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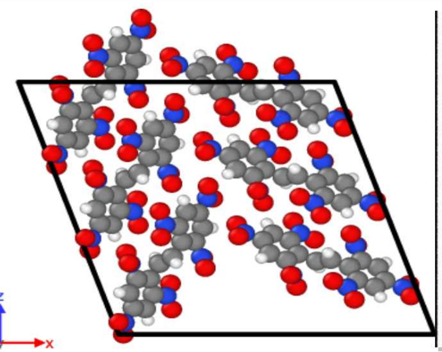
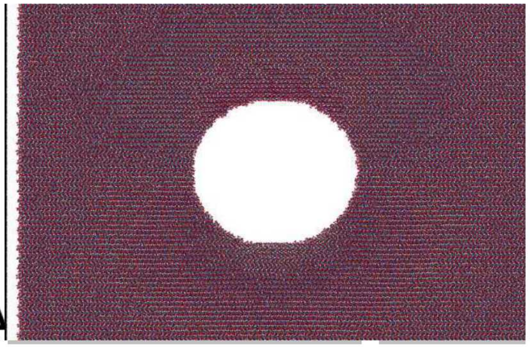
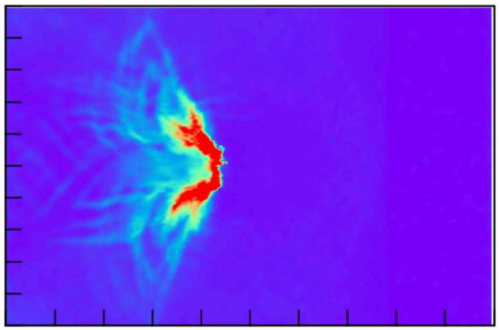
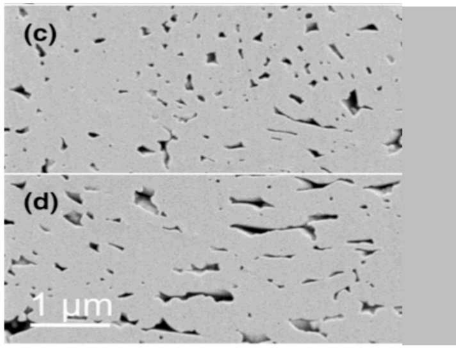

Shock Waves and Defects in Energetic Materials, a Match Made in MD Heaven

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APS March 2017 Meeting

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

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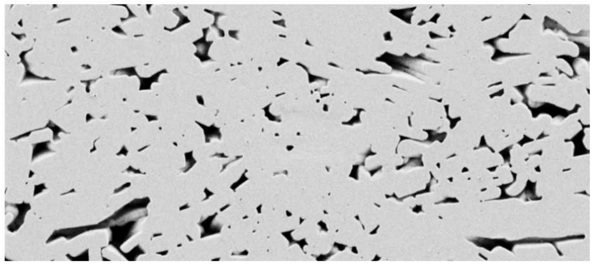
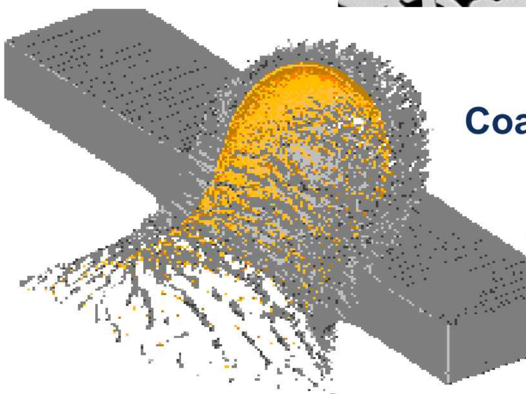
Mesoscale Materials Modelling

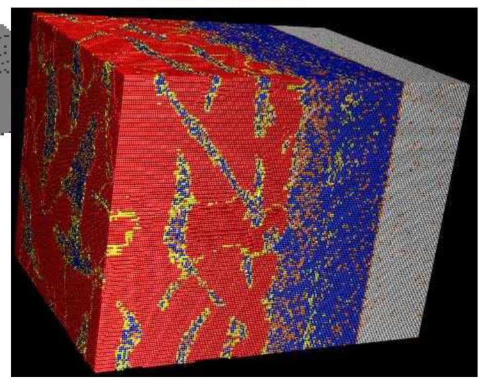


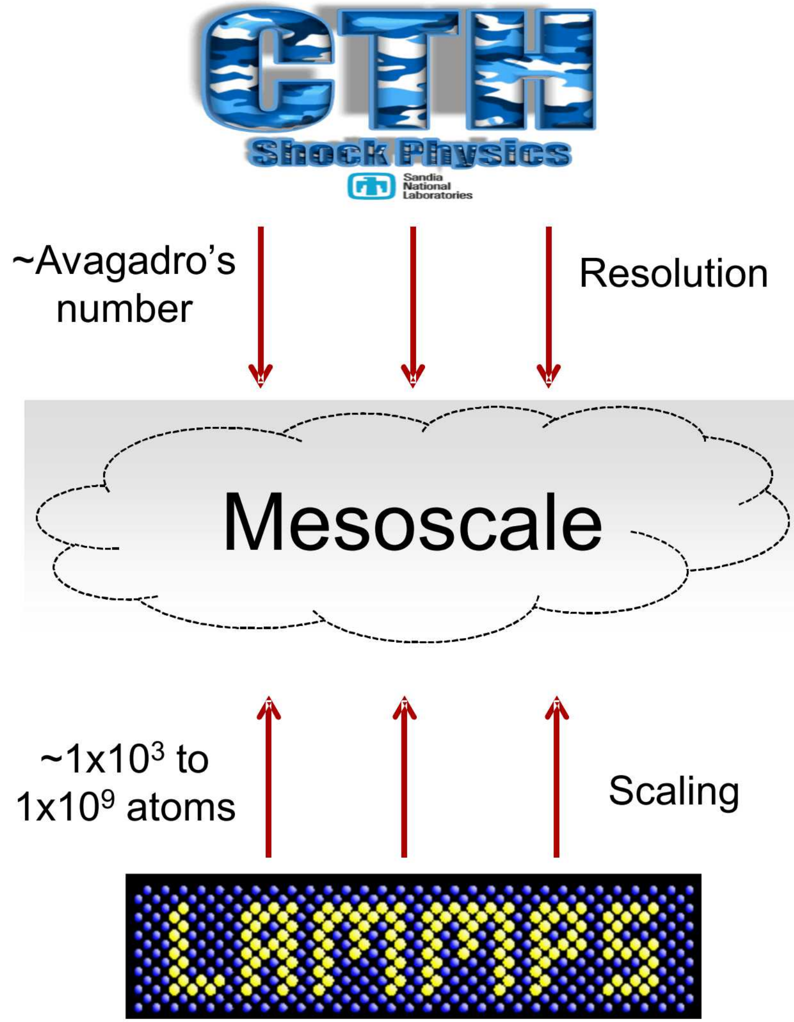
Microstructure



Coarse grain

Atomistic

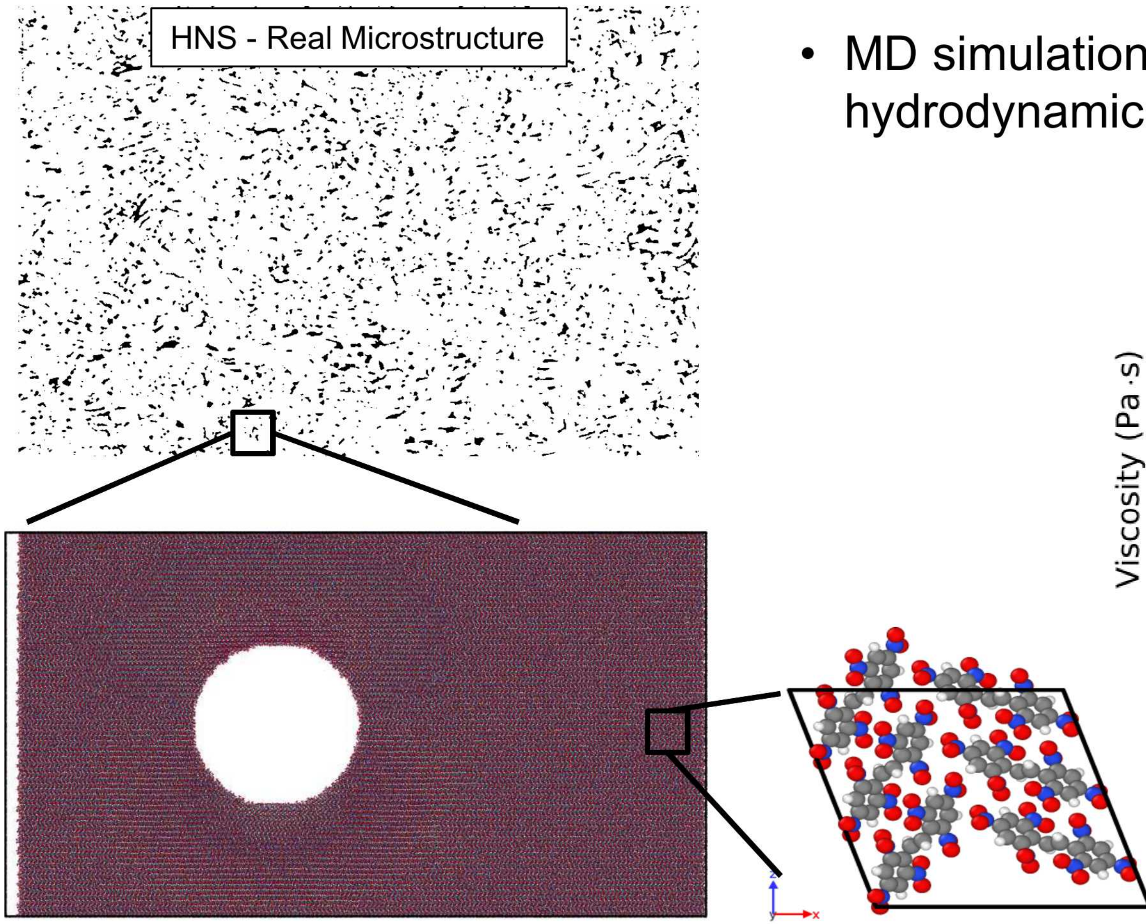




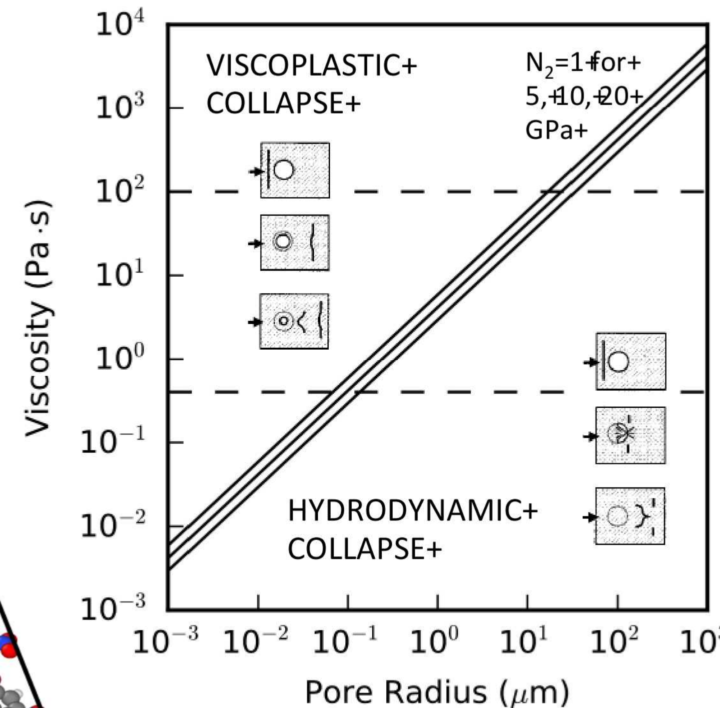
- Generally challenging problems involving physics at many length/time scales
- Shock to detonation transition in energetics fits the bill of being truly "mesoscale"

But Why Molecular Dynamics?

- Want a predictive power that spans from atoms to devices

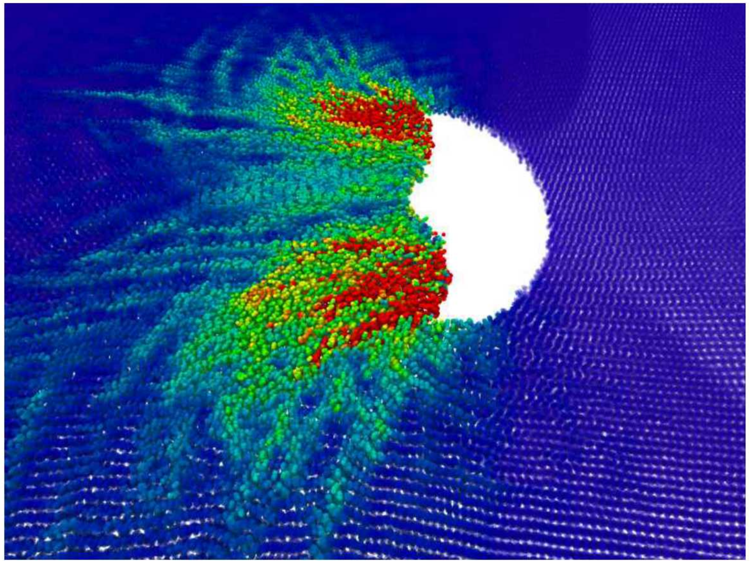


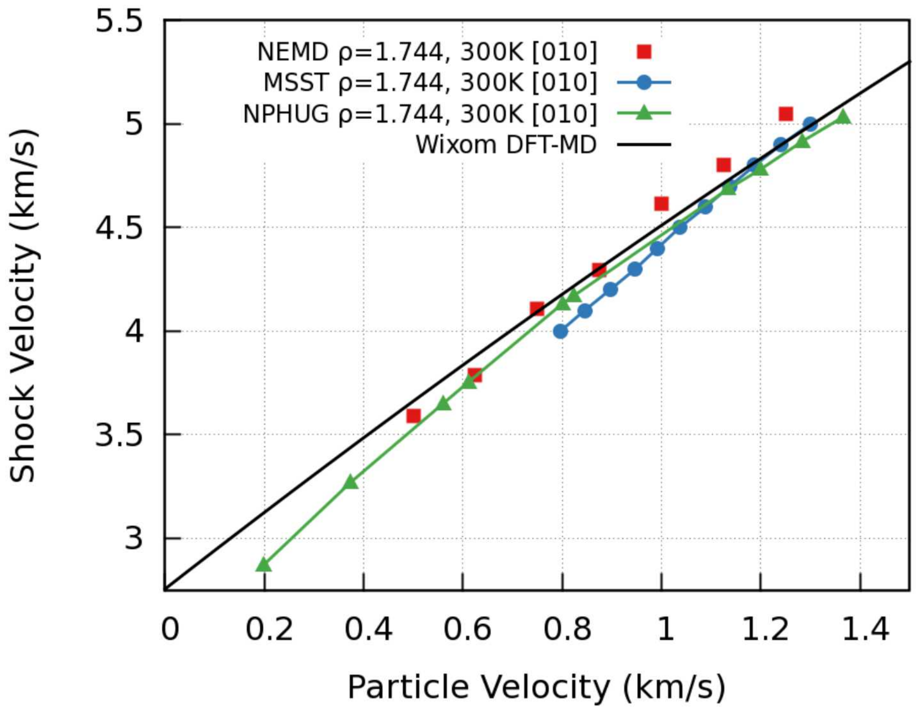
- **Results inform and train continuum models for mesoscale applications**
- MD simulations need to span the hydrodynamic to viscoplastic range

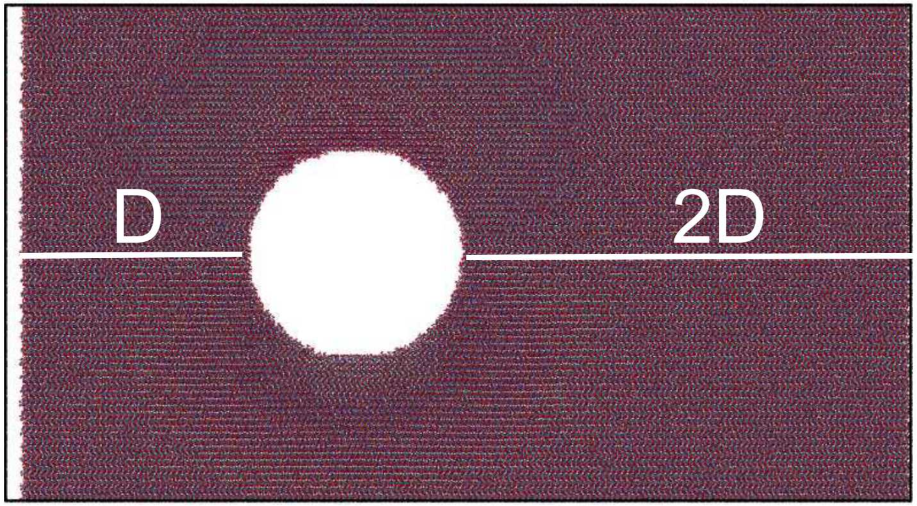


Validation of the Interatomic Potential

- Need to define a test geometry for both codes (LAMMPS, CTH)
- Small adjustments made to ReaxFF-lg potential for HNS



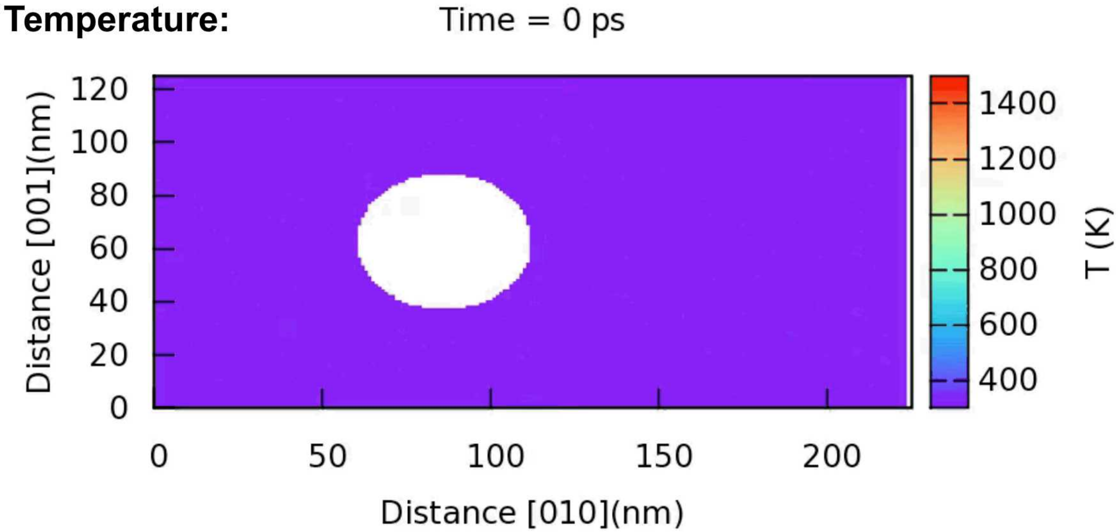




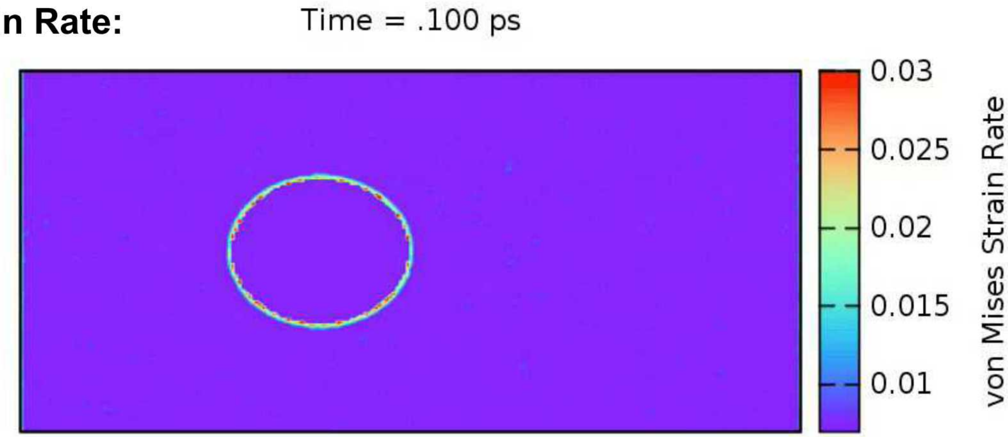
Shock to Initiation, Deflagration

- Detailed chemistry is incorporated in these MD potentials, hot spot evolution is captured naturally.
- Current computing capabilities for ReaxFF within LAMMPS is ~10^8 atoms, which is 1μm by 0.5μm of HNS
- KOKKOS-Reax/c package circumvents memory overflow errors and makes the code portable to hybrid architectures

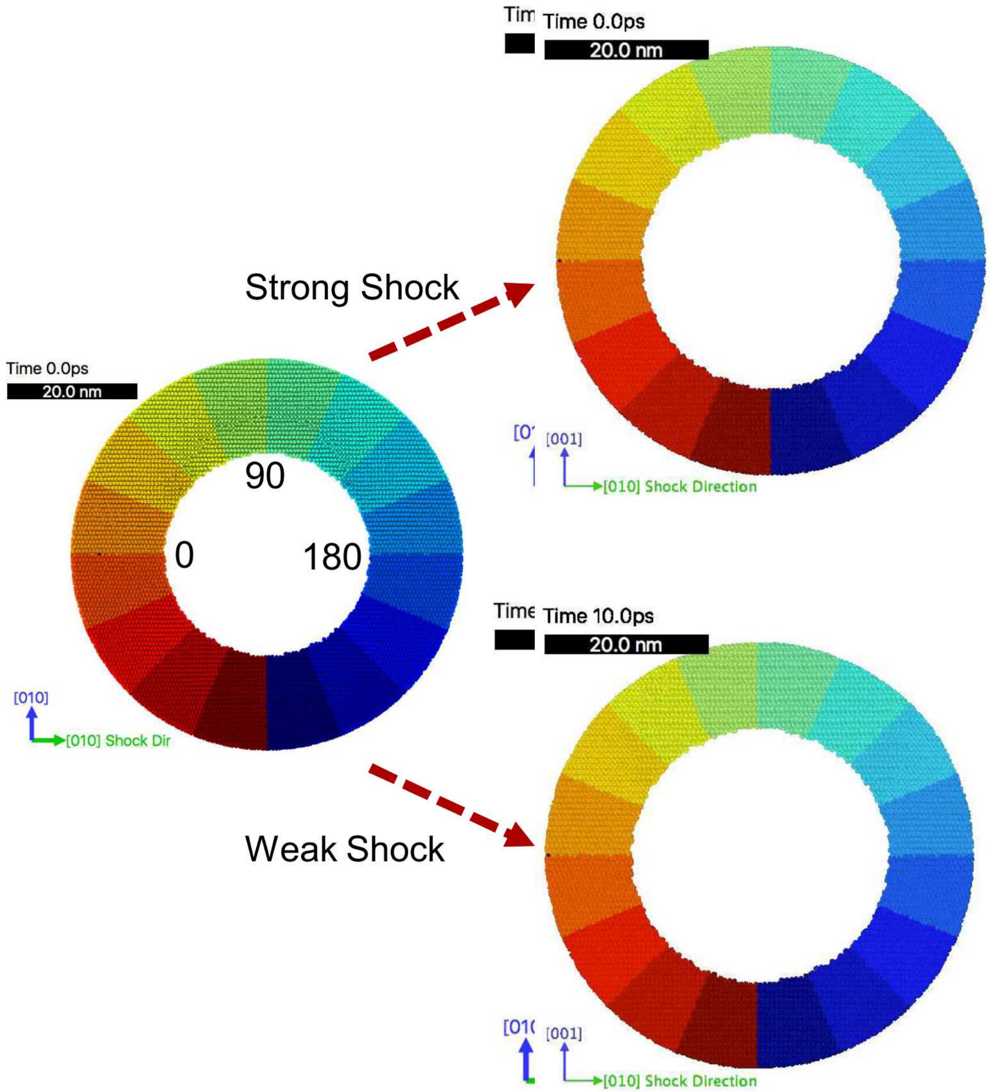
Temperature:

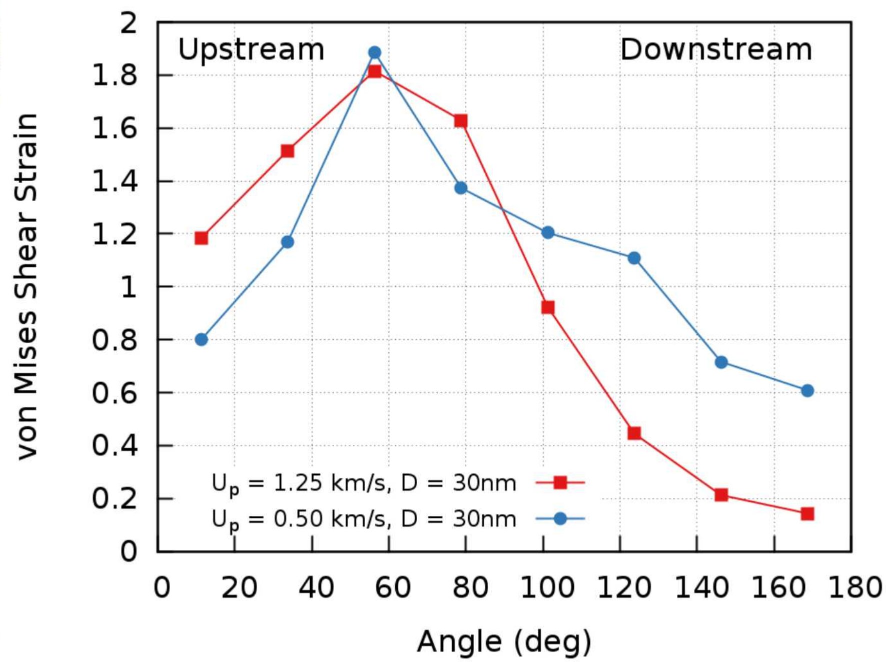


Strain Rate:



Hydrodynamic vs. Viscoplastic Pore Collapse



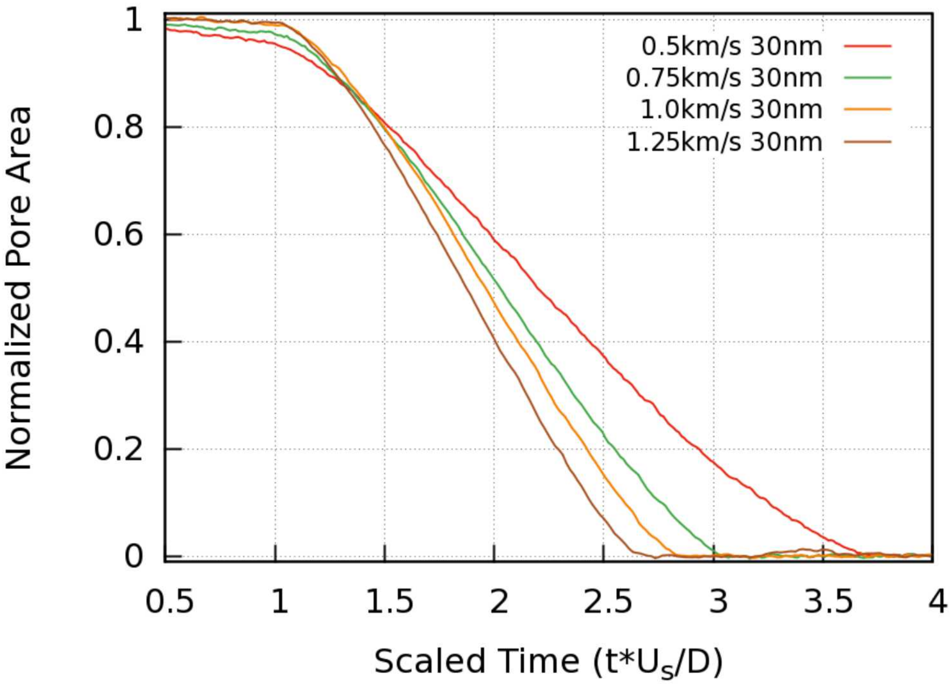


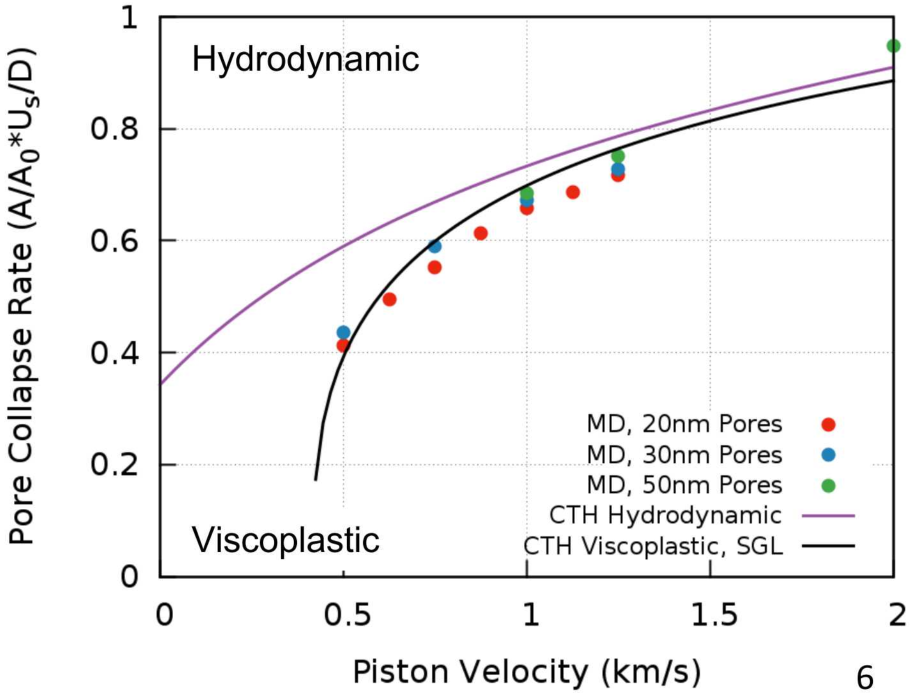
OVITO : A. Stukowski, *Modelling Simul. Mater. Sci. Eng.* 18 (2010), 015012

Connection to the Continuum Scale

- Pore size has a weak effect on pore collapse behavior, at least in the MD accessible range which for us was up to 0.25µm ($1.3 \cdot 10^8$ atoms).

- CTH strength model is fitted based on the MD prediction of pore collapse rate





Strain Rate Dependent Model – Steinberg and Lund (1989)

- 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 of $G_0 = 5686$ MPa
  - Neglect work hardening but assume $Y_A = 140$ MPa
  - Assume linear variation of the Grüneisen parameter, $\gamma_0 = 1.625$
  - Melt temperature $T_{m0} = 588$ K

SGL 4 DOF Best Fit

$C_1 = 2.025 \times 10^{11}$ s^{-1}

$C_2 = 11.25$ dyne-s/cm^2

$Y_P = 1114$ MPa

$U_K = 0.1358$ eV

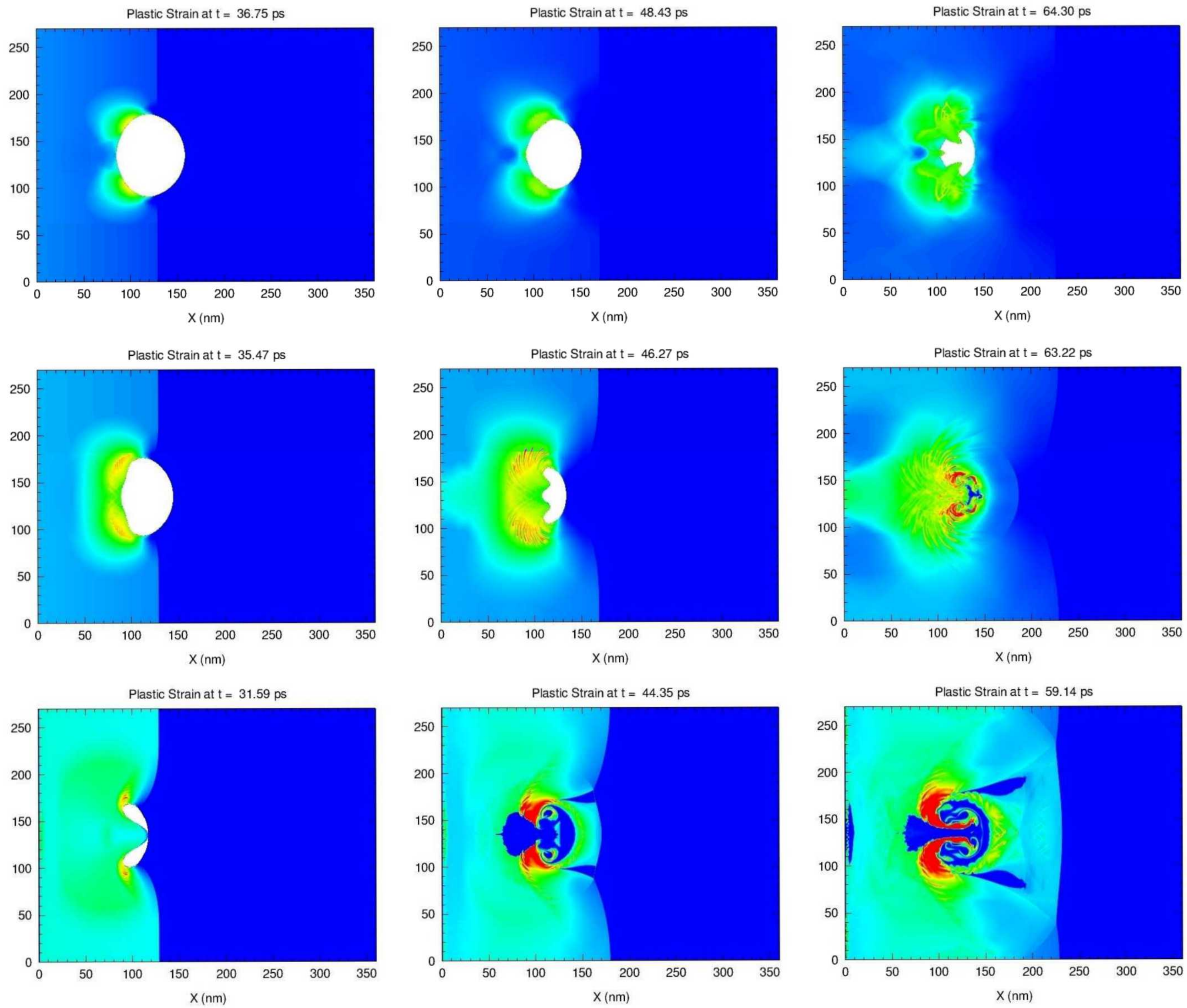
Yield Strength:	$Y = \{Y_T(\dot{\varepsilon}_p, T) + Y_A f(\varepsilon_p)\}$
Shear Modulus:	$G(P,T) = G_0$
Work Hardening:	$Y_A f(\varepsilon_p) = Y_A \leq Y^*_{max}$
Thermal Activation: (Implicit Equation)	$\dot{\varepsilon}_p = \left\{\frac{1}{C_1} exp\left[\frac{2U_K}{kT}\left(1-\frac{Y_T}{Y_P}\right)^2\right] + \frac{C_2}{Y_T}\right\}^{-1}$ $\quad Y_T \leq Y_P$
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:	$\gamma = \gamma_0/(1 + \mu)$

Strain Rate Dependent Model – Results

0.6 km/s

1.0 km/s

2.0 km/s



Viscoplastic Response

Hydrodynamic Response

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.