SAND2012-7690C

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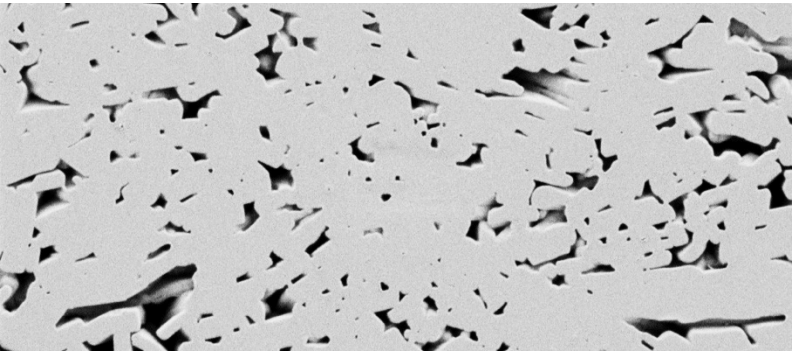
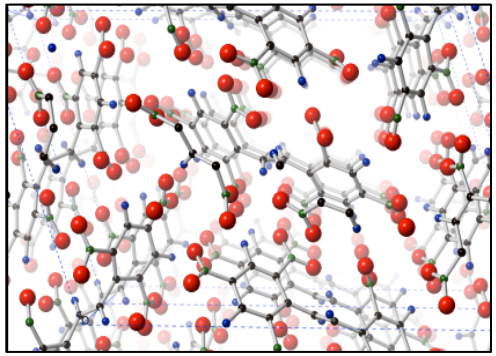
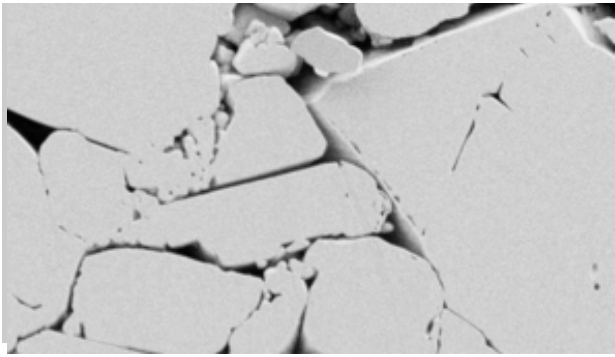

First-principles prediction of equations of state for molecular crystal explosives.

Ryan R. Wixom

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Science-based understanding of chip-slapper detonators.

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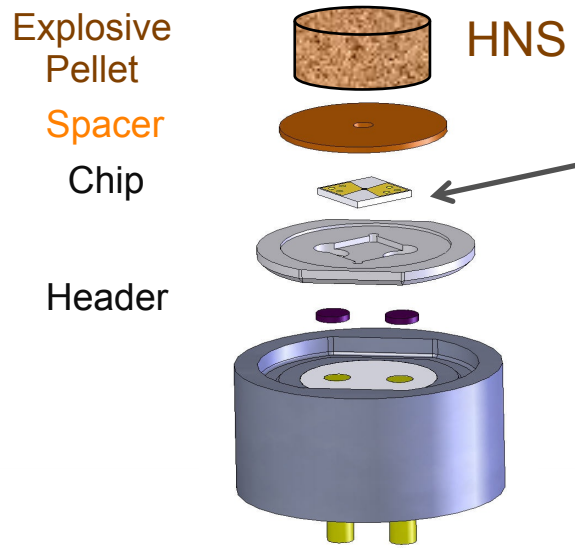
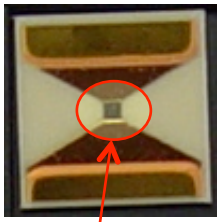
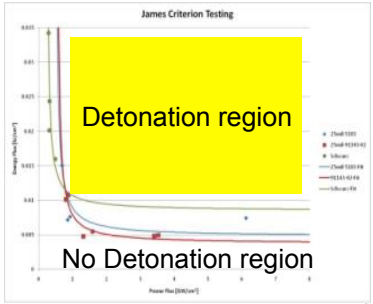




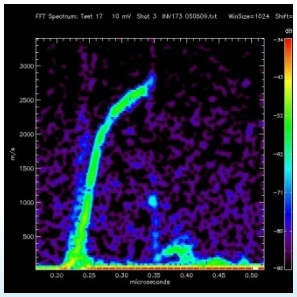
Bridge/Flyer

Empirical Go/NoGo

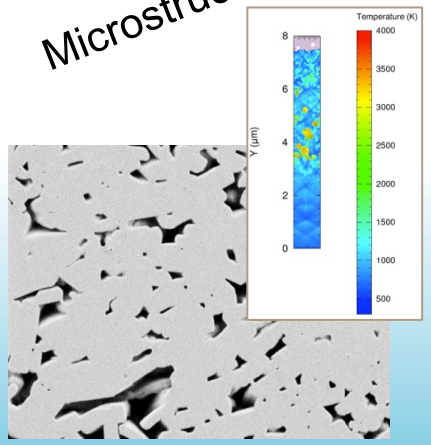


Energy flux vs. power flux of slapper for HNS-FP initiation

Microstructure Characterization

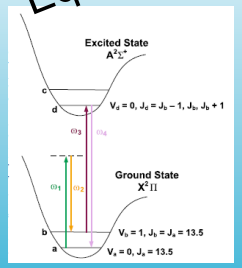


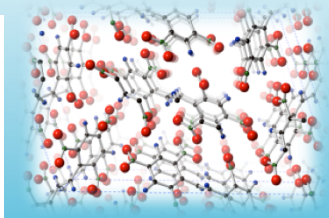
Velocimetry of flyer



X-section of HNS pellet, and grain-scale hydrocode simulation

Equation of State / Chemistry





HNS crystal structure

Time scale: 10^{-12} – 10^{-9} s

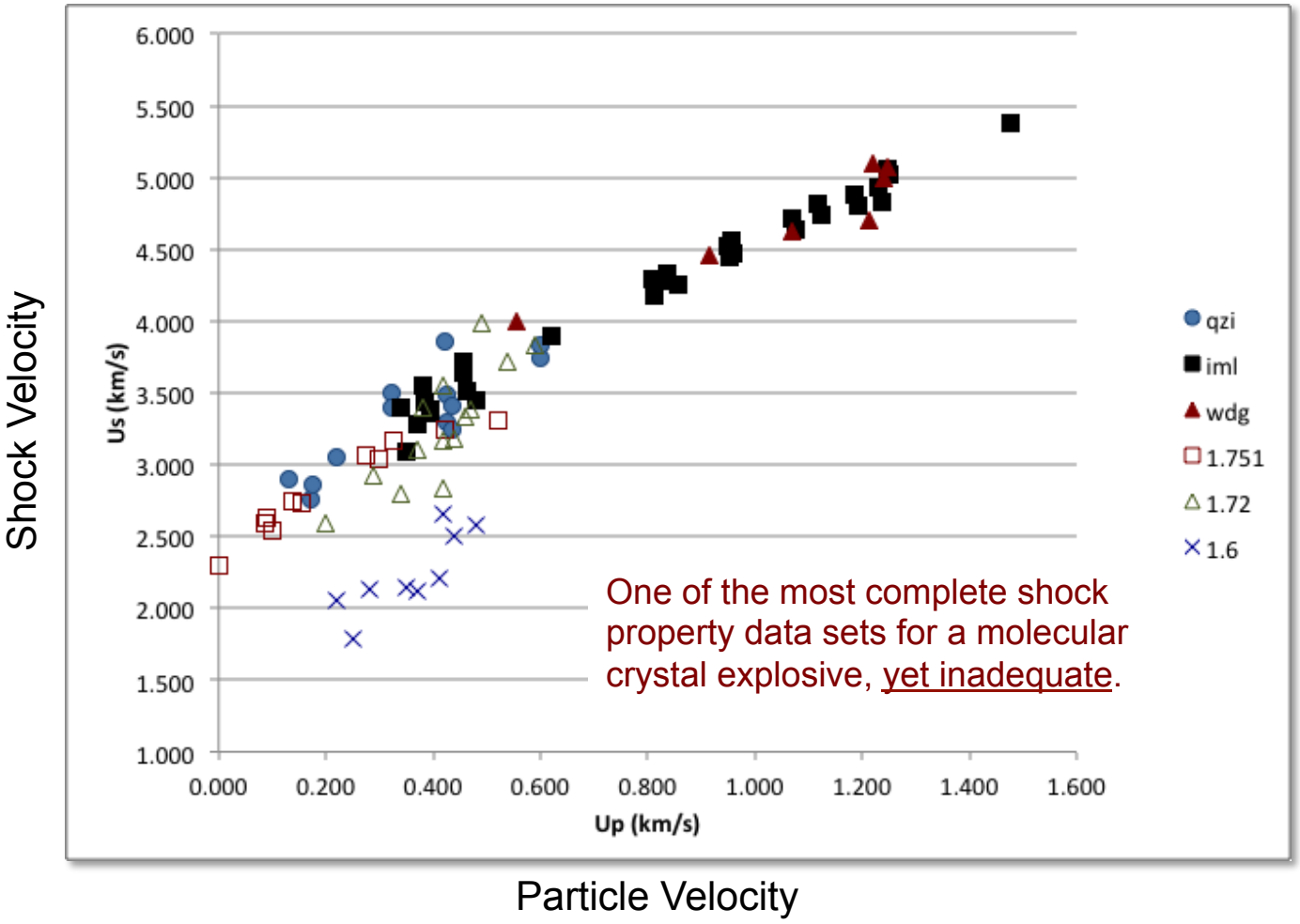
Technology

Science

Atomic | Molecular | Microscale | Mesoscale | Continuum

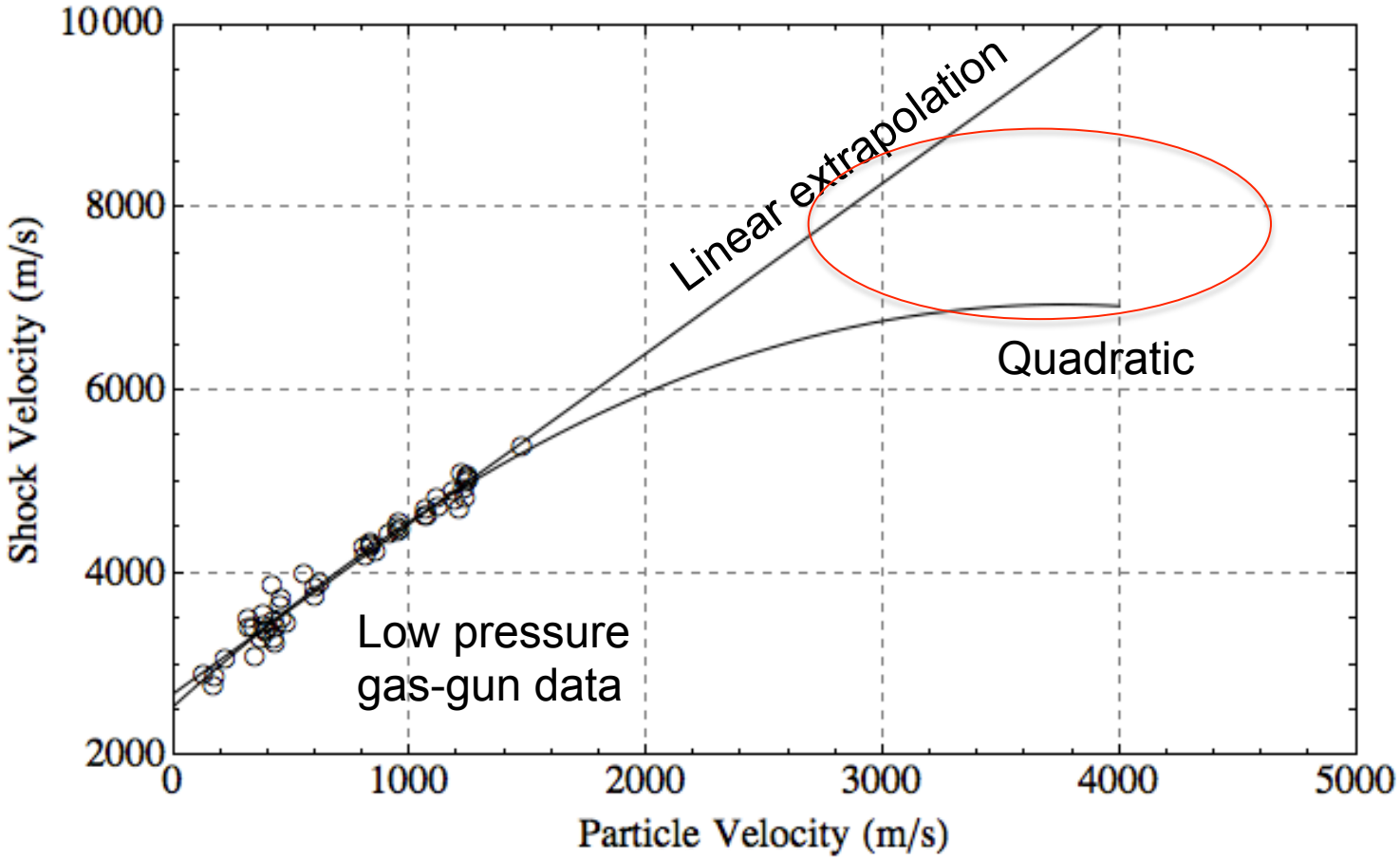
Experimental EoS for explosives

PETN Shock Hugoniot data from the LASL shock handbook (Marsh)

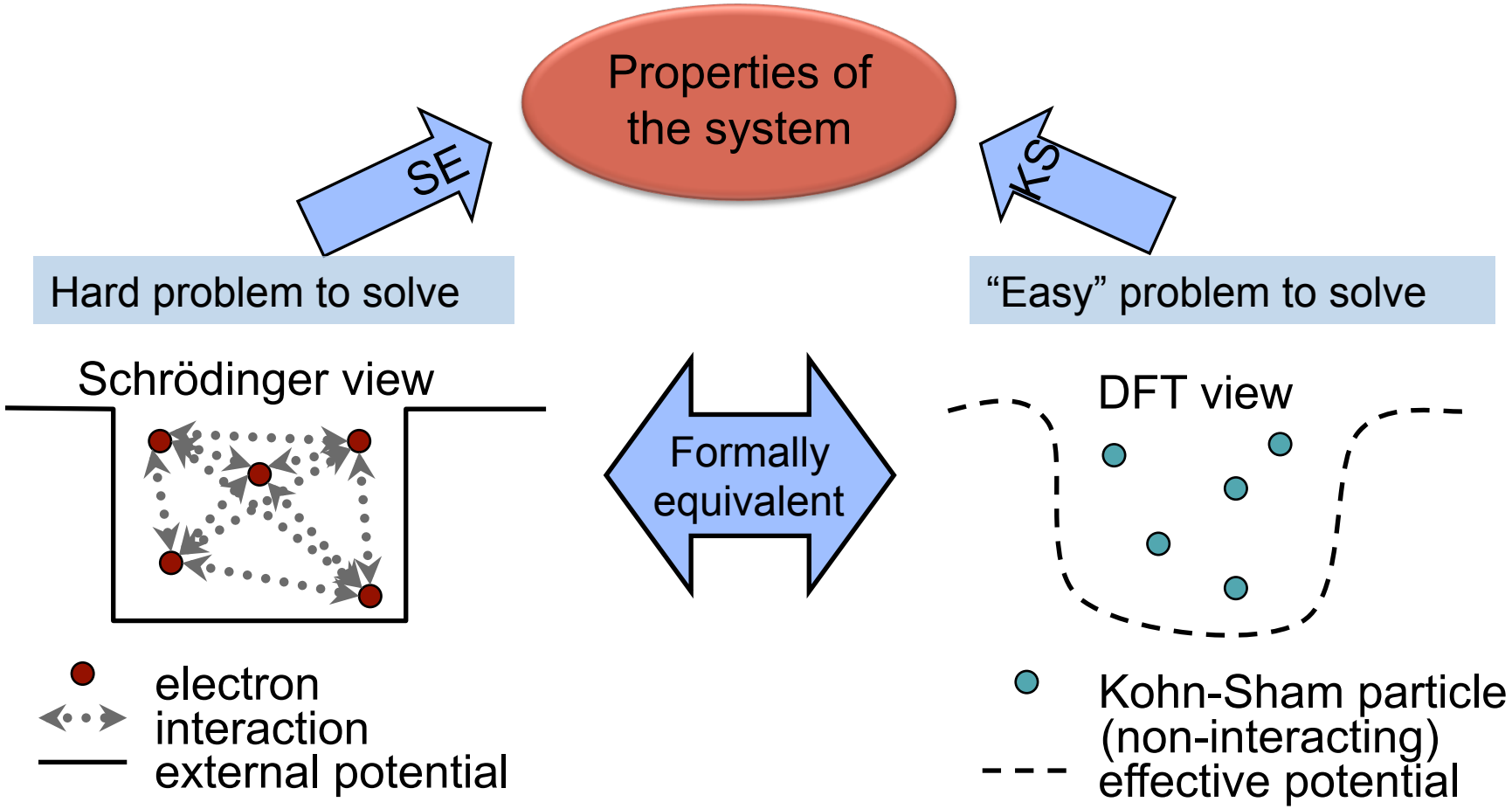


1) Not a straight line. 2) No information about temperature. 3) Data is usually low pressure.

Extrapolation = Bad.



Density Functional Theory (DFT) and XC functionals:



$$v_{eff}(\boldsymbol{r}) = v(\boldsymbol{r}) + \int \frac{n(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}\, d\boldsymbol{r}' + \frac{\delta E_{xc}[n(\boldsymbol{r})]}{\delta n(\boldsymbol{r})}$$

AM05, LDA, GGA, Meta-GGA, Hybrids

Molecular Dynamics (MD):

10,000 time-steps

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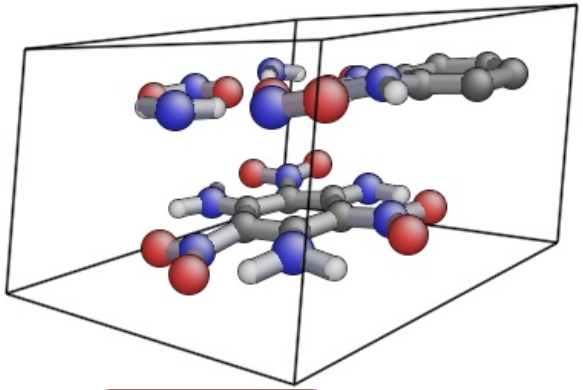
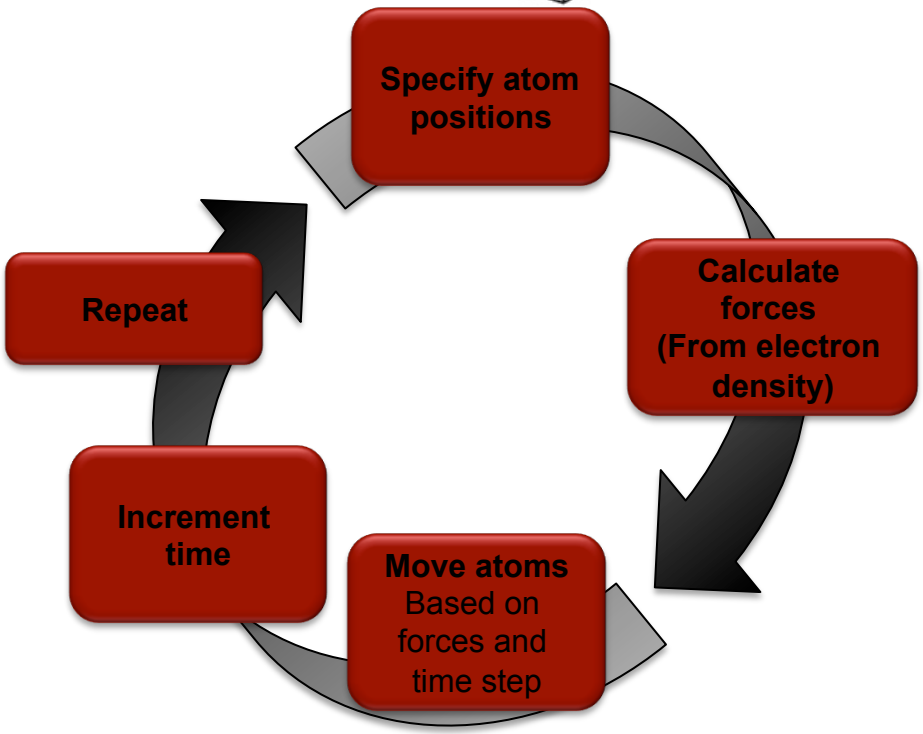
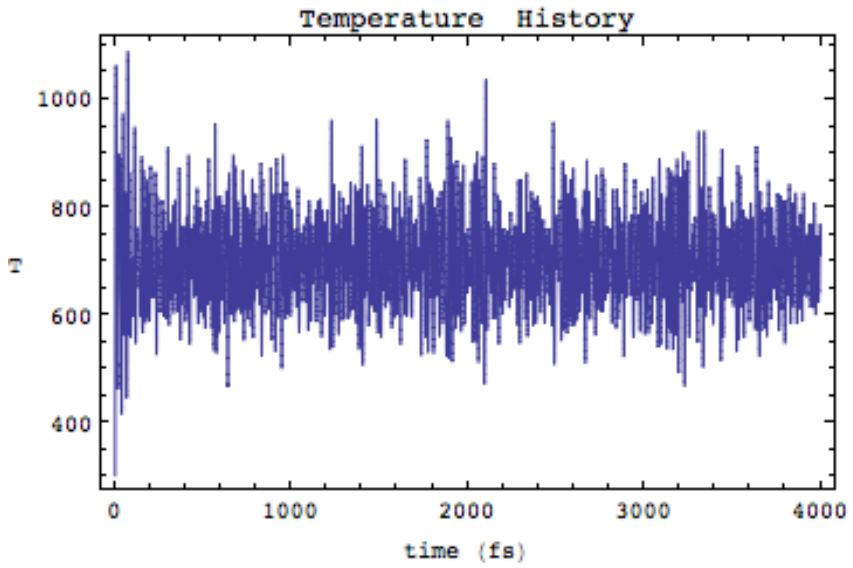
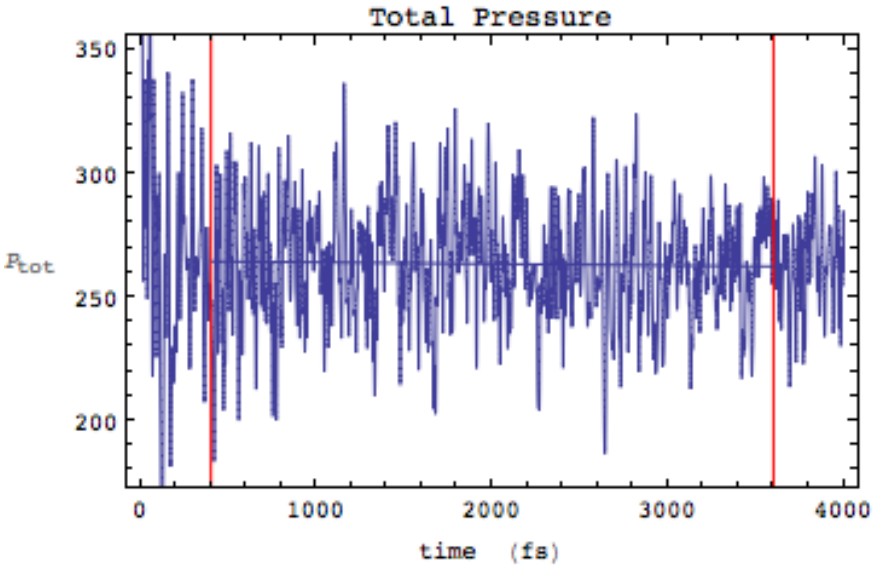
TATB
V/Vo = 0.729
T = 700 K

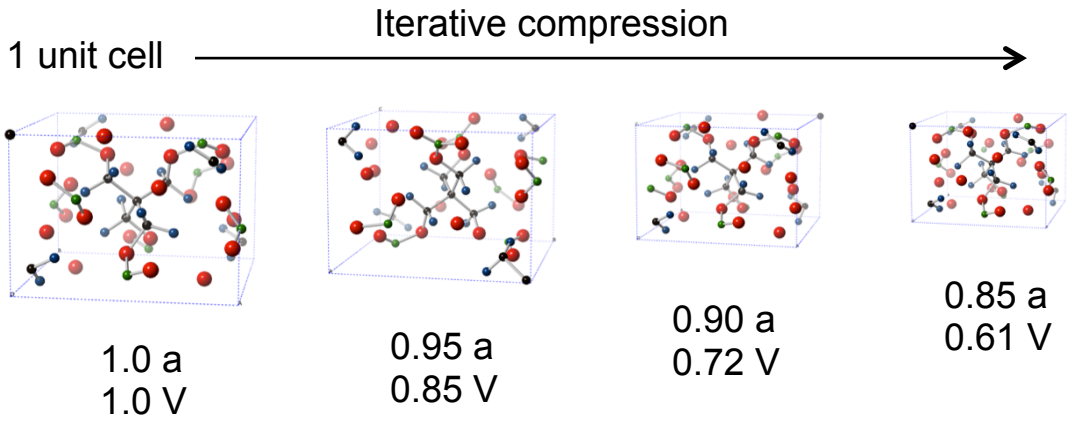


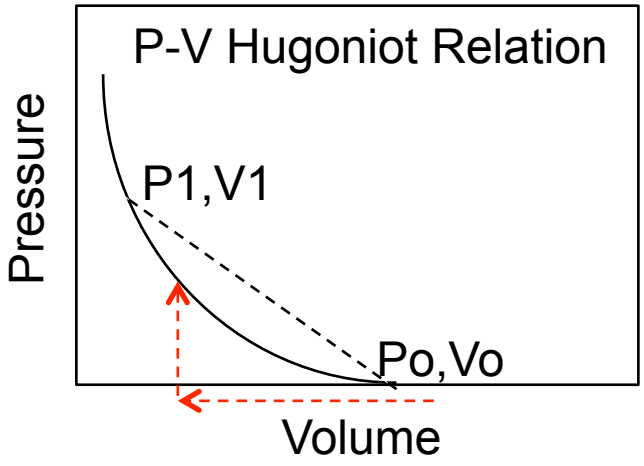






Finding the Hugoniot





Rankine-Hugoniot Relations:

Mass:

$\rho_o D = \rho_1 (D - u_1)$

Momentum:

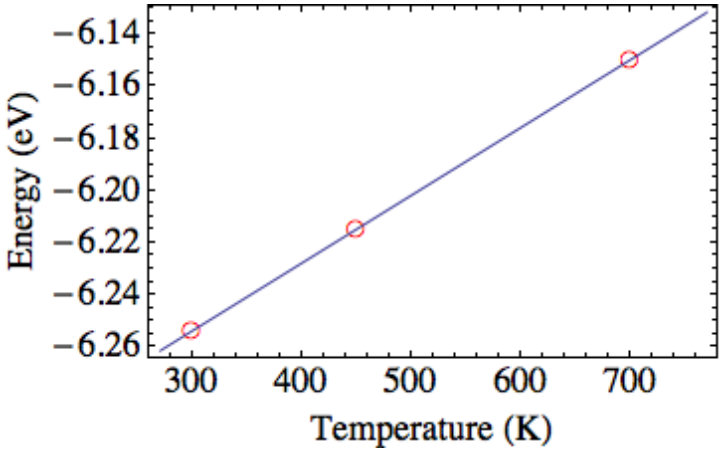
$P_1 = \rho_o D u_1$

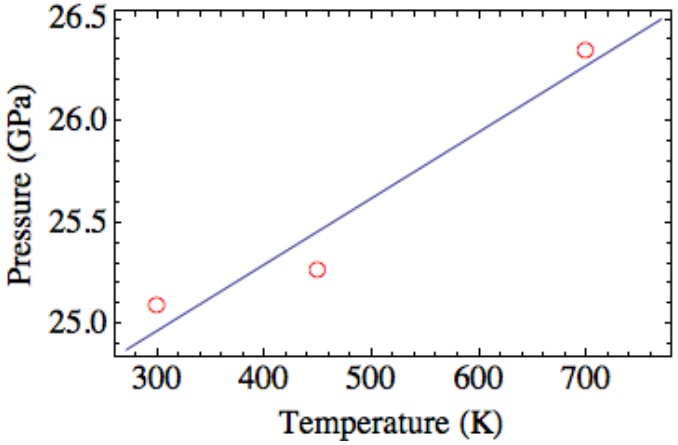
Energy:

$E - Eo = \frac{1}{2}(P + Po)(Vo - V)$

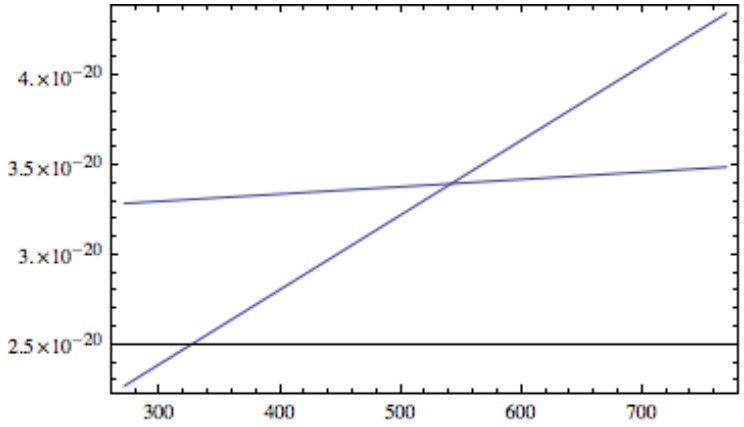
Key Point: jump conditions are only valid on the Hugoniot

Finding the Hugoniot:





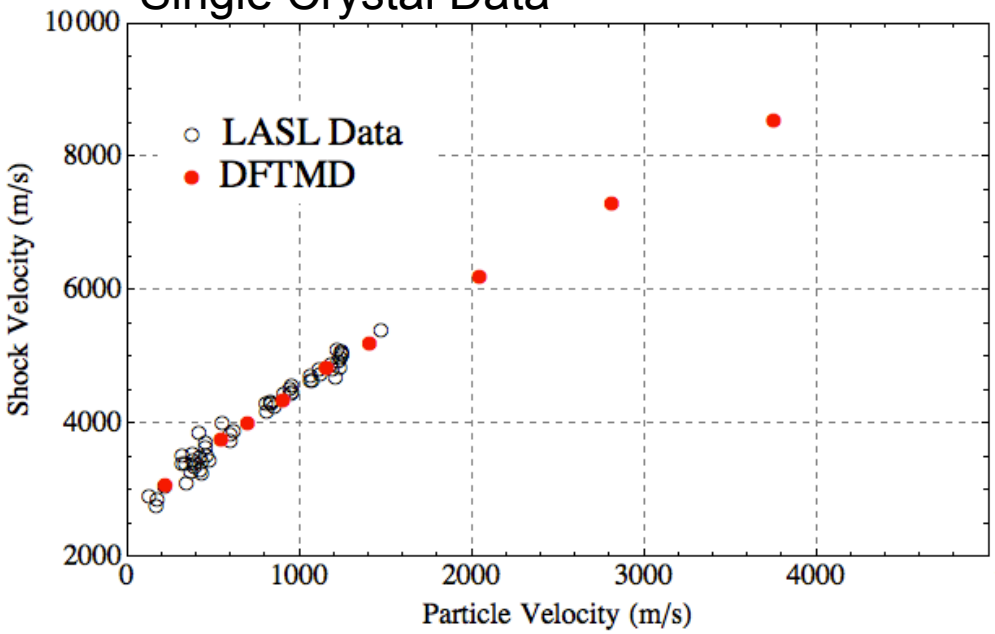
$$E - E_o = \tfrac{1}{2}(P + P_o)(V_o - V)$$



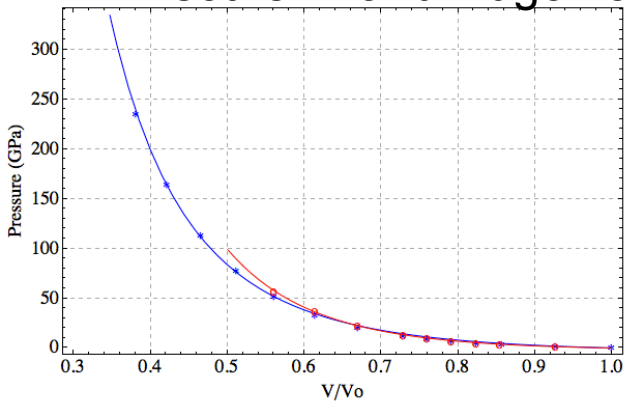
First-principles EoS for PETN

Remarkable Agreement!

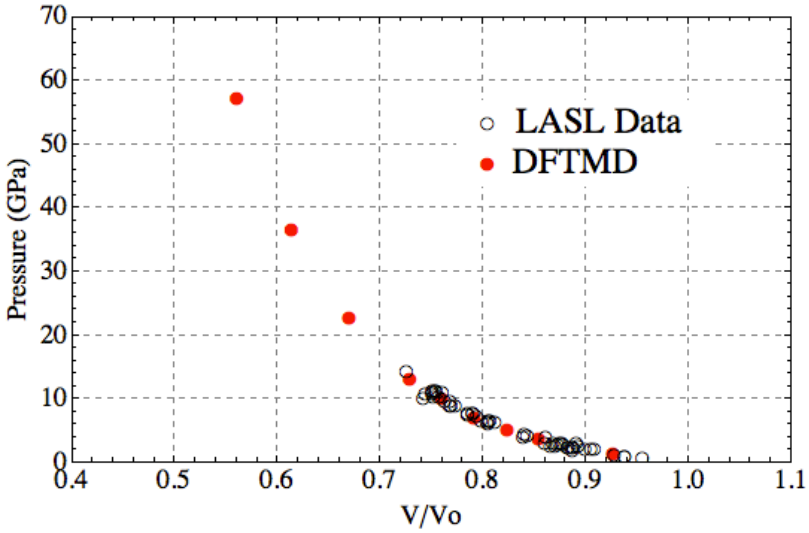
Single Crystal Data



Isotherm and Hugoniot

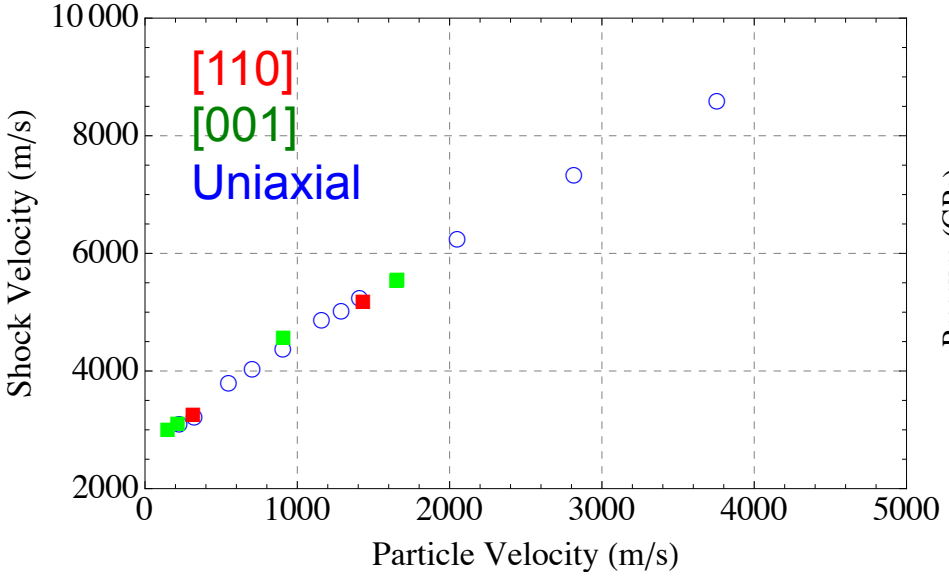


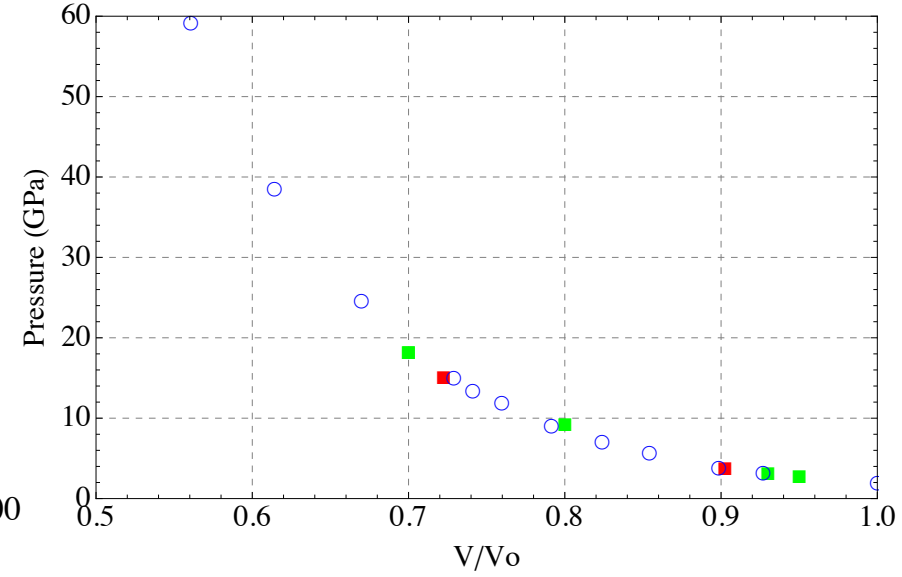
P-V Hugoniot



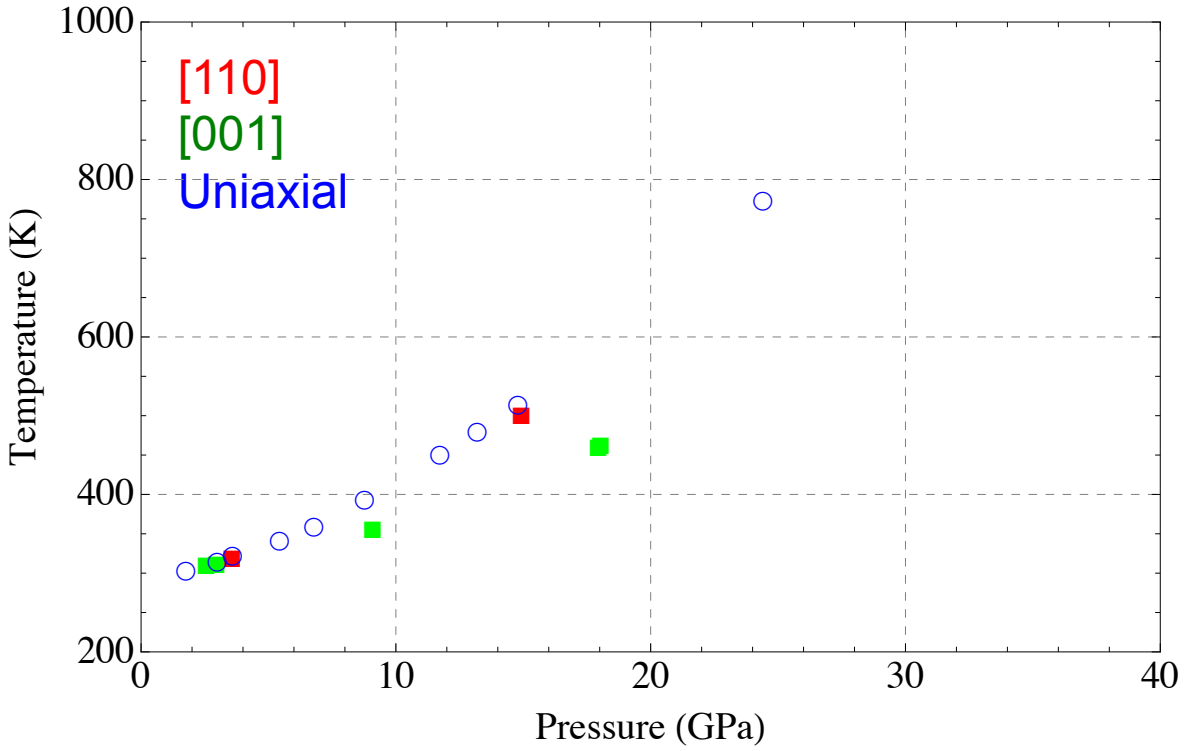
- Uniaxial compression gives similar results.
- Have all the components necessary to write a tabular EOS.

Uniaxial shocks in PETN

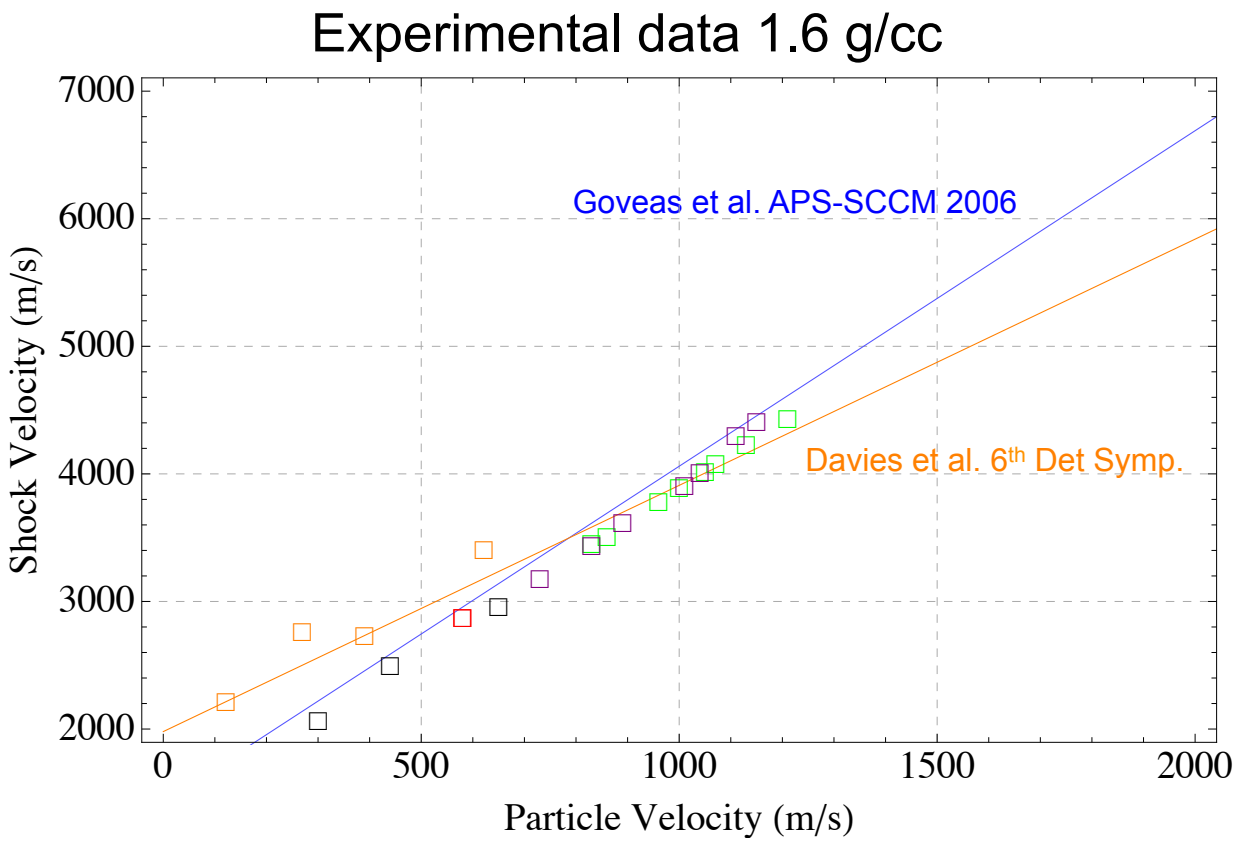




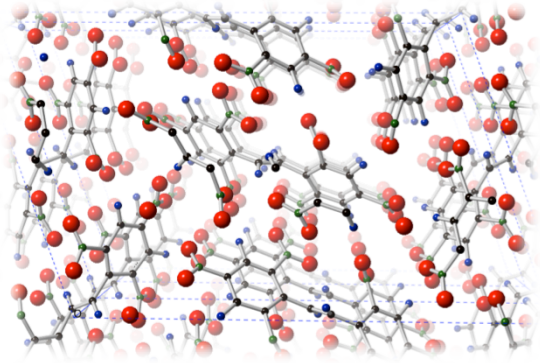
Uniaxial shocks in PETN: Different Temperatures ???

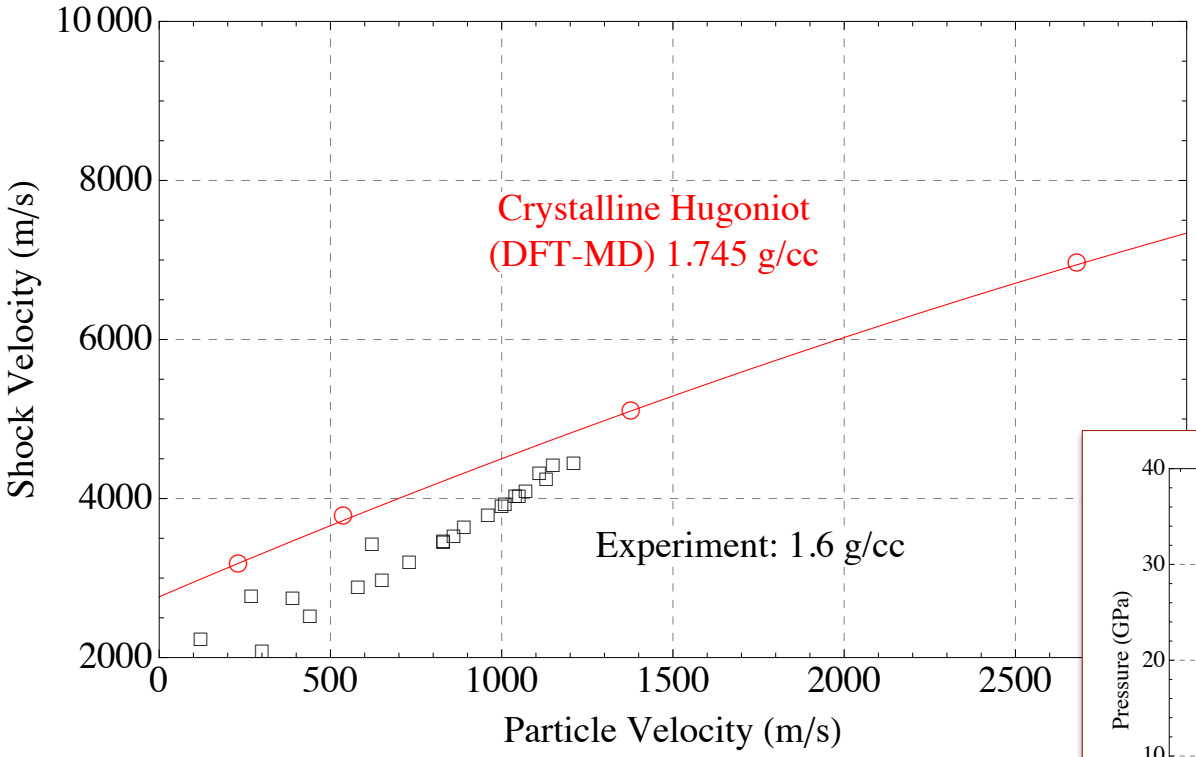


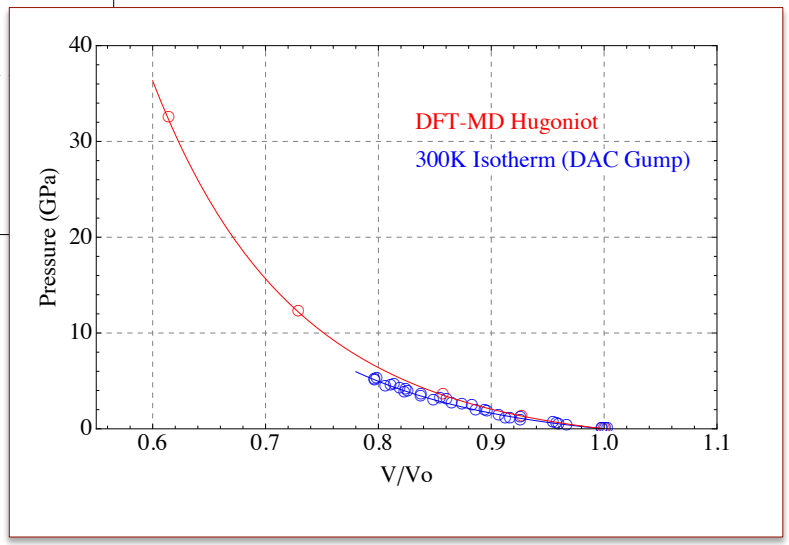
Experimental data for Hexanitrostilbene (HNS) No Crystalline data



EoS for Hexanitrostilbene (HNS) from DFT-MD







Predicted the shock response for any density?

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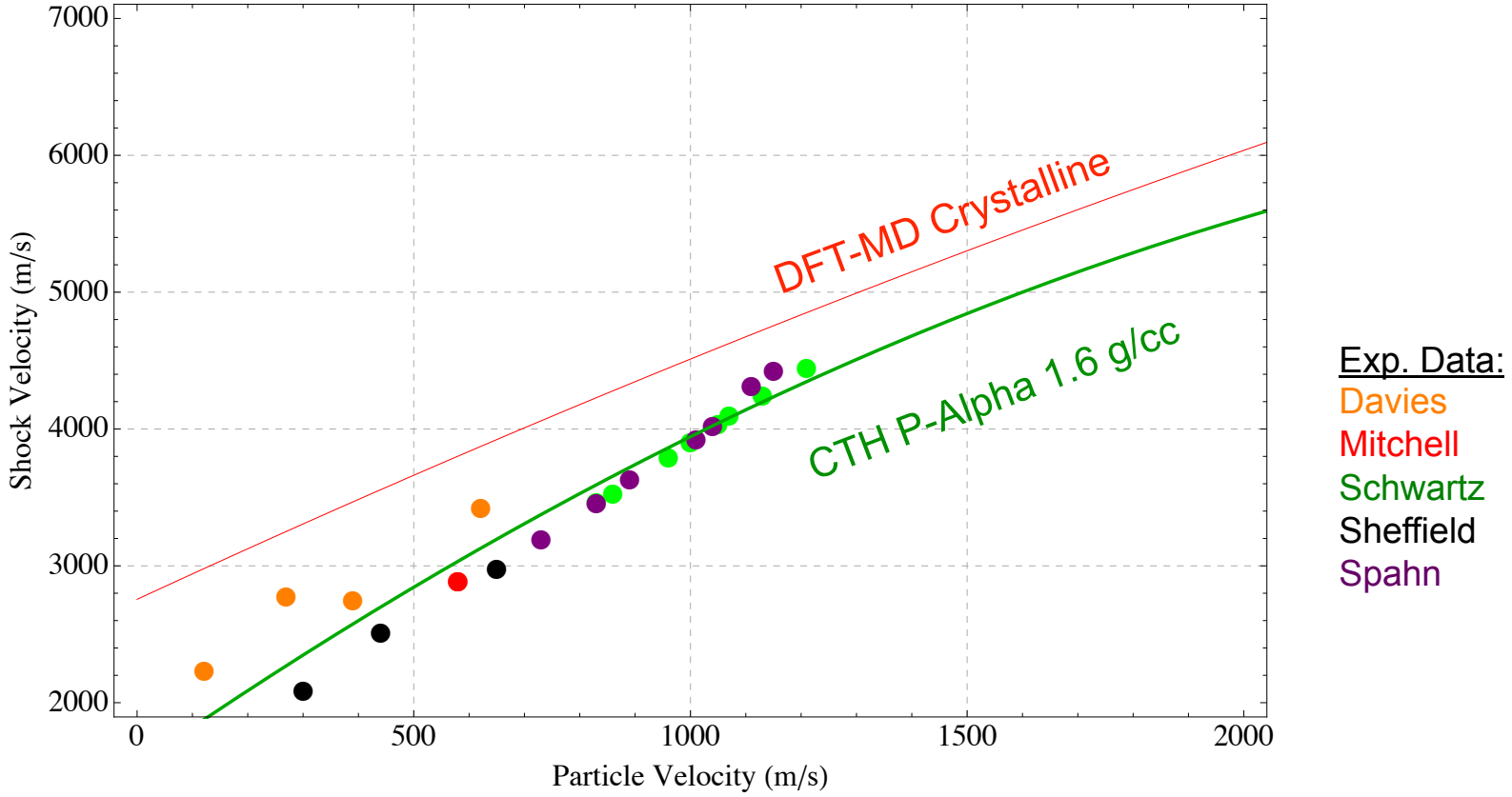
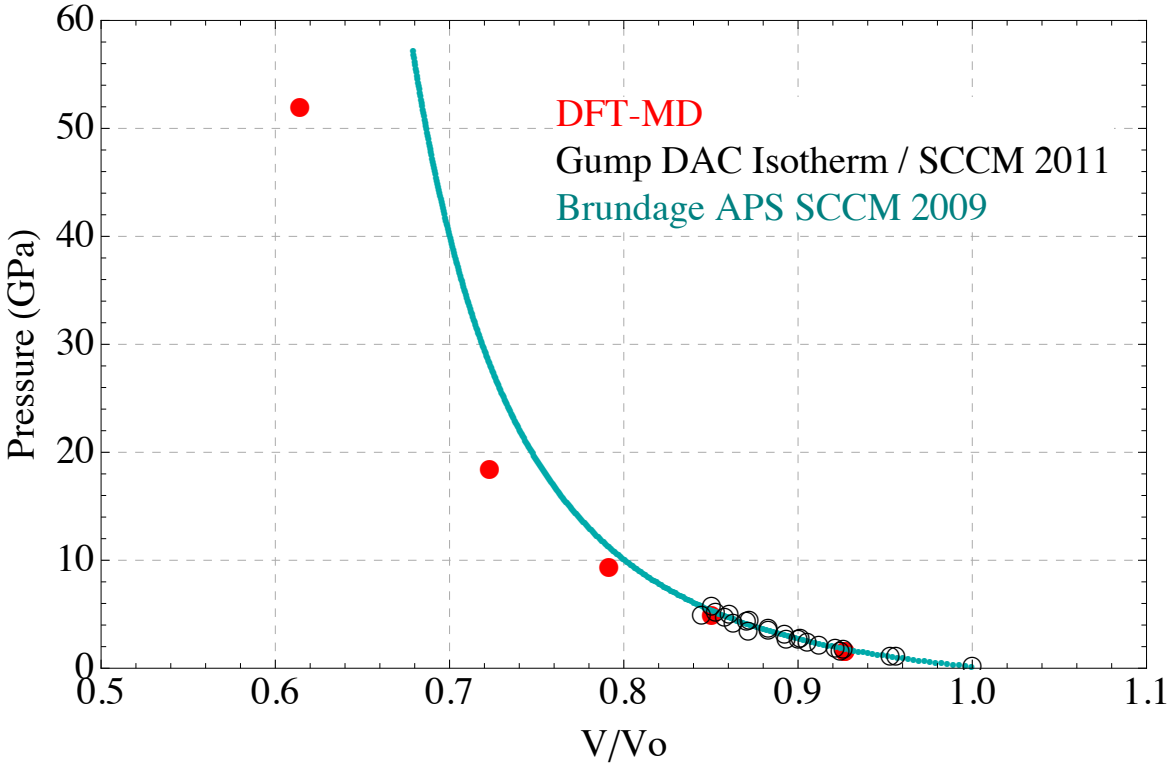
P-alpha model in CTH w/ crush pressure of 1.43 GPa [Kipp et al.]

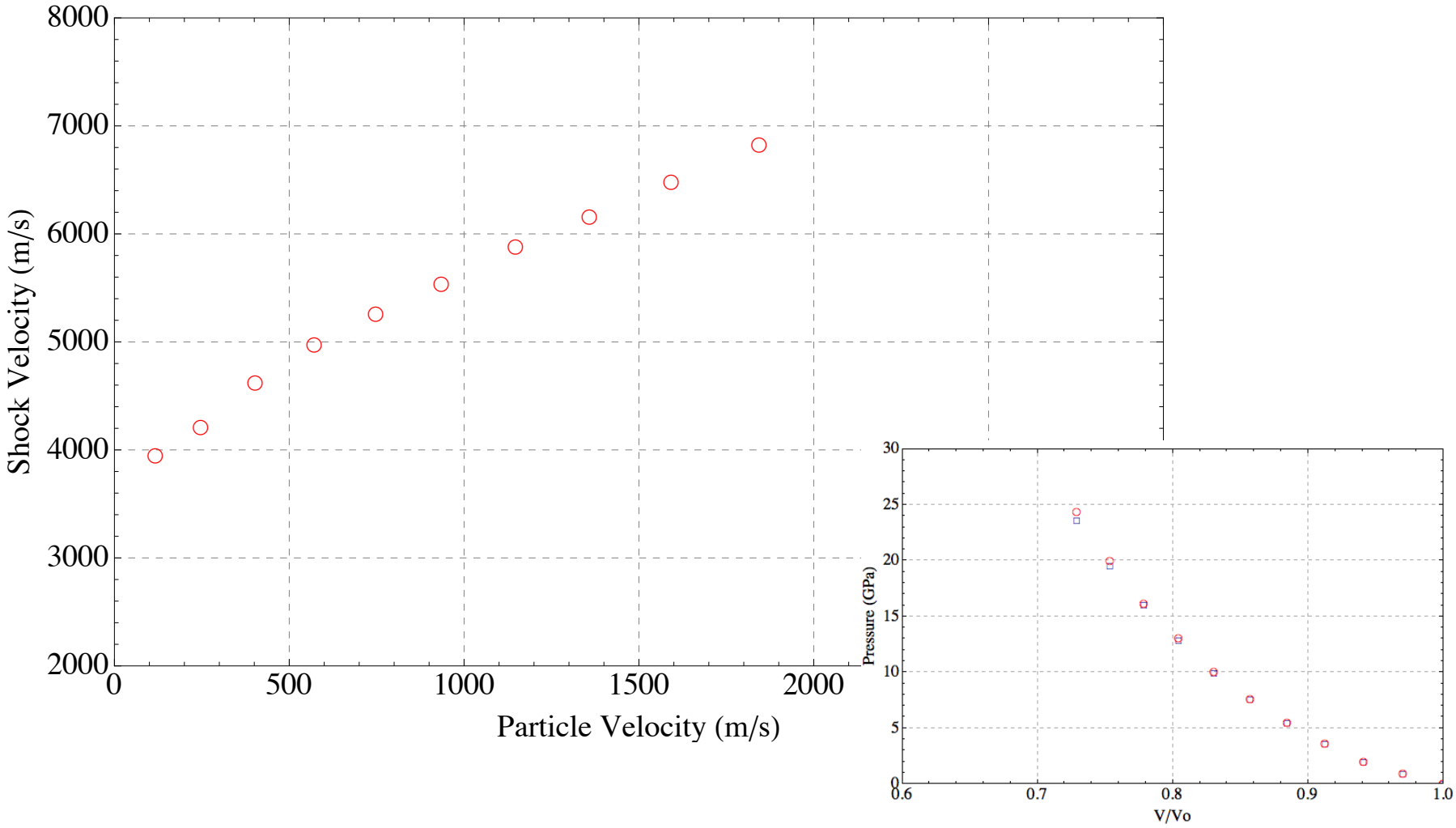
- This is great, if you want to simulate the continuum scale and you don't care about the low pressure regime.
- We have repeated this exercise with microstructure (grain-scale simulation)
- Still need a tabular EoS for accurate temperature predictions. We have all the data necessary.



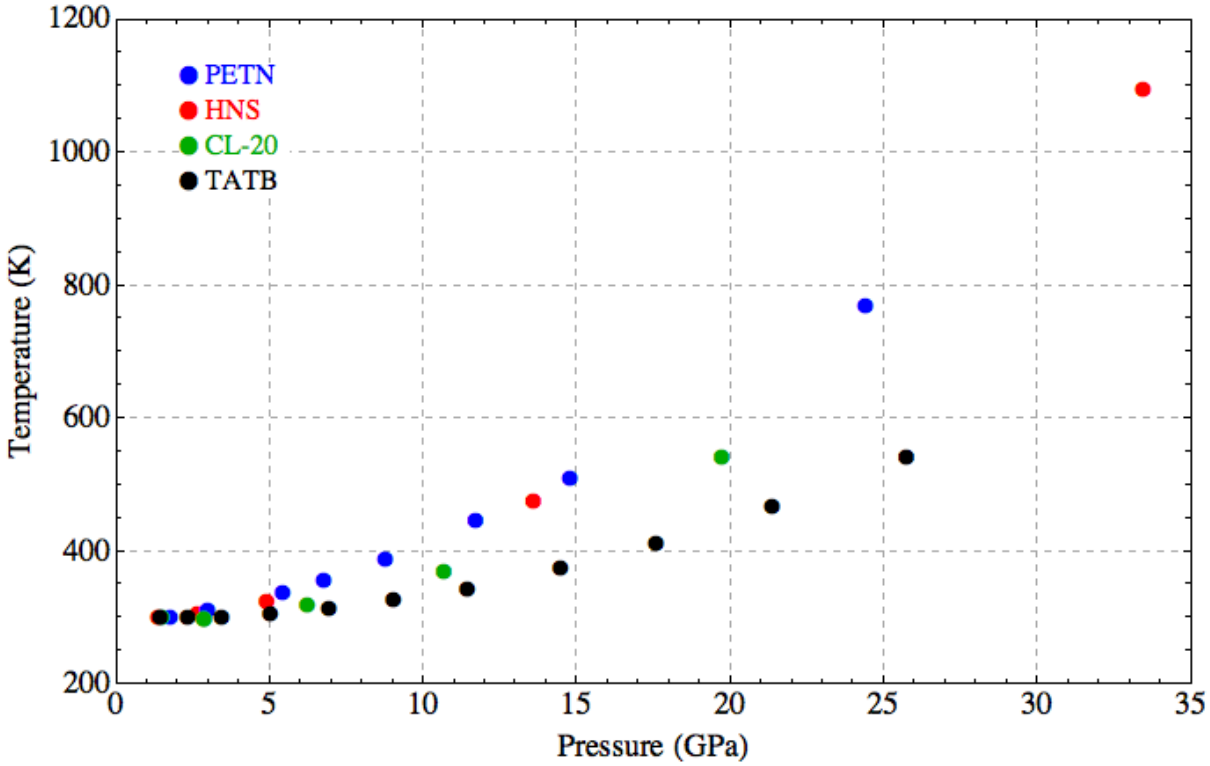
Hexanitrohexaazaisowurtzitane
CL-20 Hugoniot



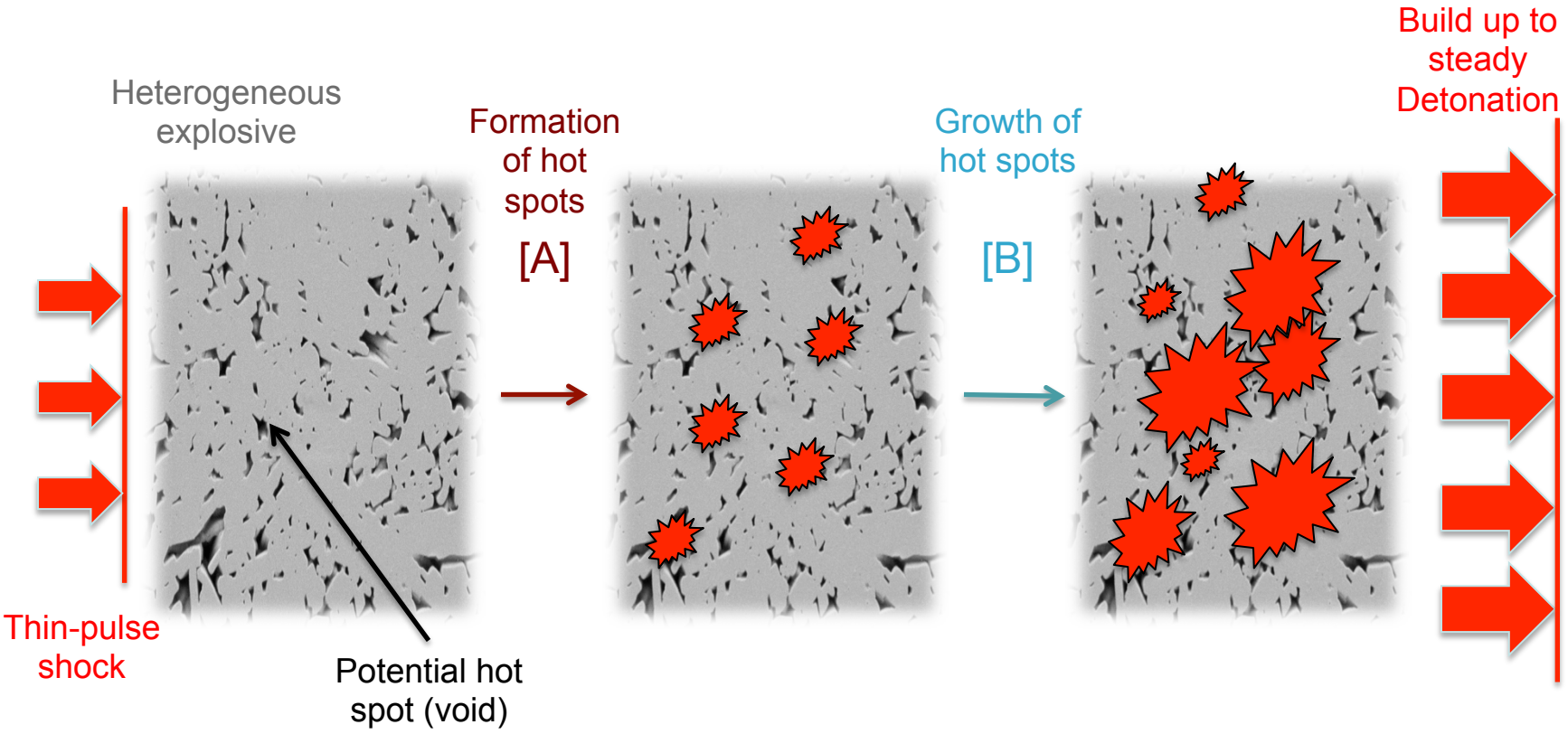
TATB Hugoniot:



Comparison of shock temperature: Implications for sensitivity?



Shock Initiation:
Energy is localized at heterogeneities (pores)

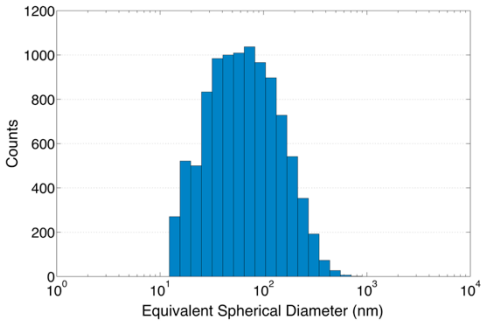


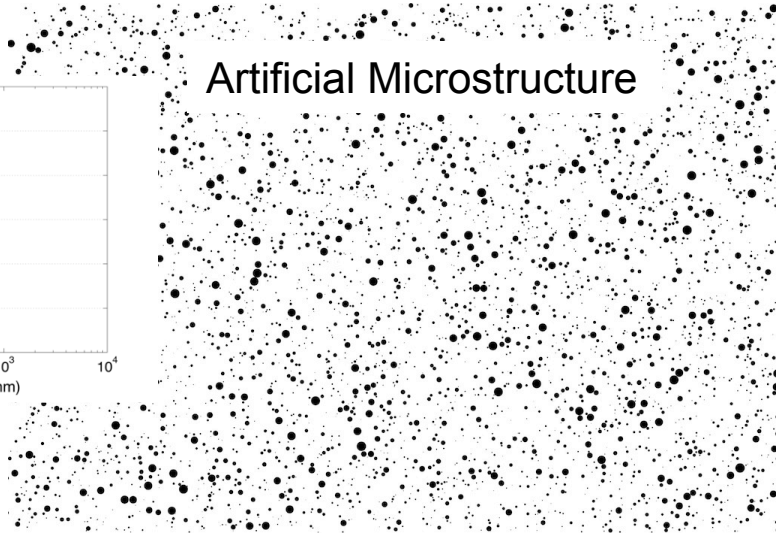
Adapted from Khasainov et al. Shock Waves (1997) 7:89-105

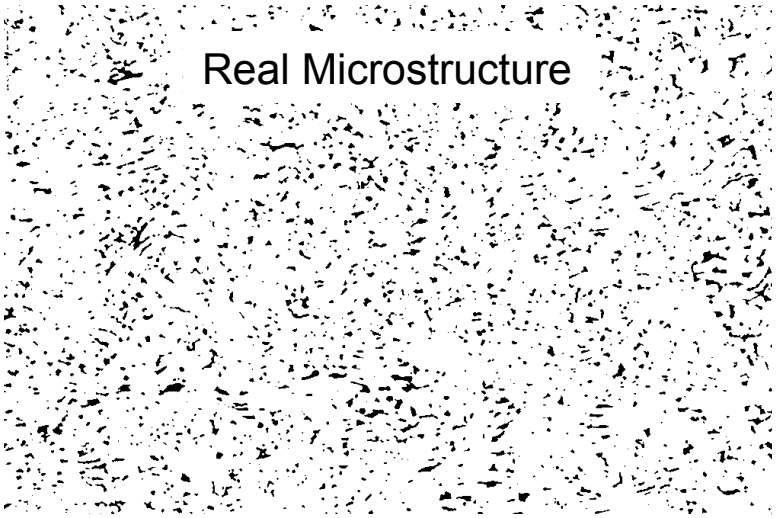
[A] Ignition of hot spots –> average size of heterogeneity

[B] Growth to sustained detonation –> interface area

Grain-scale w/ statistically equivalent microstructure



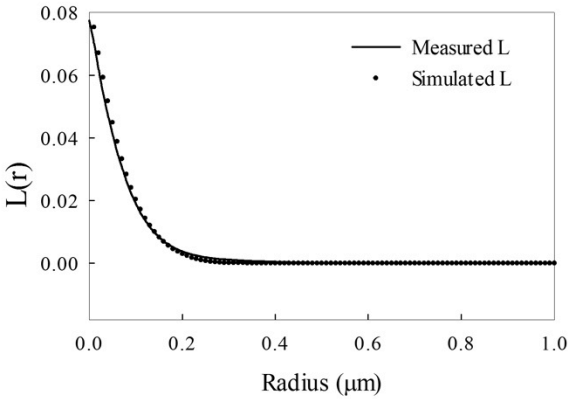


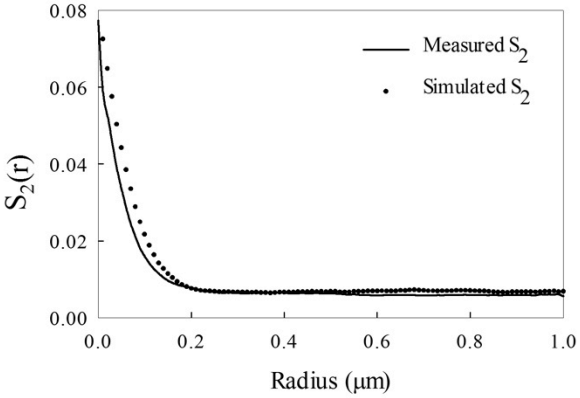


25 microns

What features are important to initiation?

Statistical comparison





Simulation with **microstructure** and **crystalline EoS**

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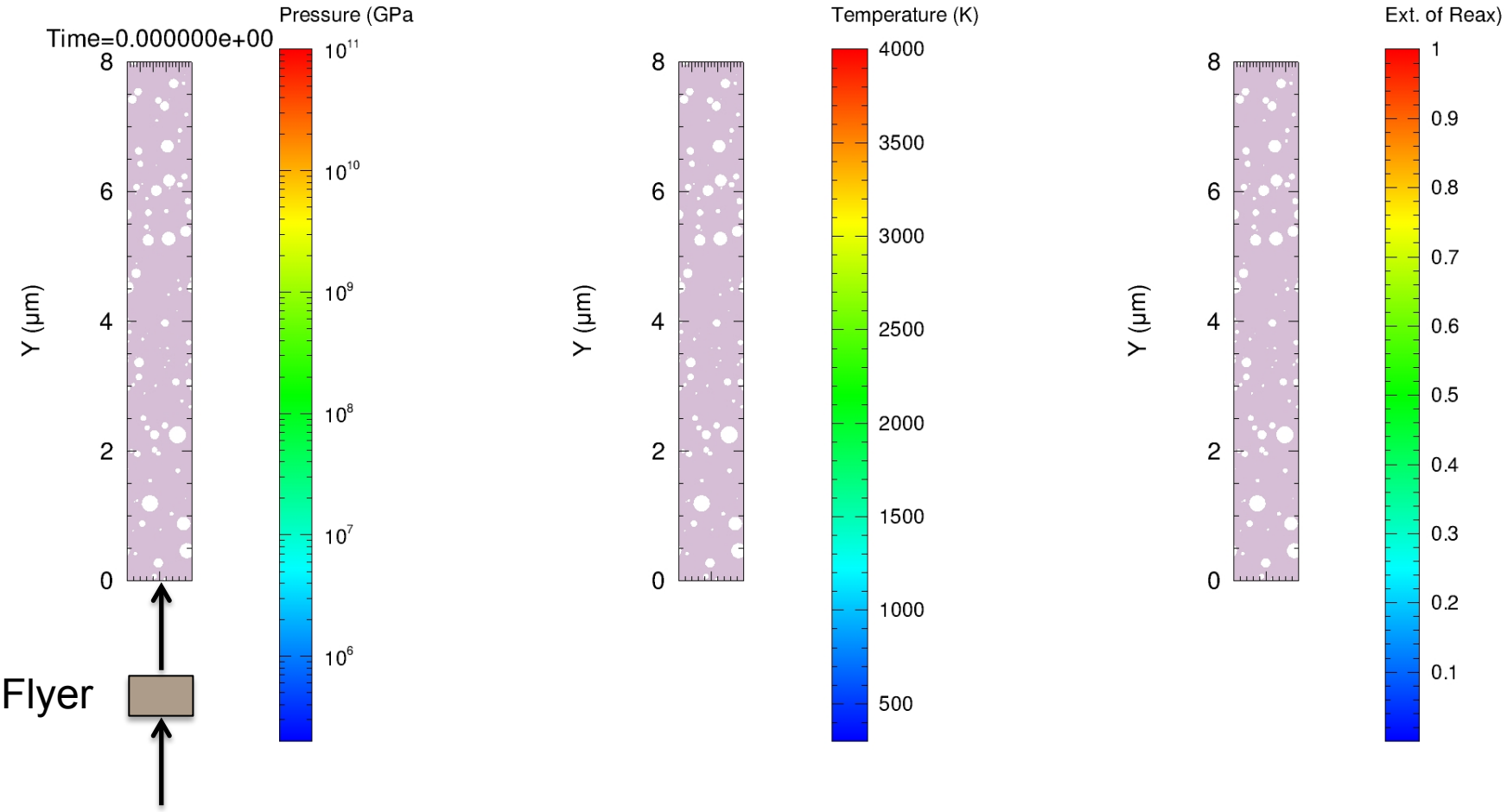
Initial state.



Simulations are still missing accurate temperature and reaction model

Simulation with **microstructure** and **crystalline EoS**

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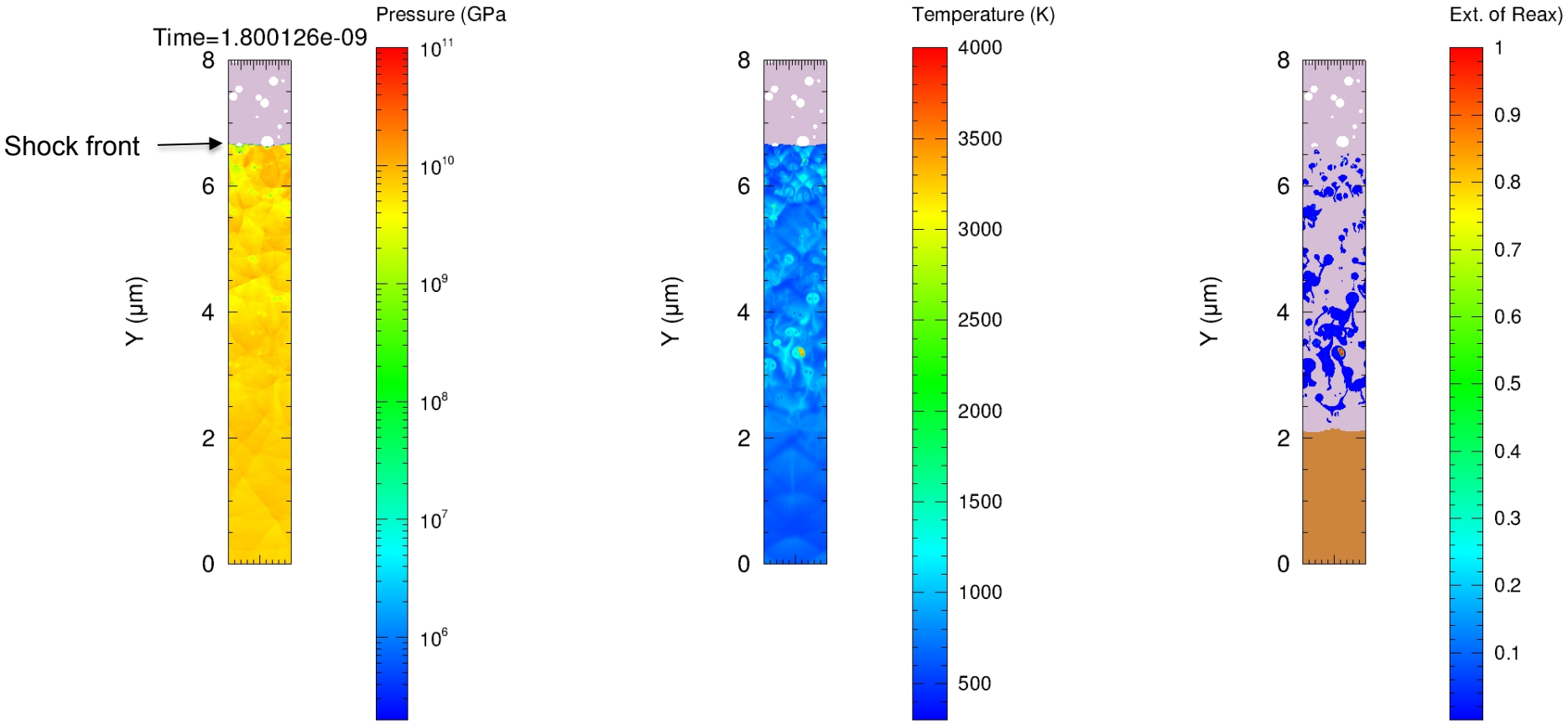
1.8 ns after flyer impact at 2.5 km/s



Simulations are still missing accurate temperature and reaction model

Simulation with **microstructure** and **crystalline EoS**

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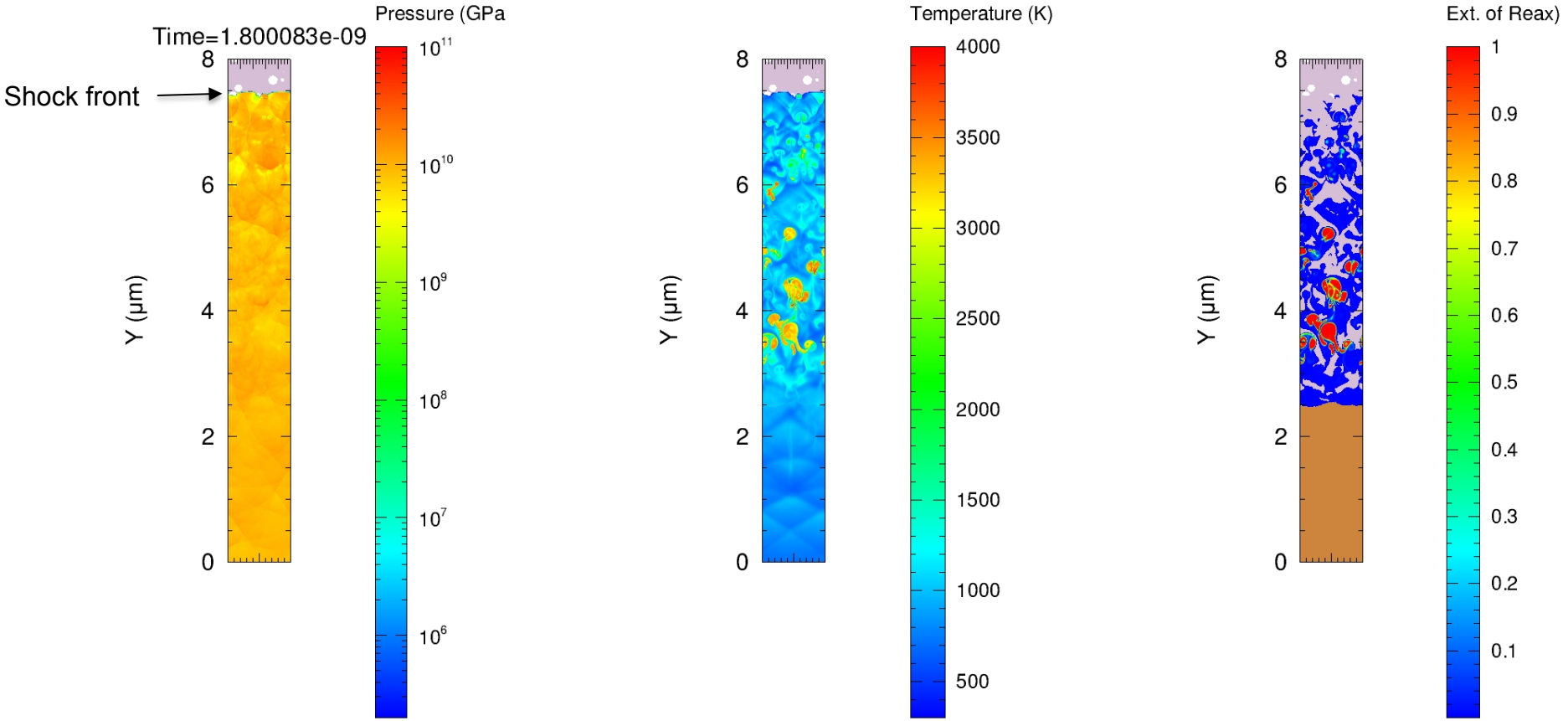
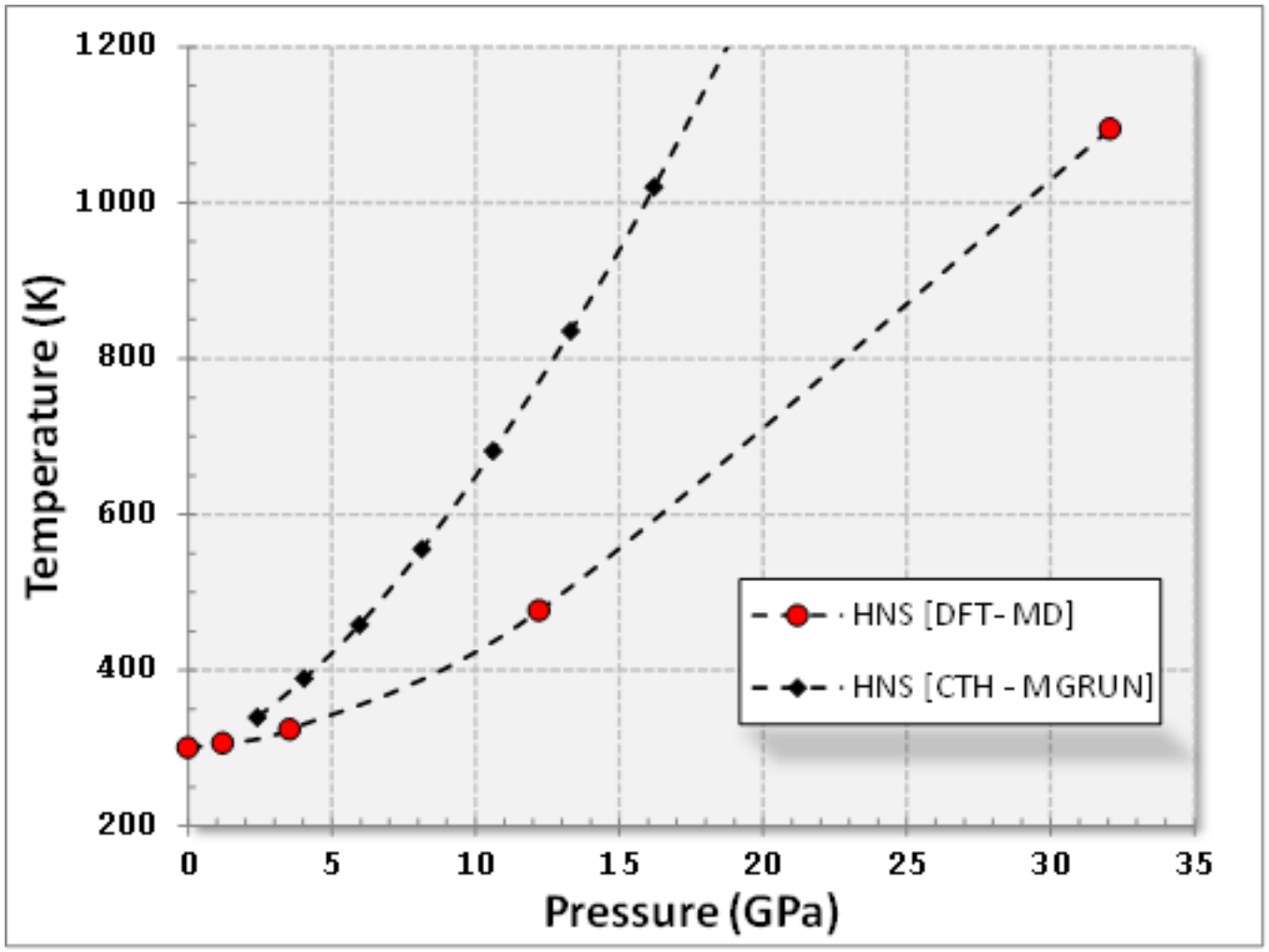
1.8 ns after flyer impact at 3.0 km/s



Simulations are still missing accurate temperature and reaction model

Demonstrating the EoS problem:



Conclusions / Future Work

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1. Extrapolation from low pressure is bad.

2. We can predict EoS using DFT-MD

3. We can make a tabular EoS and remove the need for making approximations to C_v and Gamma. Temperatures are predicted… need to be validated.

4. Shock temperature is linked to sensitivity.

5. Working to incorporate DFT-MD EoS with microstructural characterization and reactive process to build a predictive grain-scale simulation of shock initiation.

Extras:

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Extras:

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Extrapolation = Bad. Kerley = mysteriously good.