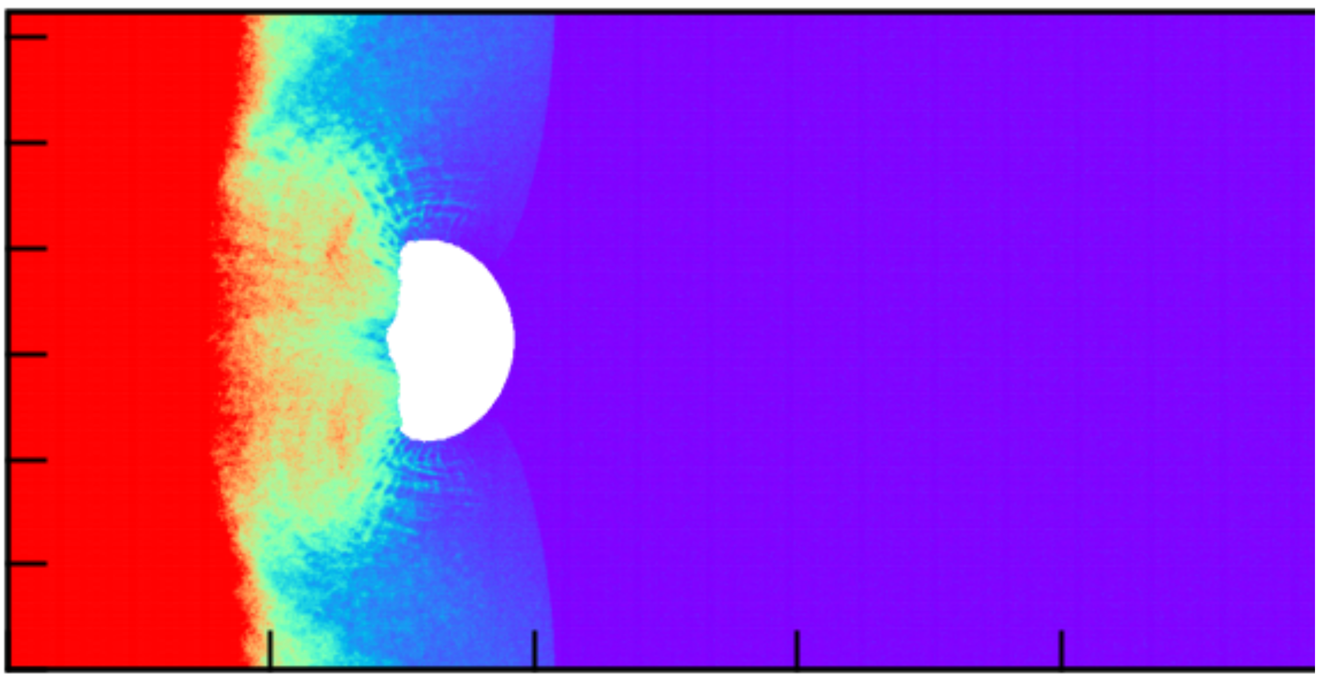
Evolution of Reactive Simulations of Energetic Materials

2010: 244nm x 4nm x 3nm with 240k atoms, perfect crystal (GRASP)

2013: 50nm x 20nm x 20nm with 2M atoms, 10nm void (LAMMPS USER-REAXC)



2017: 1000nm x 600nm x 10nm, 129M atoms, 200nm void (LAMMPS KOKKOS)

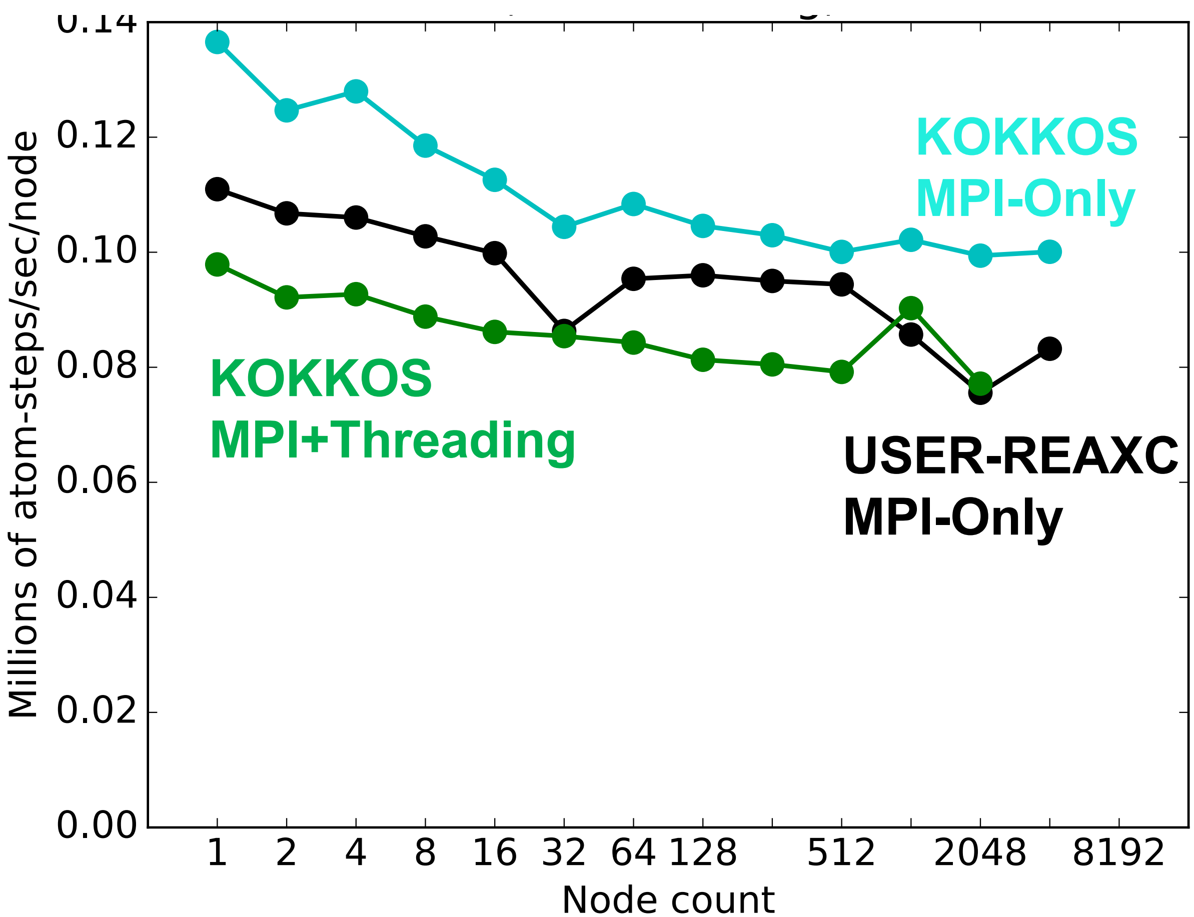


LAMMPS KOKKOS ReaxFF Implementation

- **Current capabilities for ReaxFF within LAMMPS is ~100M atoms running routinely on ~100k processors**

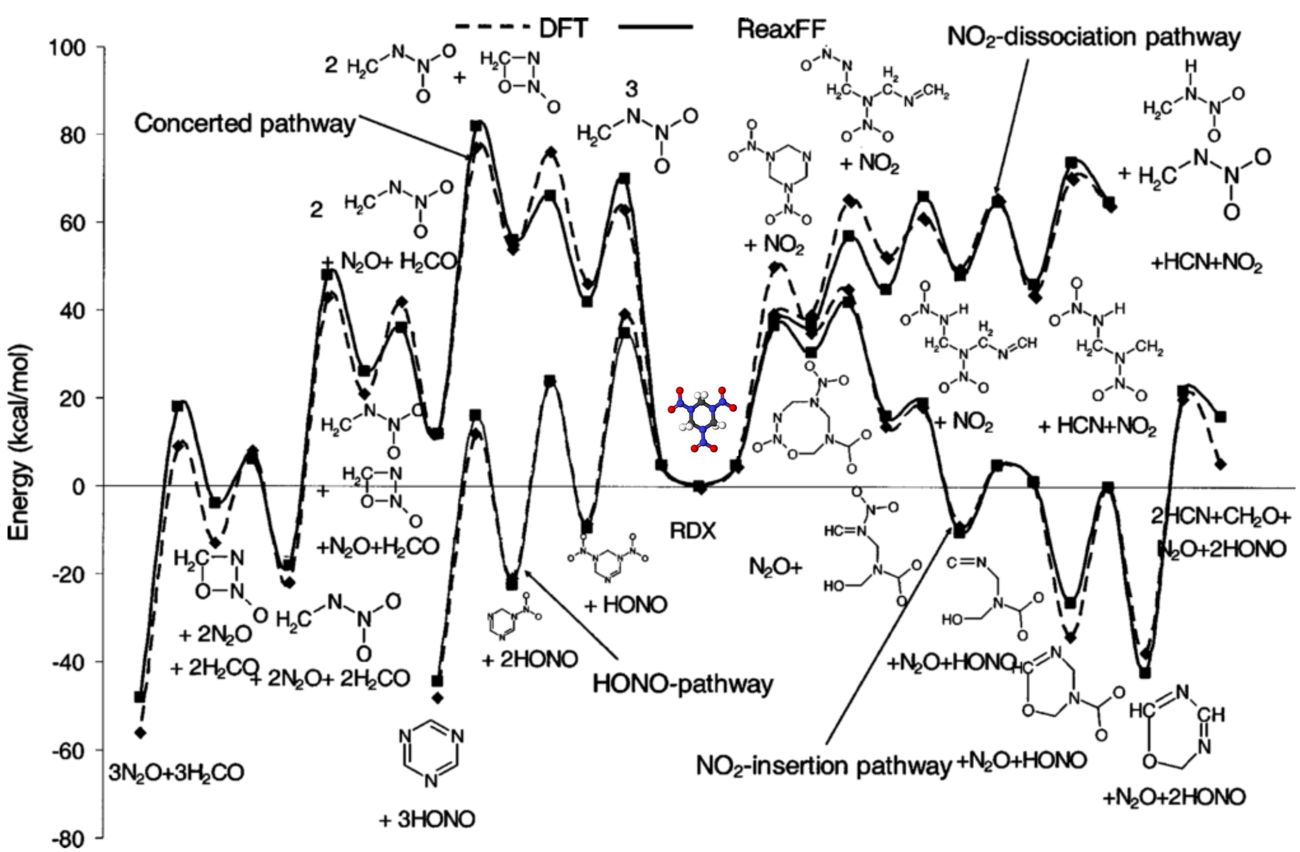
- KOKKOS-Reax/c package circumvents memory overflow errors and makes the code portable to modern architectures (GPU, KNL, HSW)
- MPI-Only KOKKOS performance surpasses USER-REAXC
- KOKKOS w/ threading slower that expected

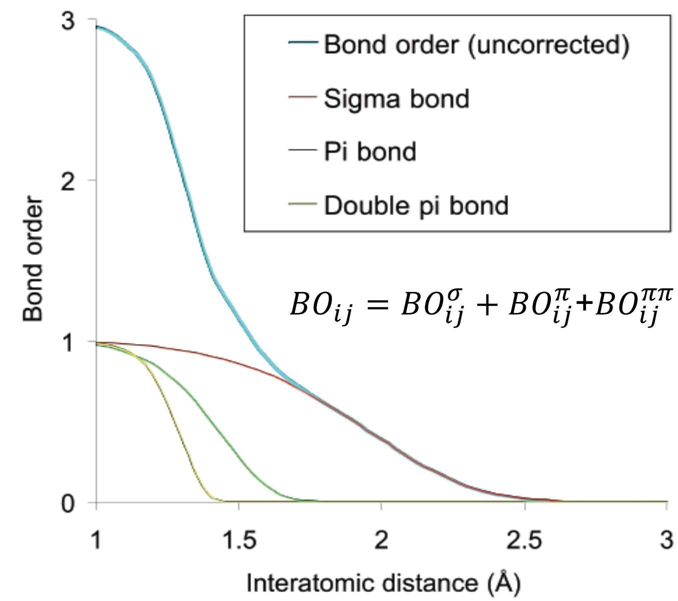
Trinity KNL, weak scaling, 32K atoms/node
Up to 4096 nodes, 130M atoms



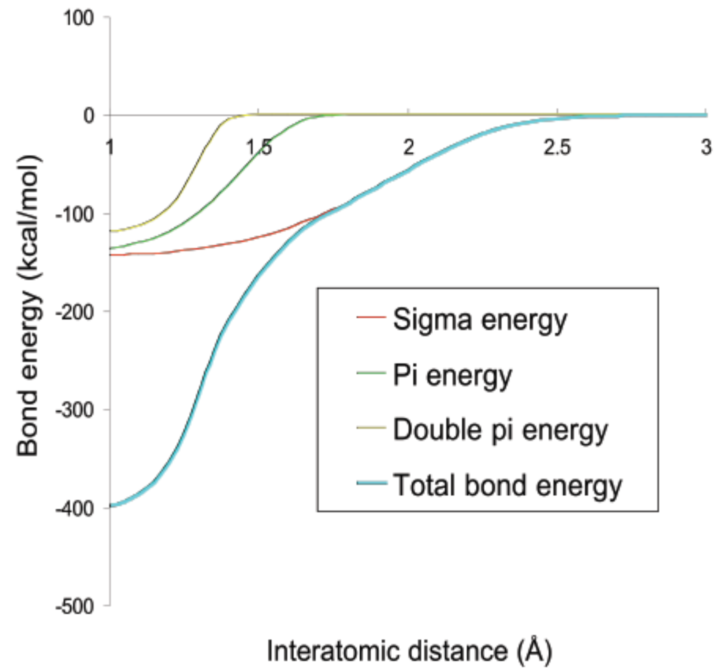
ReaxFF Potential

- Complex formulation is challenging to parameterize.
- Energetic materials have been a focus of ReaxFF training for decades





$$BO_{ij} = BO_{ij}^{\sigma} + BO_{ij}^{\pi} + BO_{ij}^{\pi\pi}$$



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

Validation of the HNS Potential

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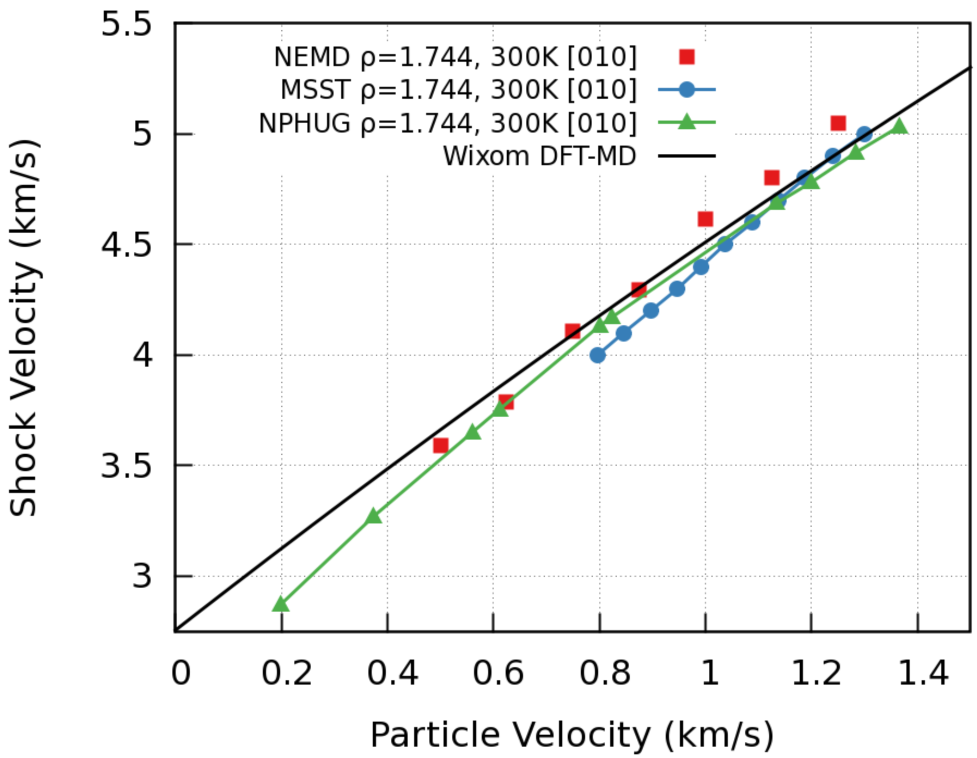
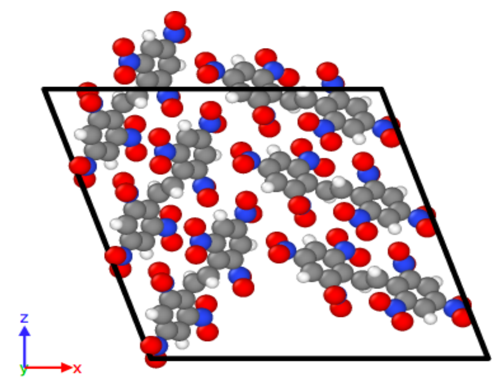
- HNS parameterization based on standard ReaxFF nitramine potential [1,2]
- Added low-gradient correction tuned to HNS DFT data
- Reproduces high-pressure equation of state for HNS





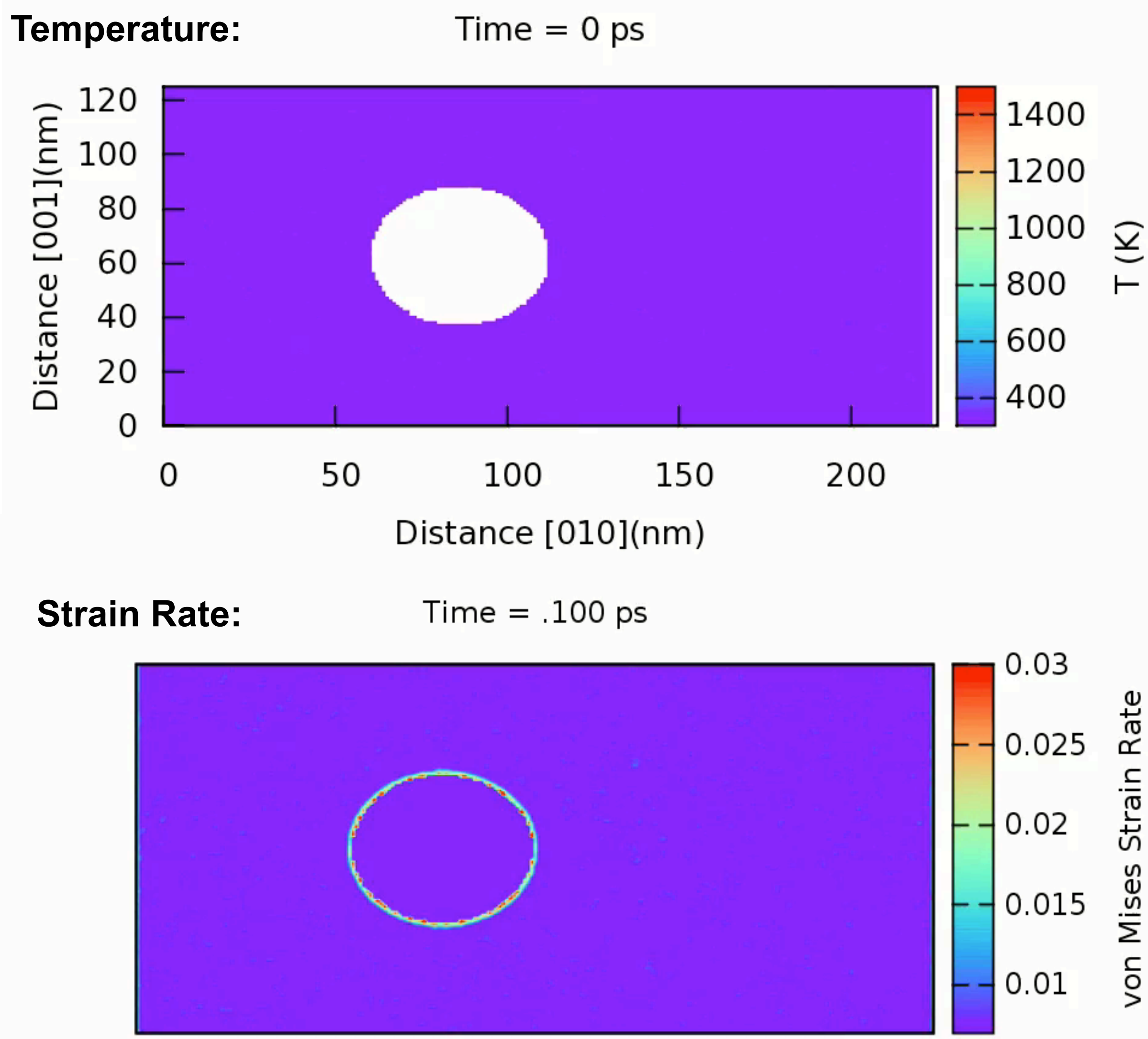
[1] Chenoweth, van Duin and Goddard, J. Phys. Chem. A, 112, 1040-1053 (2008)
[2] Strachan *et al.* J. Chem. Phys. 122, 054502 (2005)

Shock to Initiation, Deflagration

- Detailed chemistry is incorporated in these MD potentials, hot spot evolution is captured naturally.

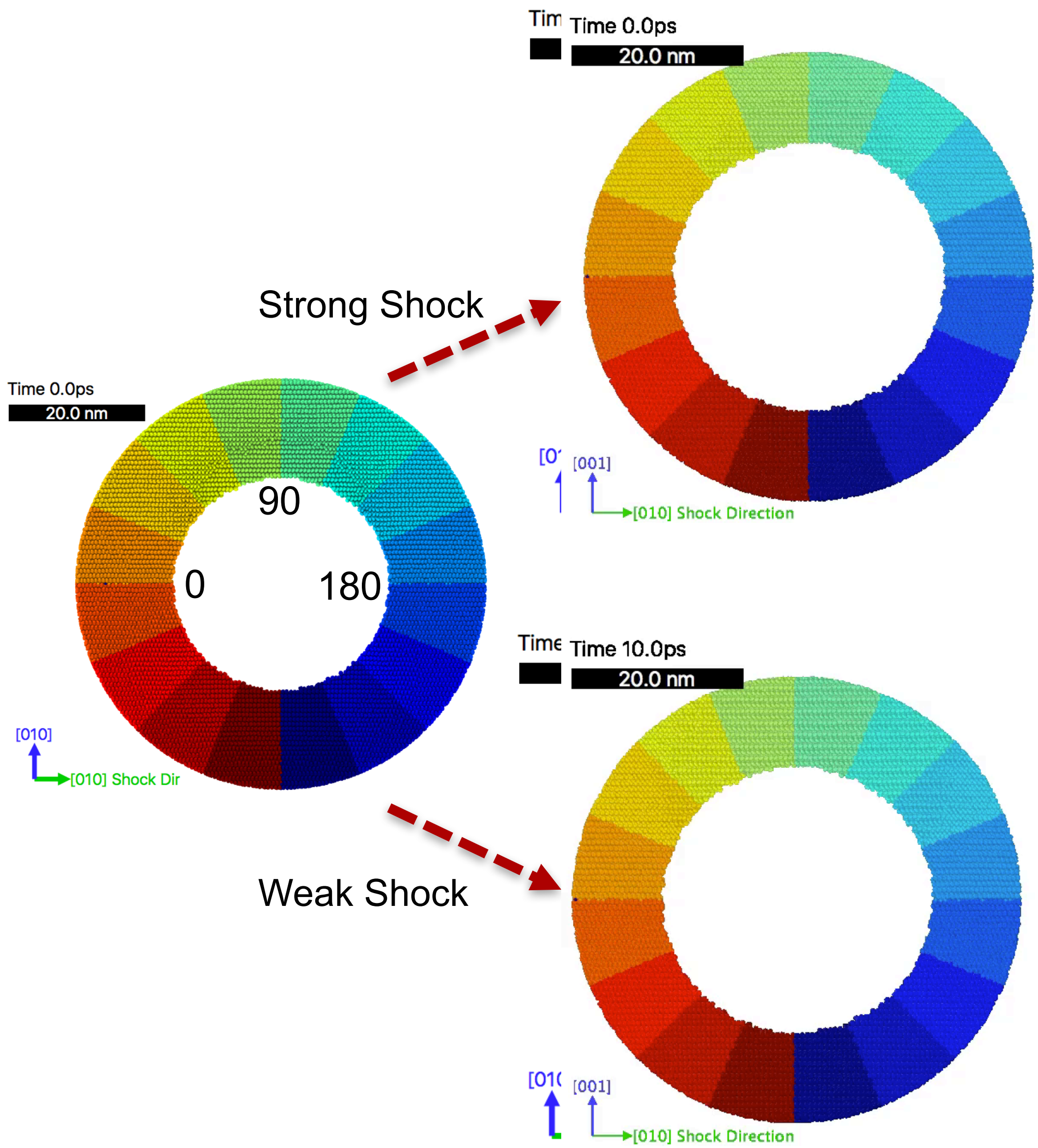
- **Current capabilities for ReaxFF within LAMMPS is ~100M atoms running routinely on ~100k processors**

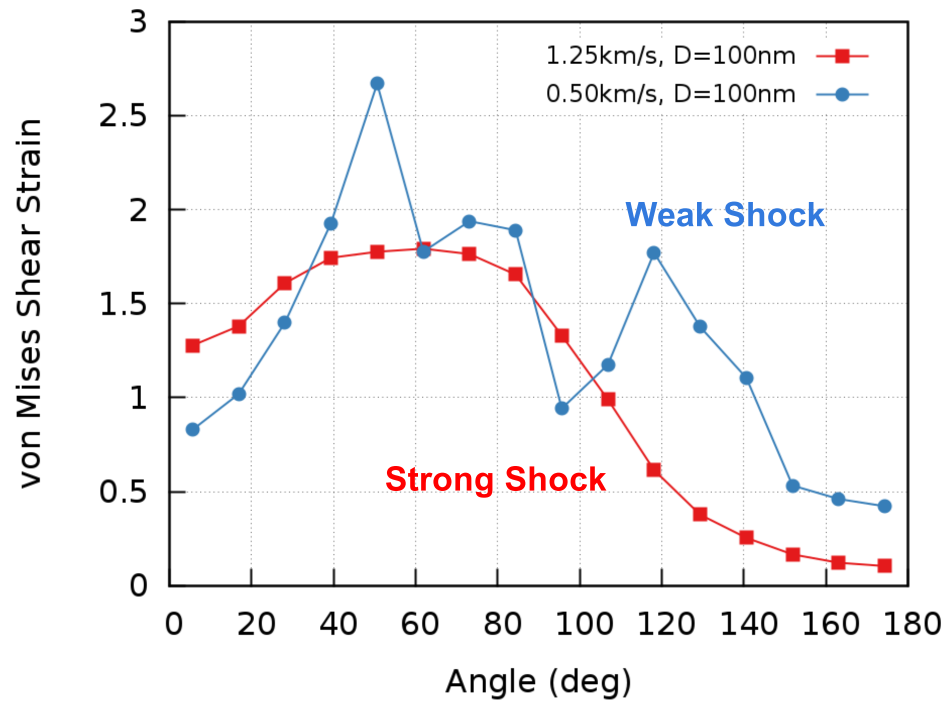
- KOKKOS-Reax/c package circumvents memory overflow errors and makes the code portable to modern architectures (GPU, KNL, HSW)



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

Hydrodynamic vs. Viscoplastic Pore Collapse





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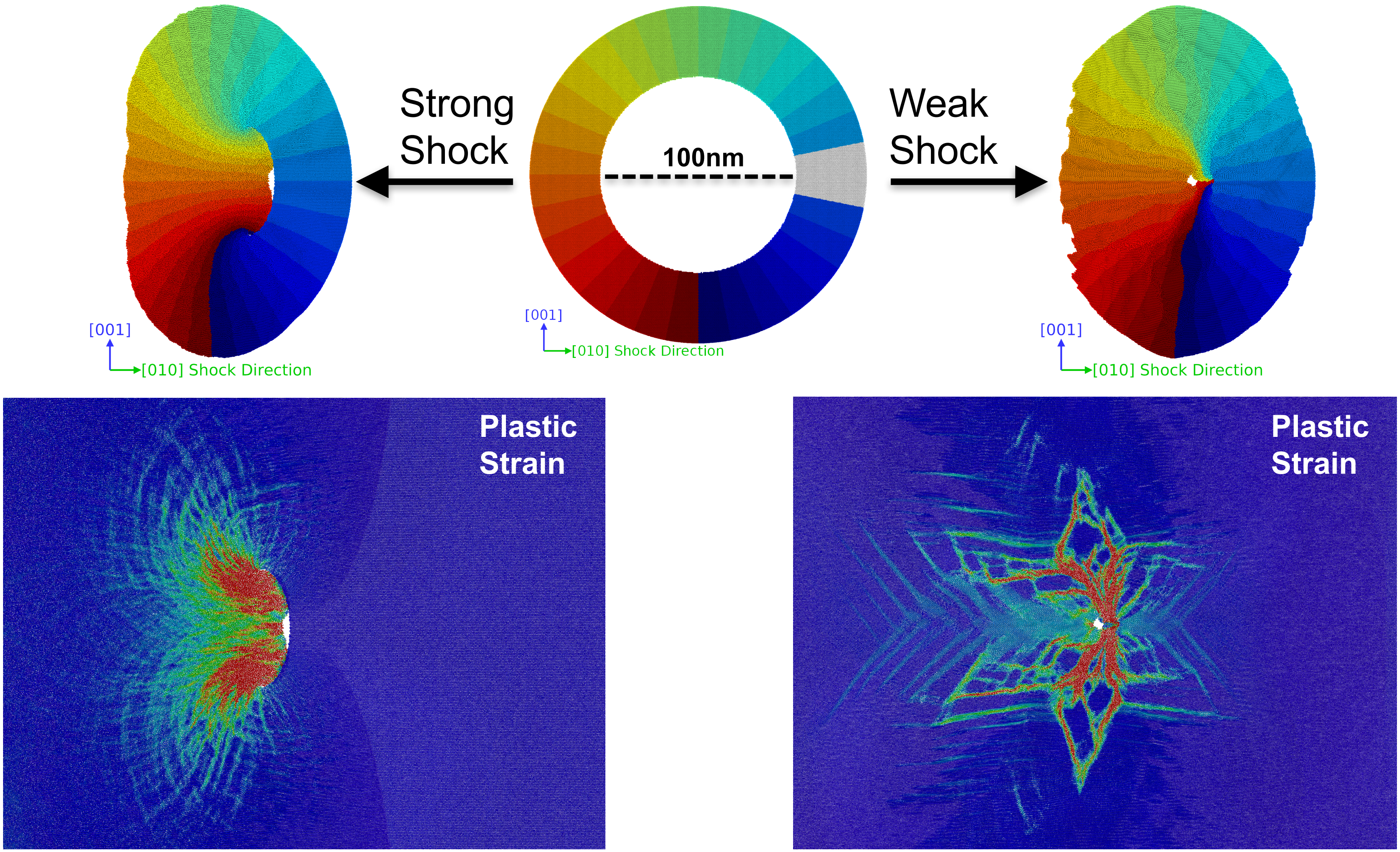
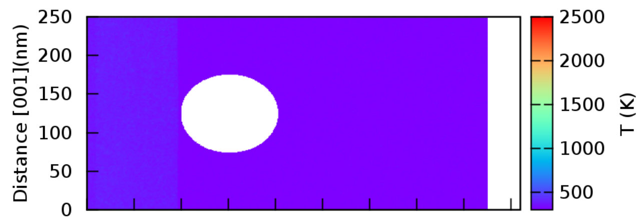
Hydrodynamic vs. Viscoplastic Pore Collapse



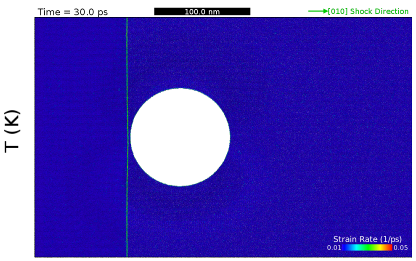
Viscoplastic Pore Collapse Hot Spot

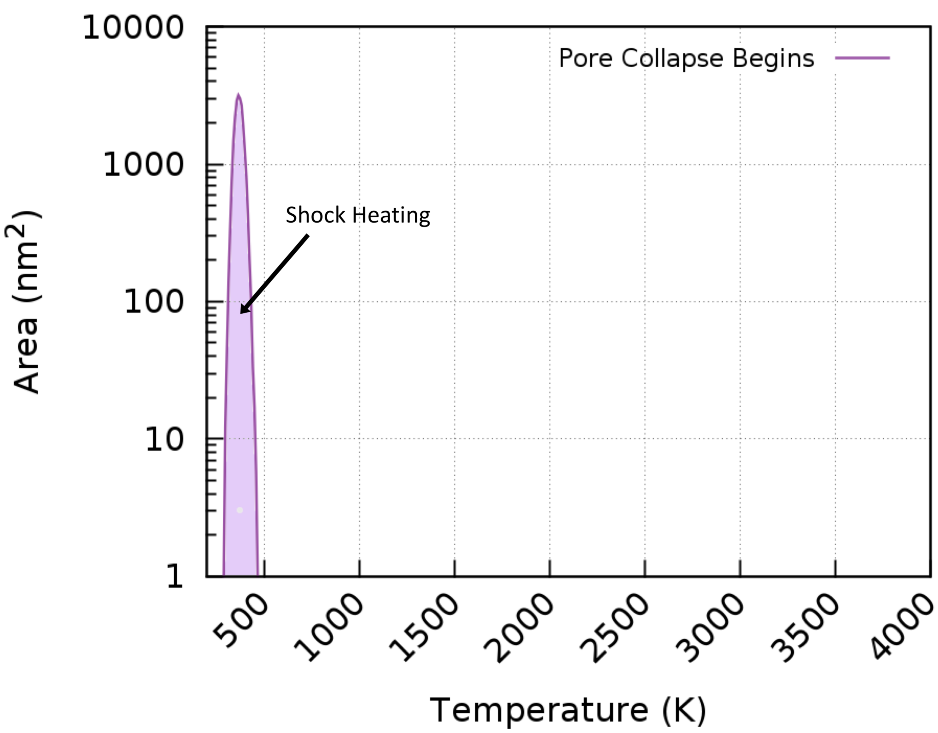
- How is the heat generated in the resultant hot spot?
- Up = 0.75km/s, mixed hydrodynamic / viscoplastic

Local Temperature



Local Strain Rate





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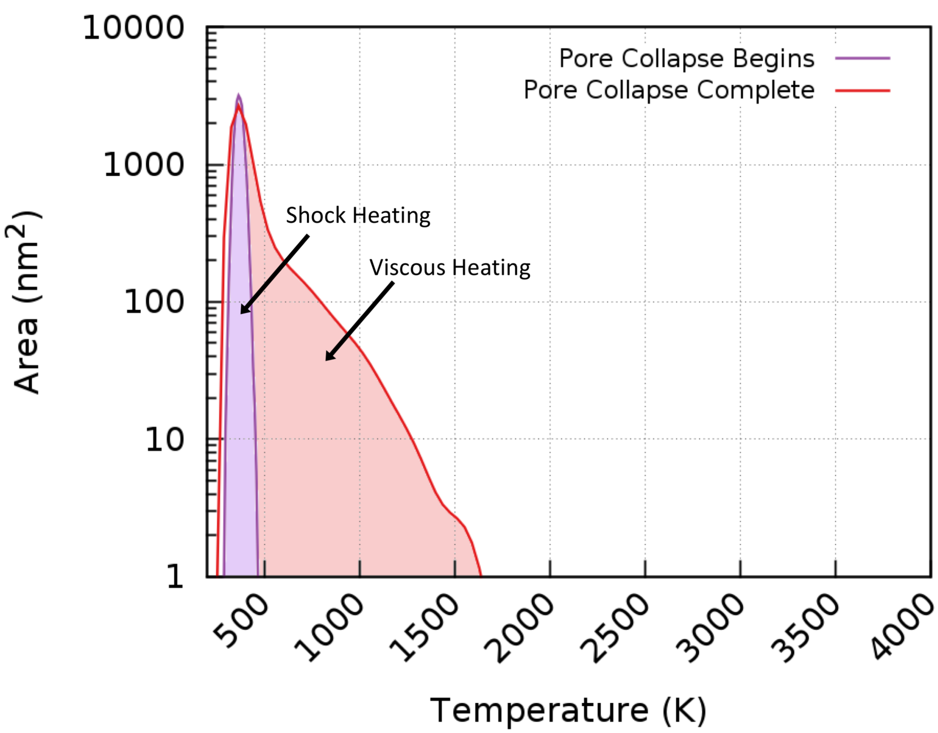
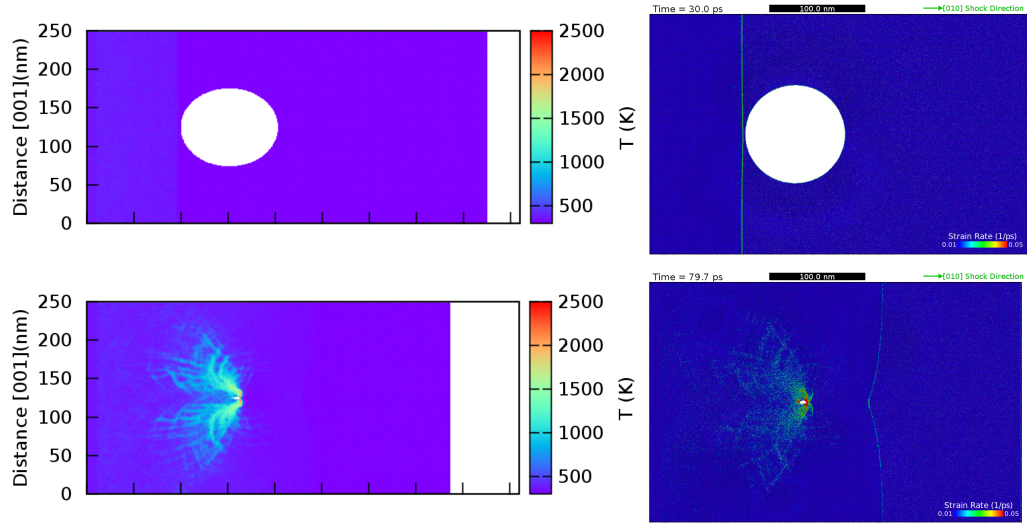


Local Temperature

Local Strain Rate



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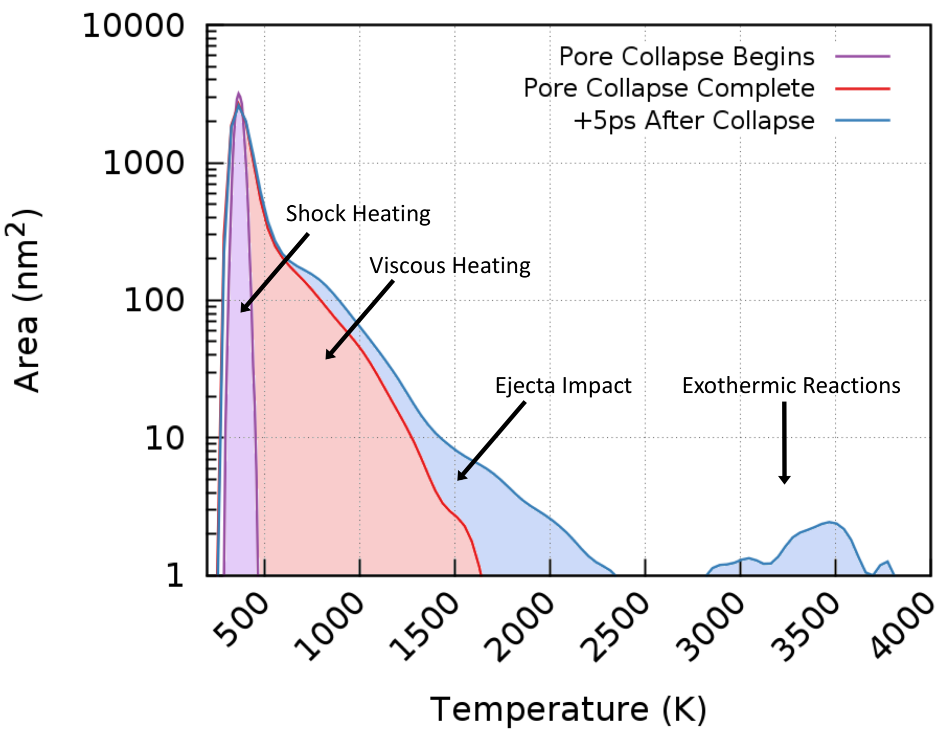

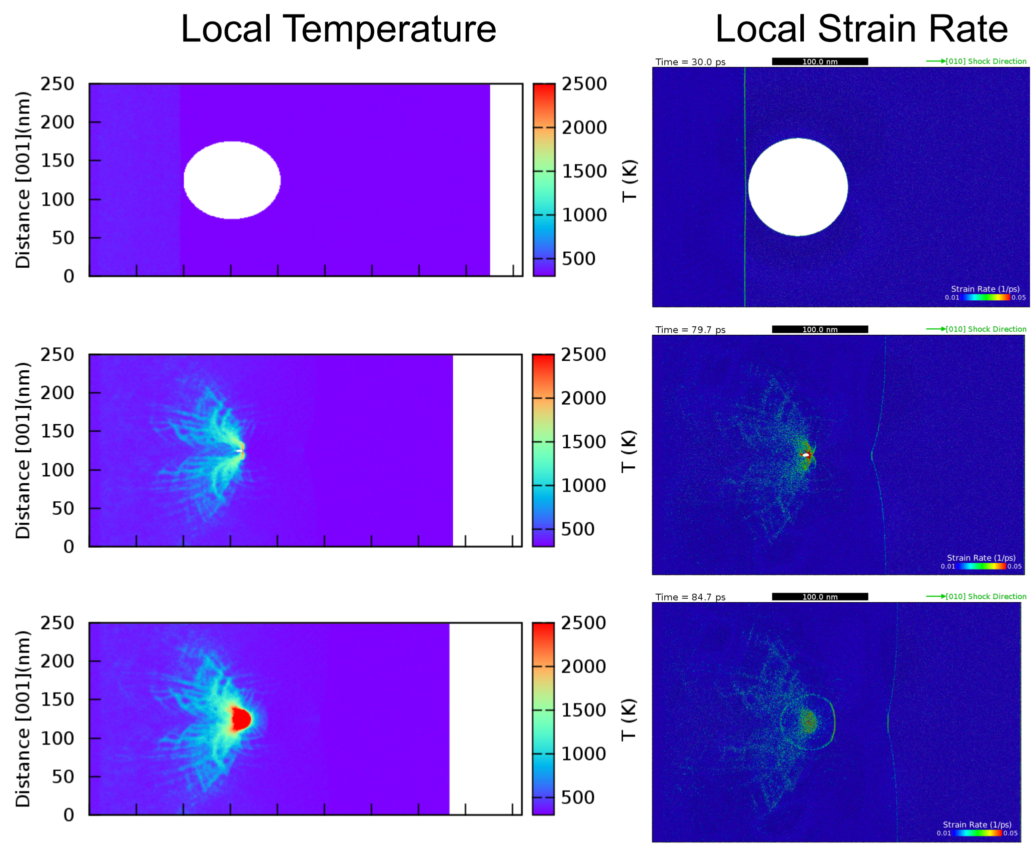

Viscoplastic Pore Collapse Hot Spot

Sandia National Laboratories

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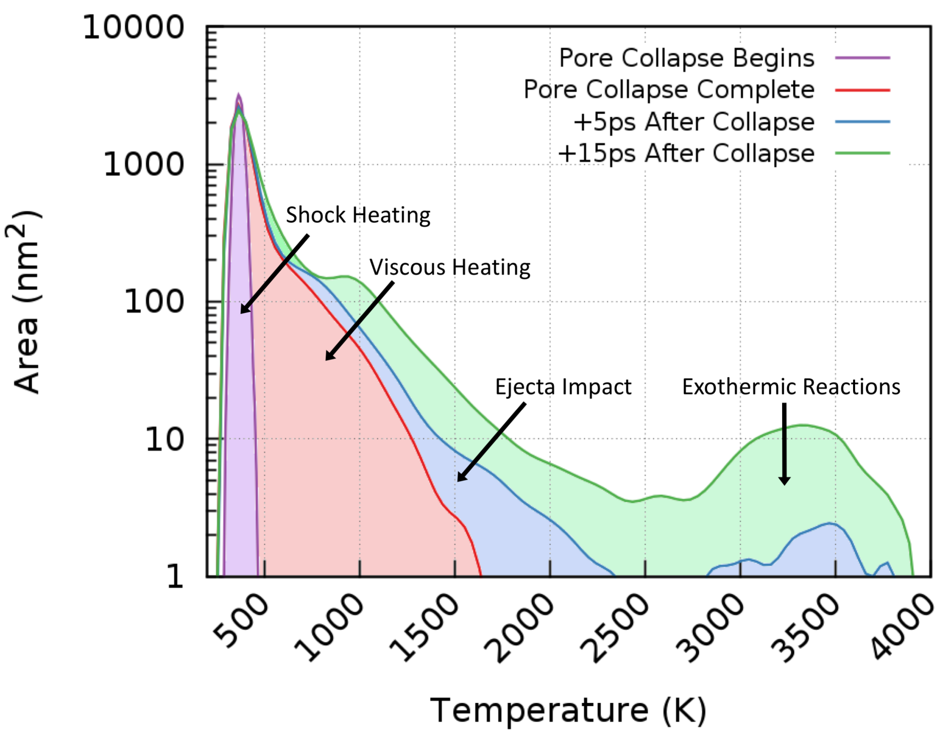
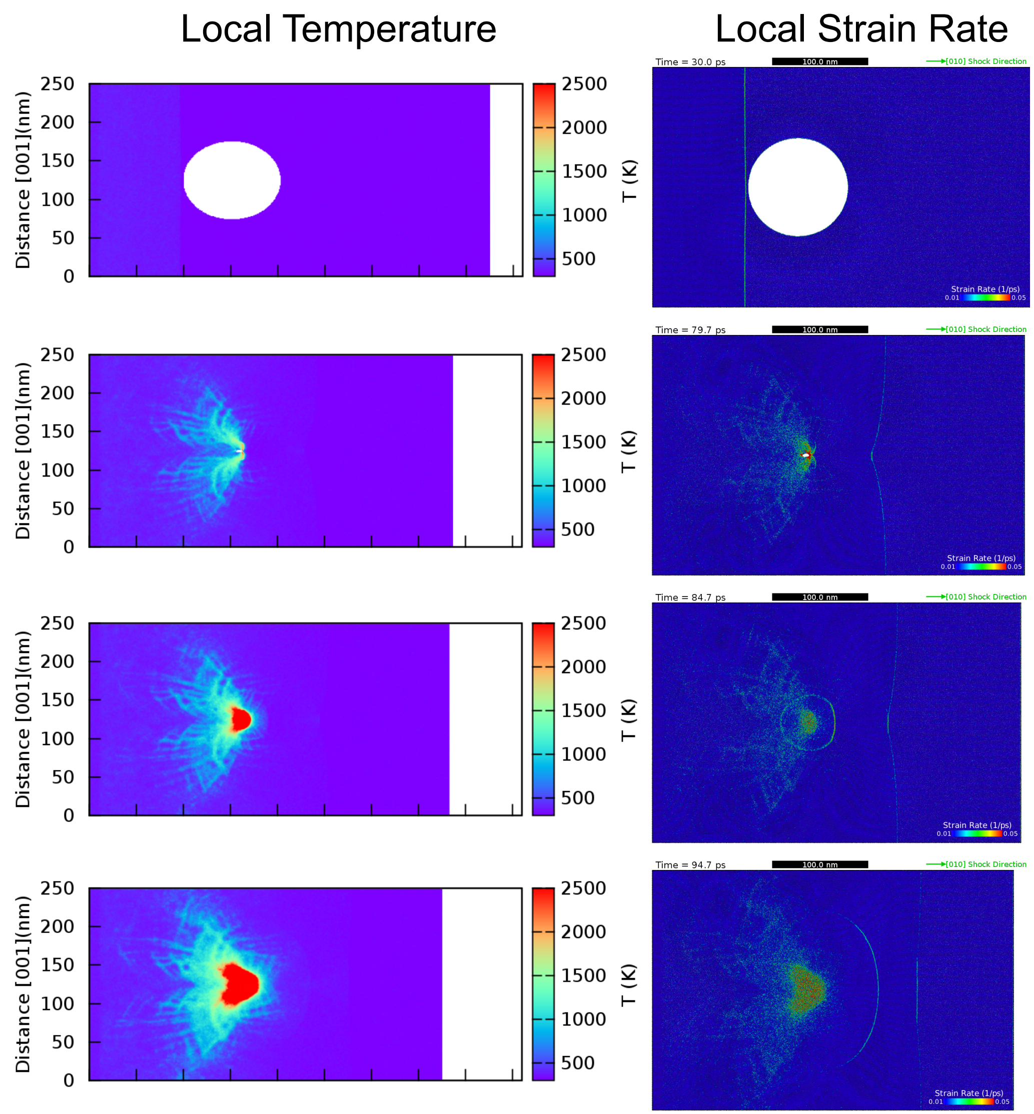
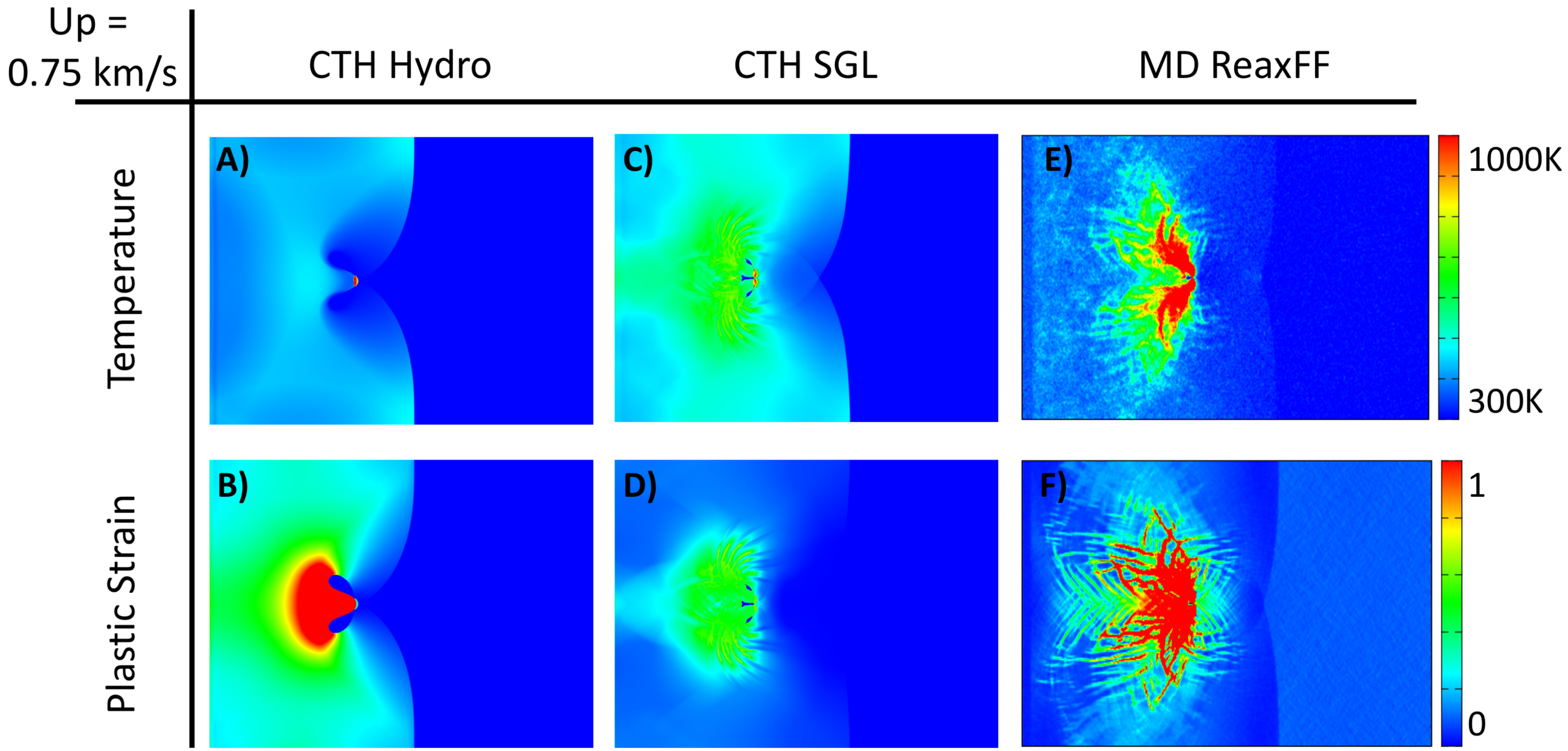




CTH Strain Rate Dependent Model – Results

- MD results were used to train a strain rate dependent strength model in CTH, significant improvement over previous model forms



Conclusions and Path Forward

- By training a strain-rate dependent CTH strength model for HNS to reproduce MD predicted viscoplastic shock response, we have been able to obtain consistent pore collapse behavior.
- Initiation behavior as a function of this viscoplastic character is an avenue for future work on both the MD and CTH codes (+ training on reaction paths).