

**RYAN R. WIXOM**

# SHOCK INITIATION: ATOMIC TO COMPONENT SCALES

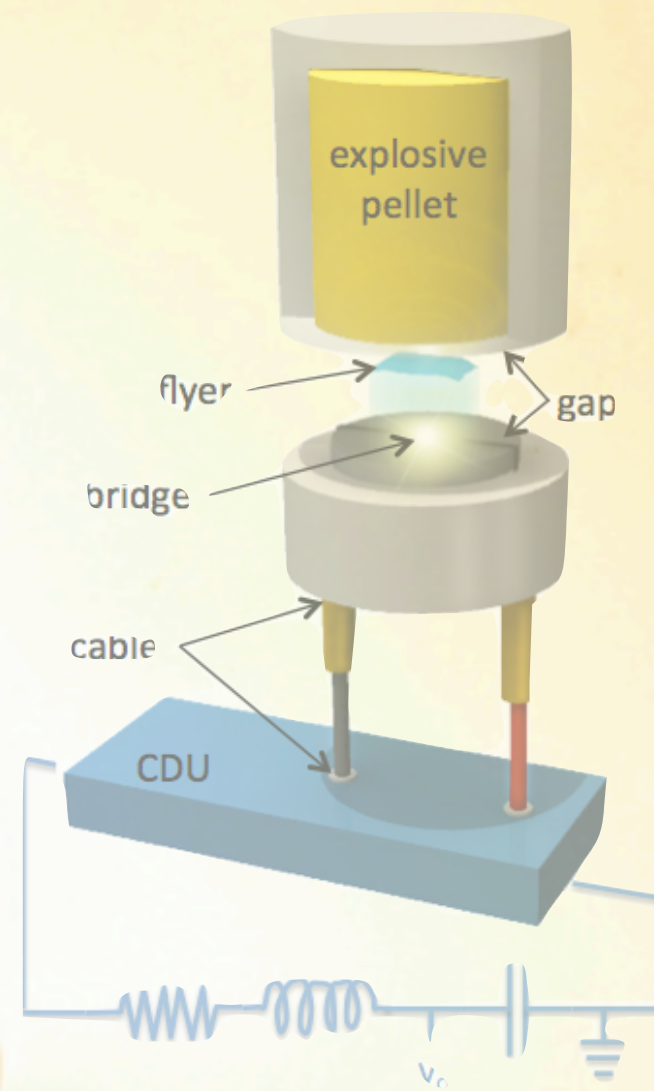


---

# COLLABORATORS

- ▶ Aidan Thompson, Cole Yarrington, Tzu-Ray Shan : SNL
- ▶ Joe Olles, Barry Ritchey, Alex Tappan, Rob Knepper, ...  
SNL
- ▶ David Damm : Schlumberger
- ▶ Eric Welle, Chris Molek : AFRL
- ▶ ~ Min Zhou : Georgia Tech (through AFRL)

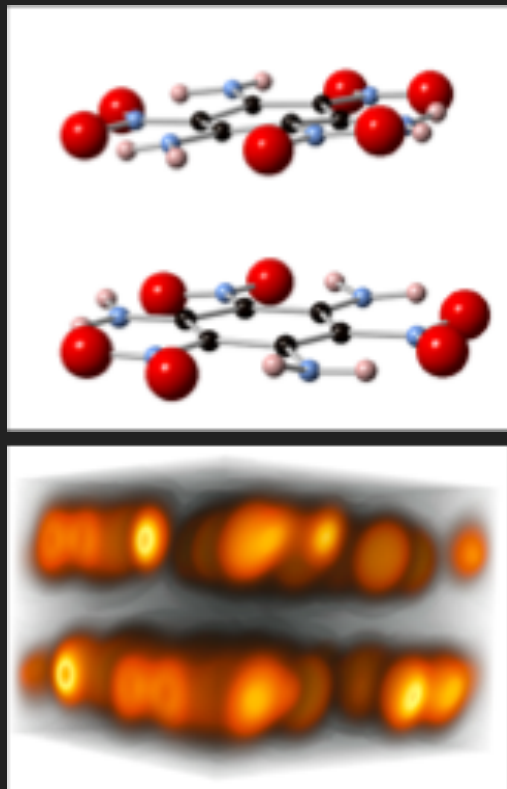
# Is a truly predictive model in our future?



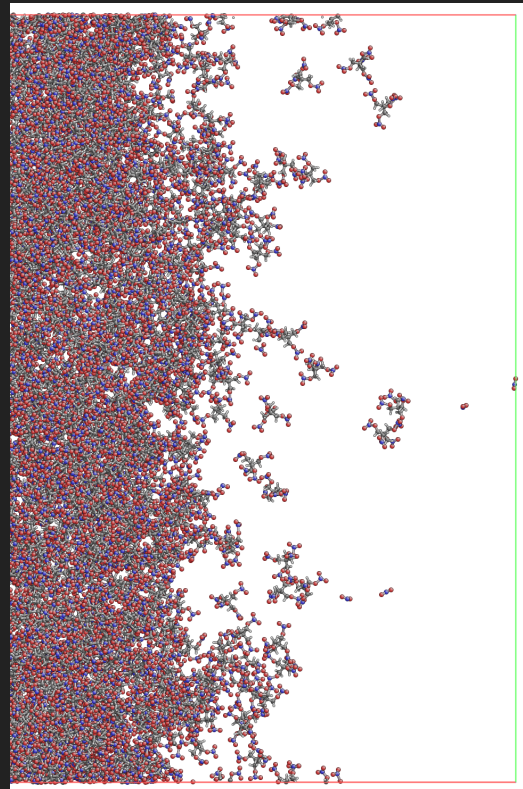
tenable timescale : this process is fast



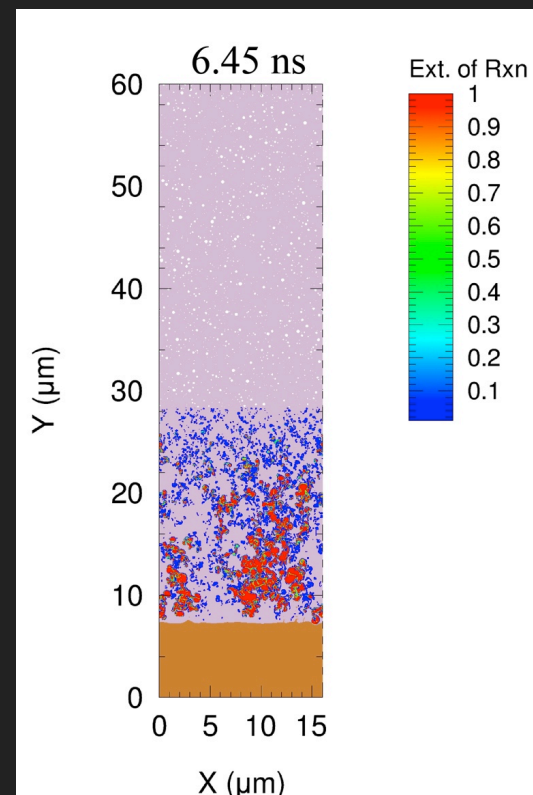
DFT-MD



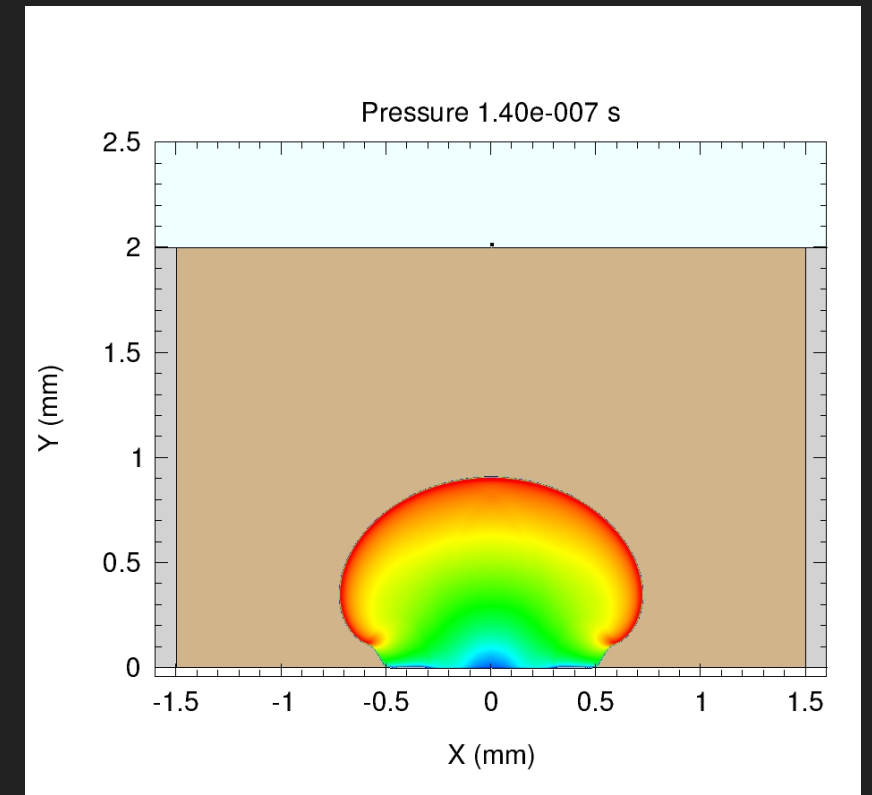
Reactive MD



Grain scale



Continuum Scale



QMC

Coarse-Grain

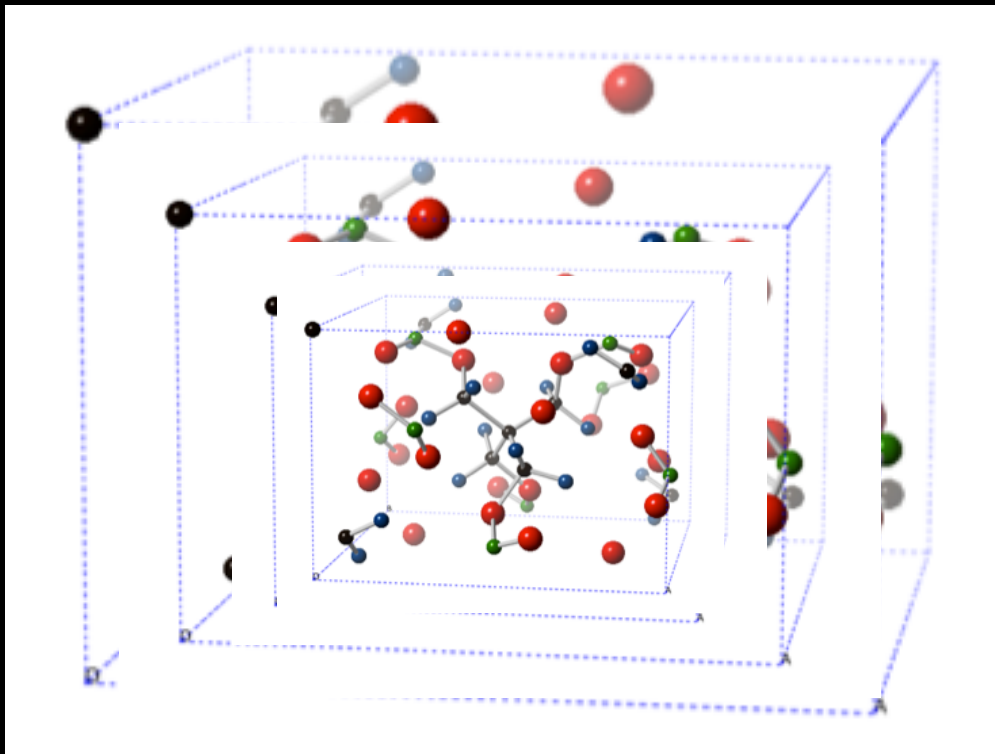
Sub-grid methods

Diagnostics / Experiments

Can the scales be overlapped?



# Equation of state of single crystal PETN: DFT-MD

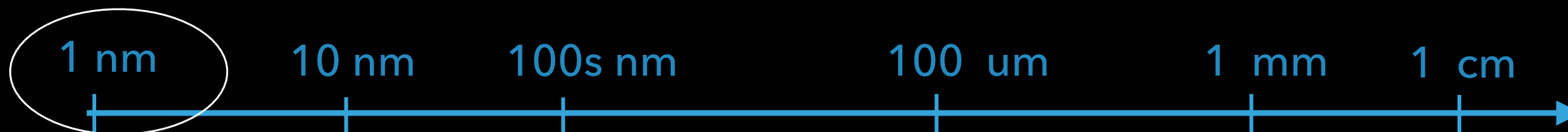
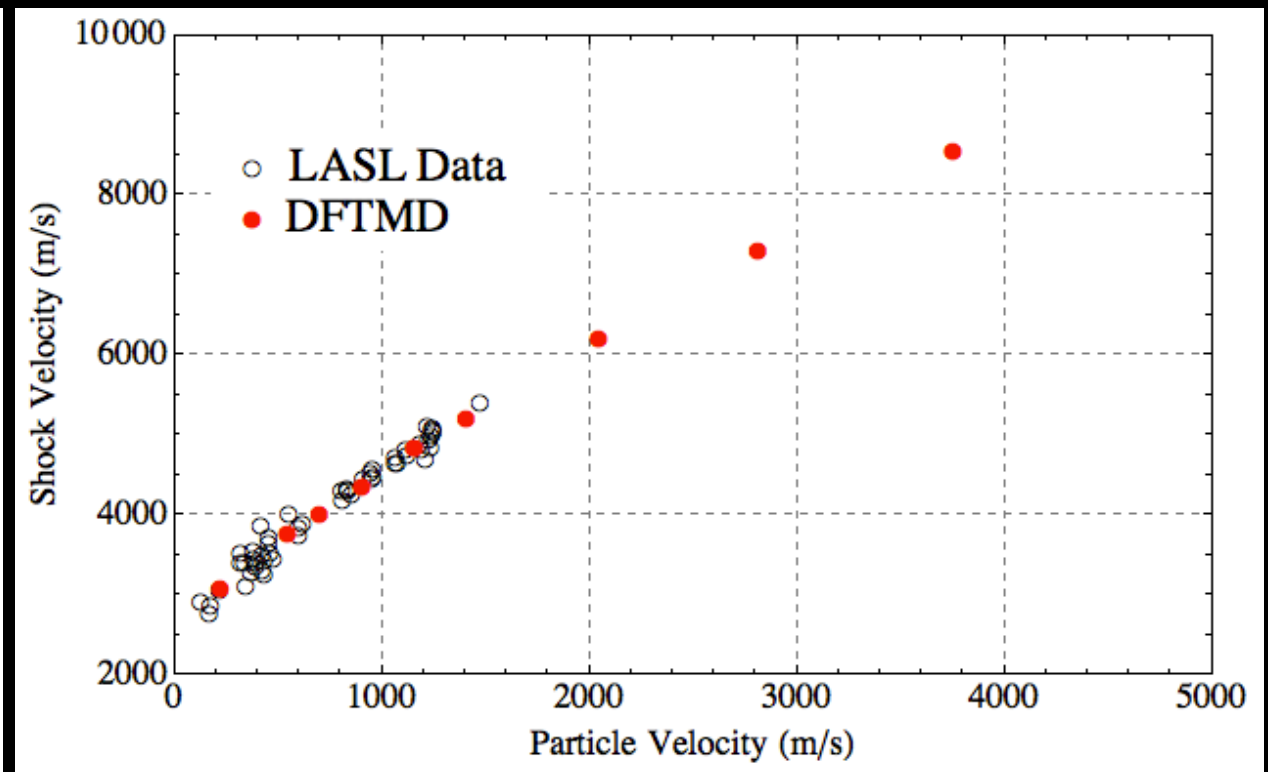
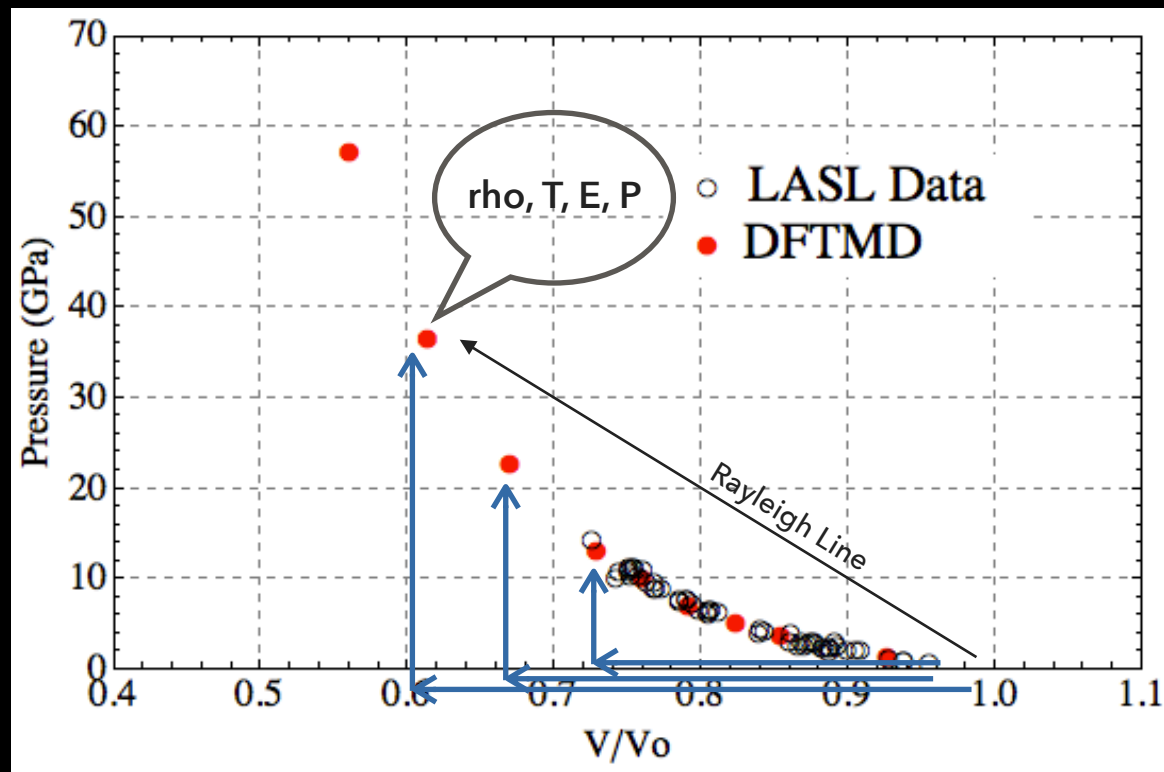


## Rankine-Hugoniot Jump Conditions

$$\rho_0 D = \rho_1 (D - u_1)$$

$$P_1 = \rho_0 D u_1$$

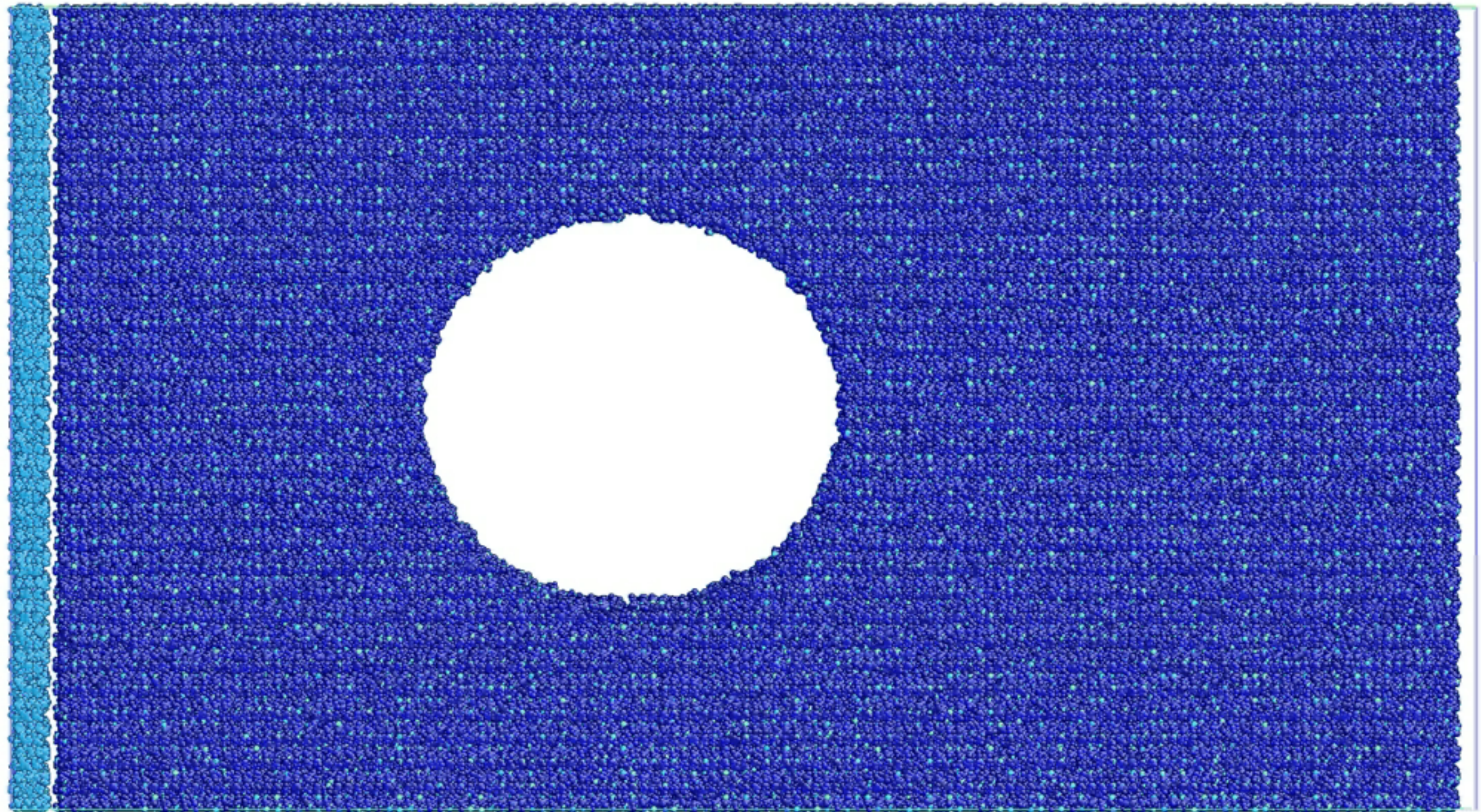
$$E - E_0 = \frac{1}{2}(P + P_0)(V_0 - V)$$





# Can MD be used to define material models?

REAX-FF MD: PARTICLE VELOCITY DURING PORE COLLAPSE IN HEXANITROSTILBENE (HNS)



22 nm

1 nm

10 nm

100s nm

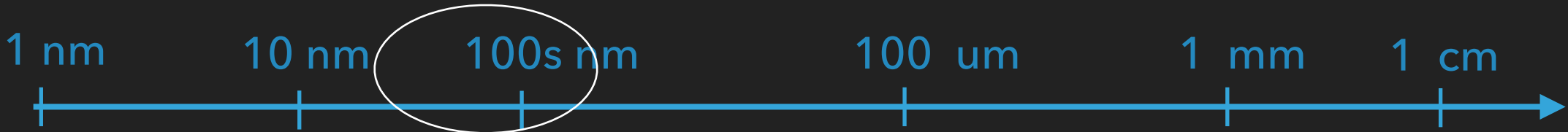
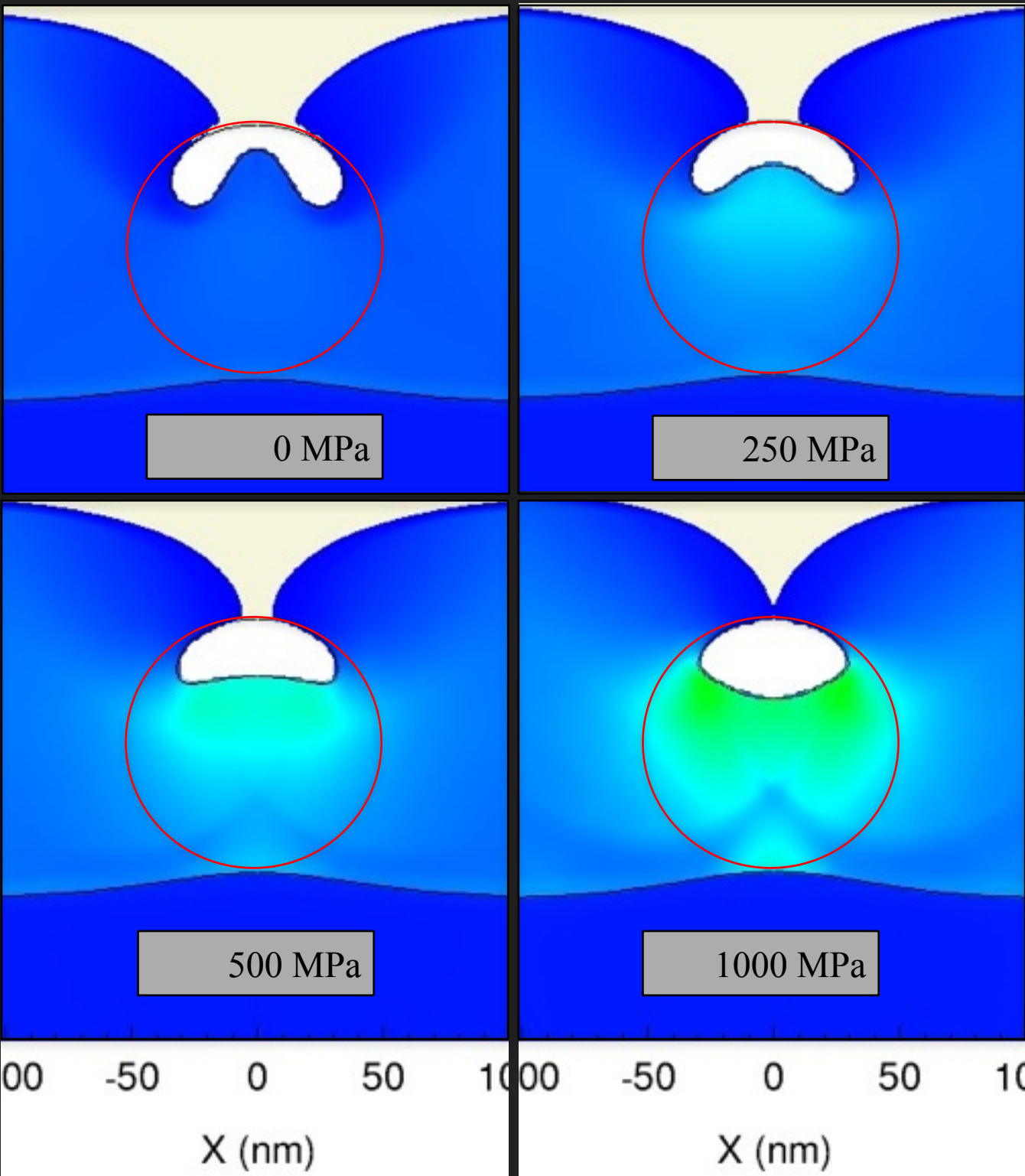
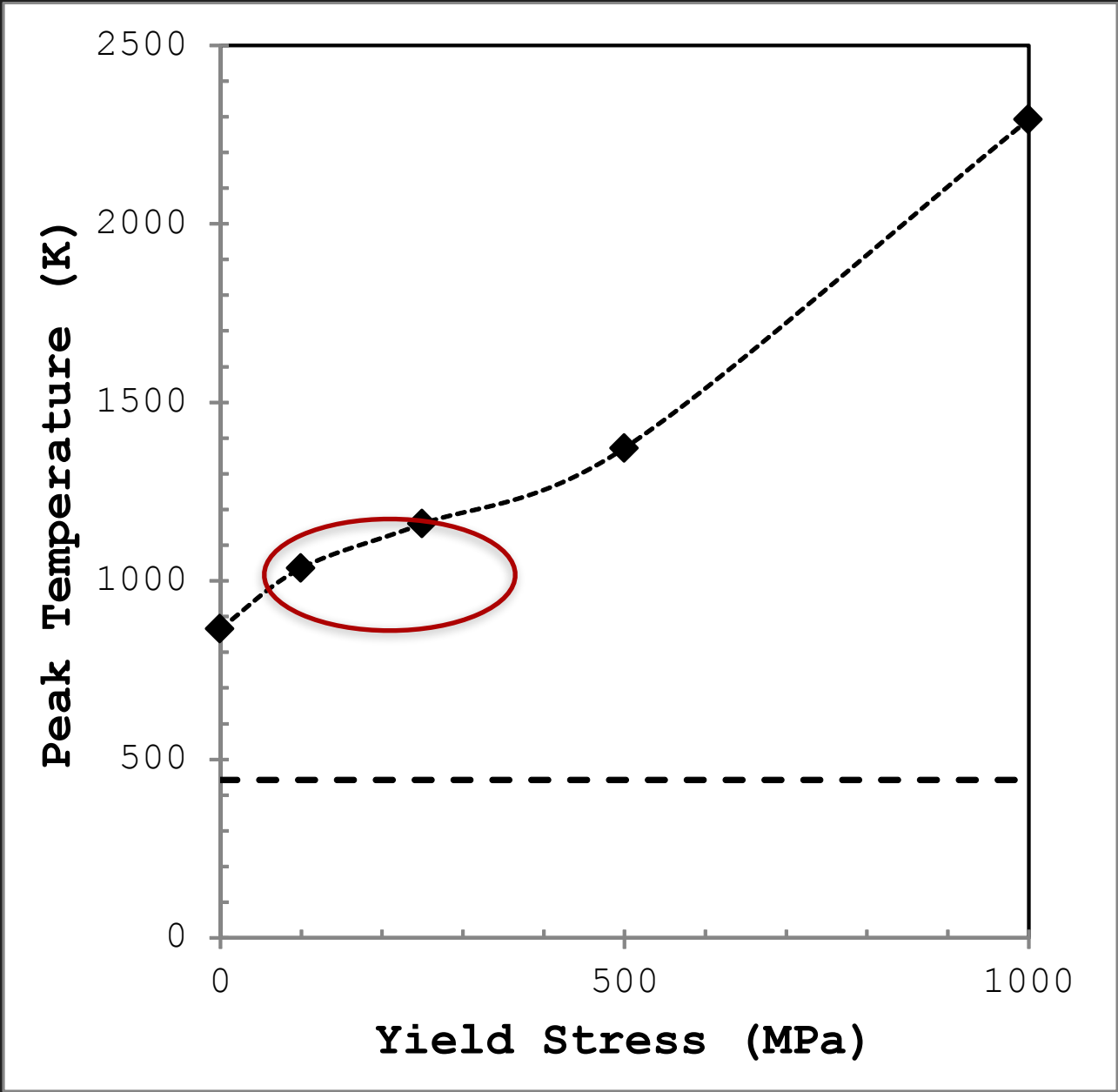
100 um

1 mm

1 cm



# Strength model effects pore collapse, but does it matter?



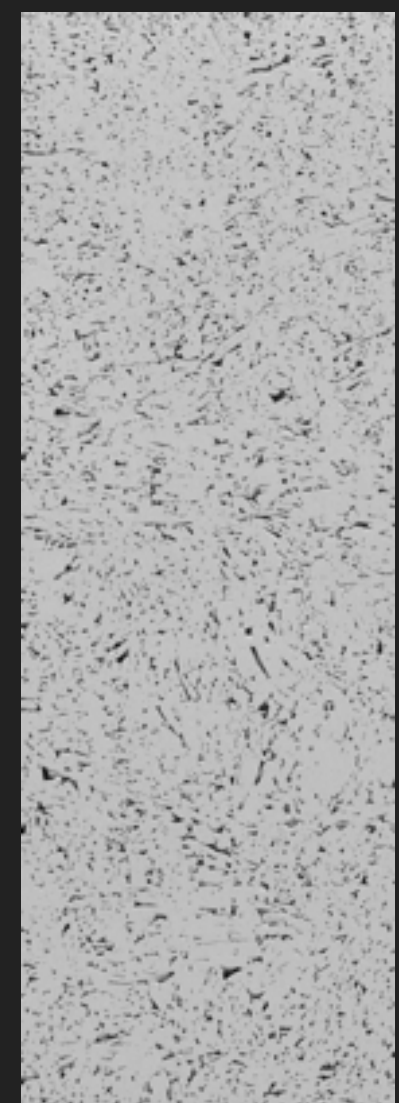


# GRAIN-SCALE (MESO) SIMULATION

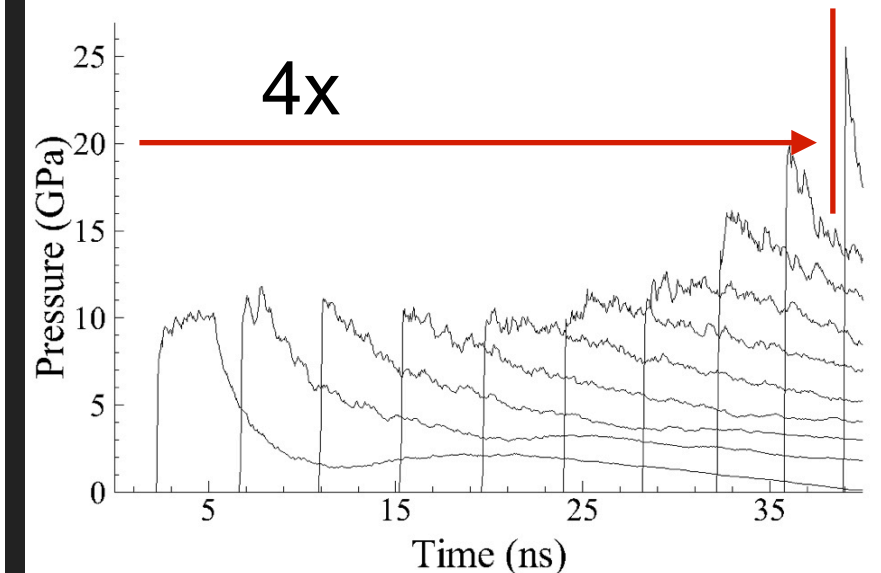
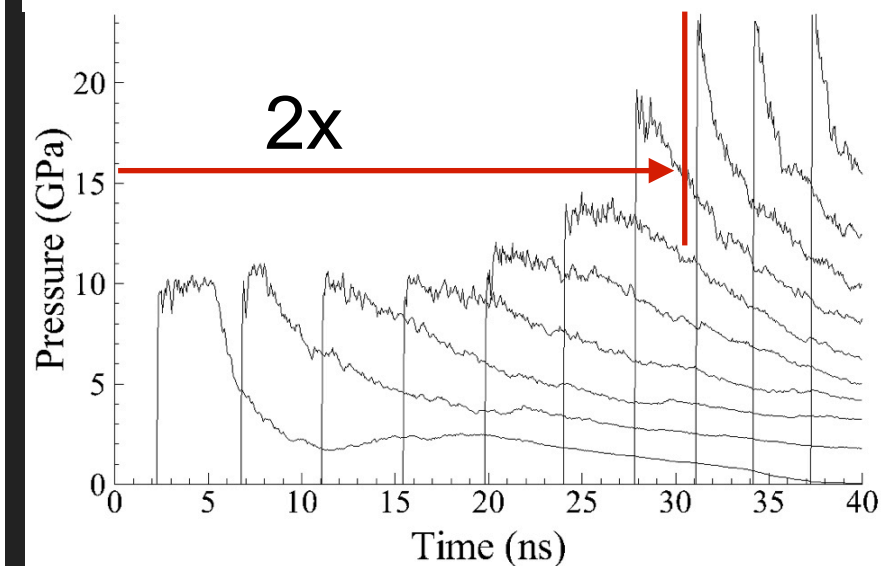
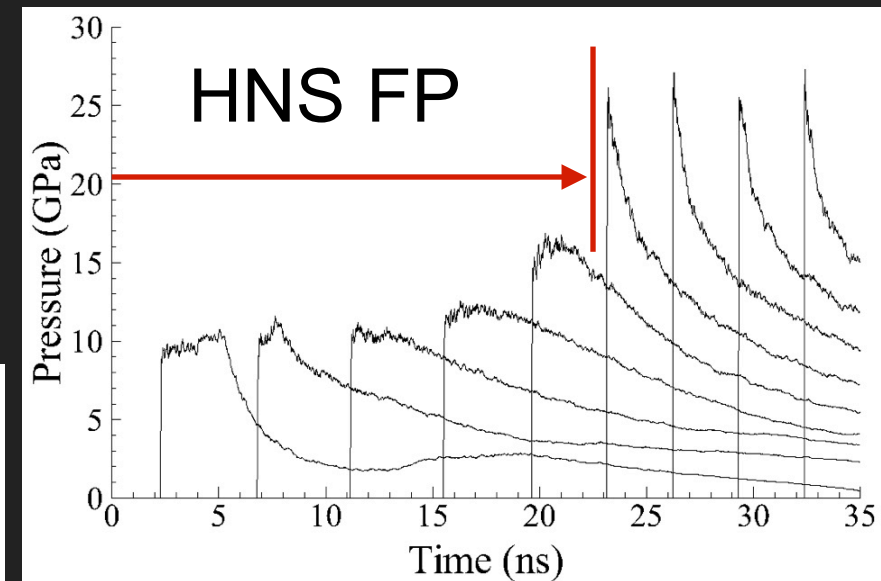
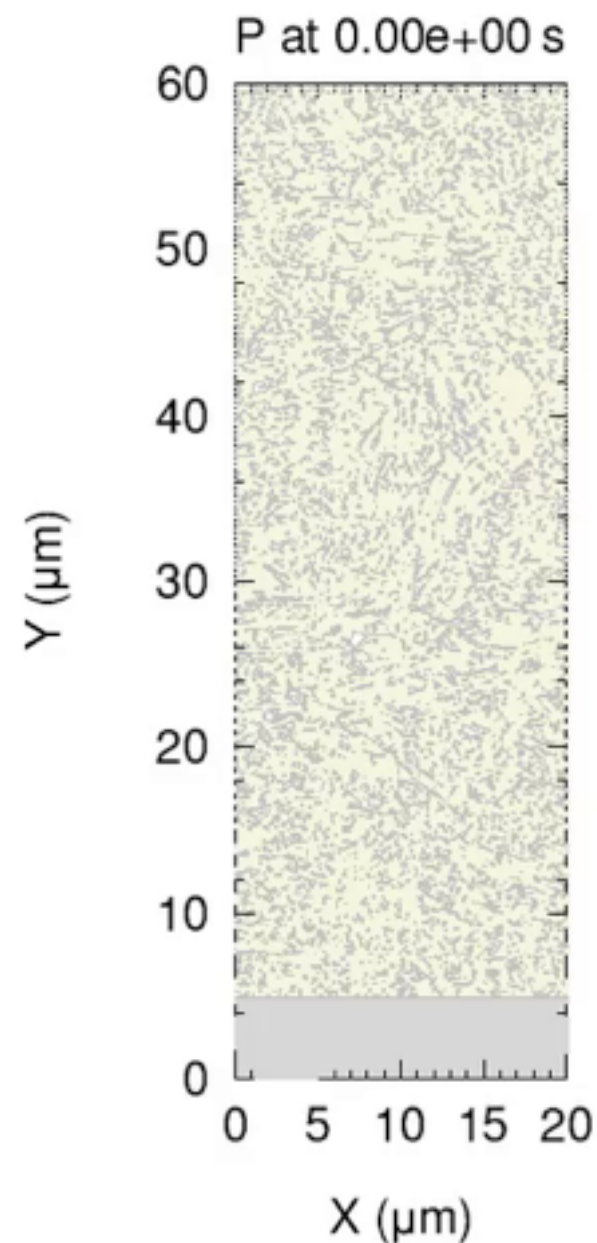
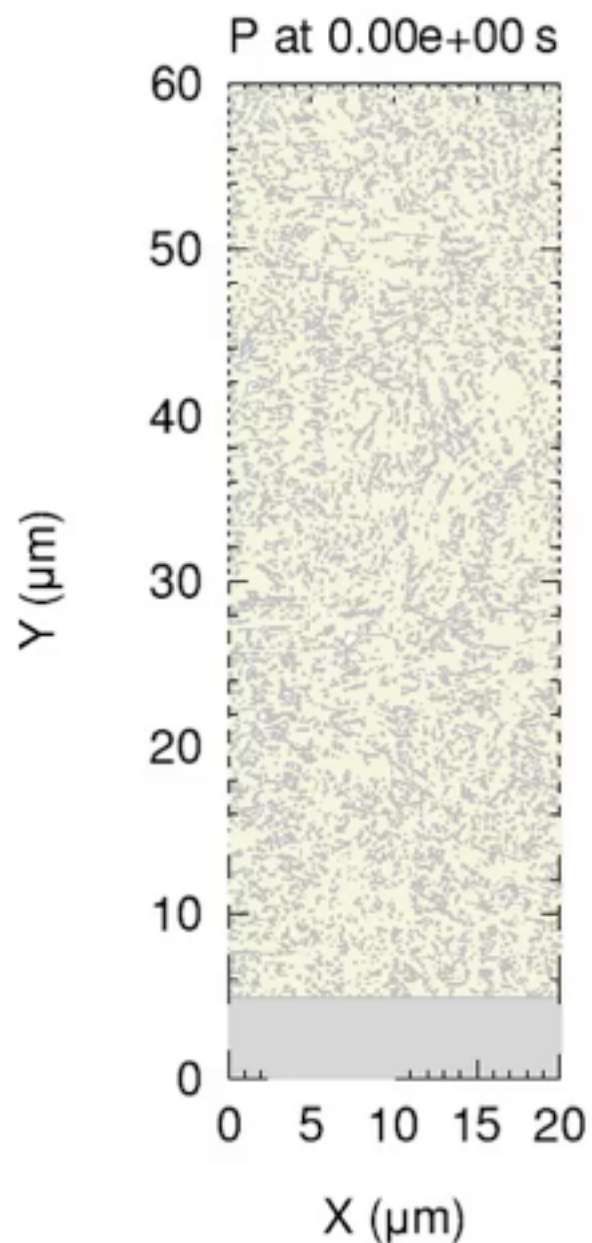
Prediction of initiation threshold and run-distance

1.5 km/s impact

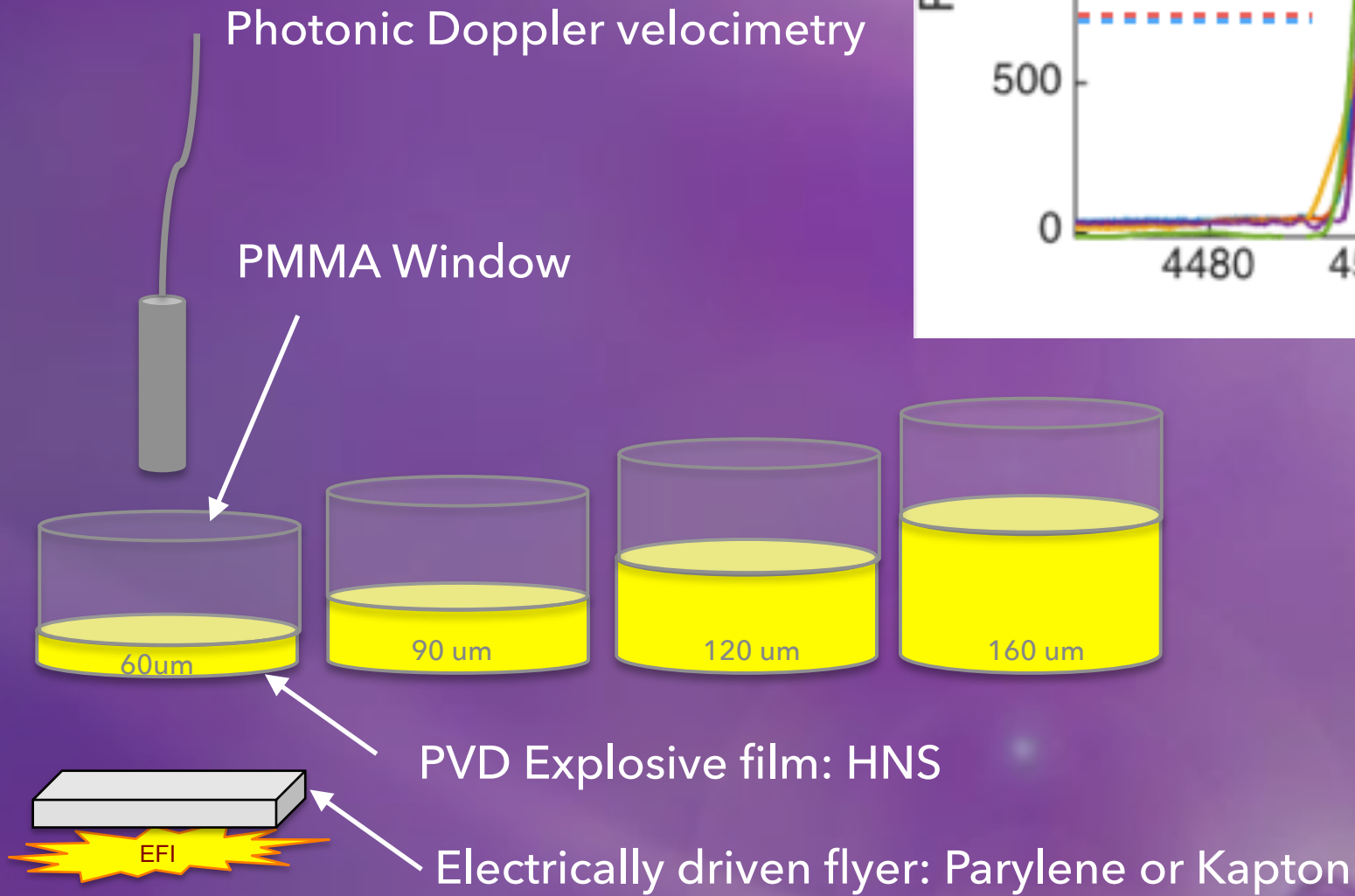
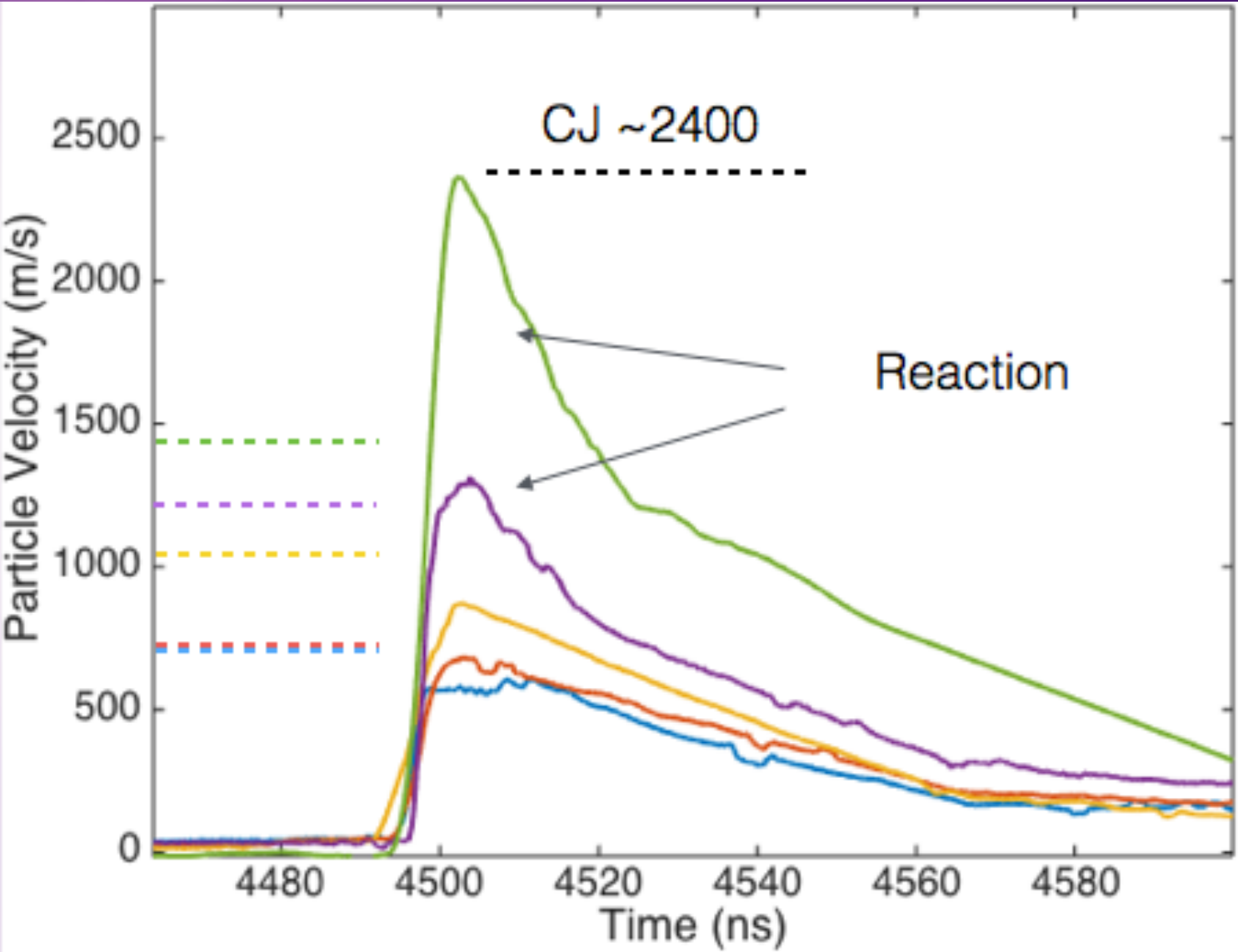
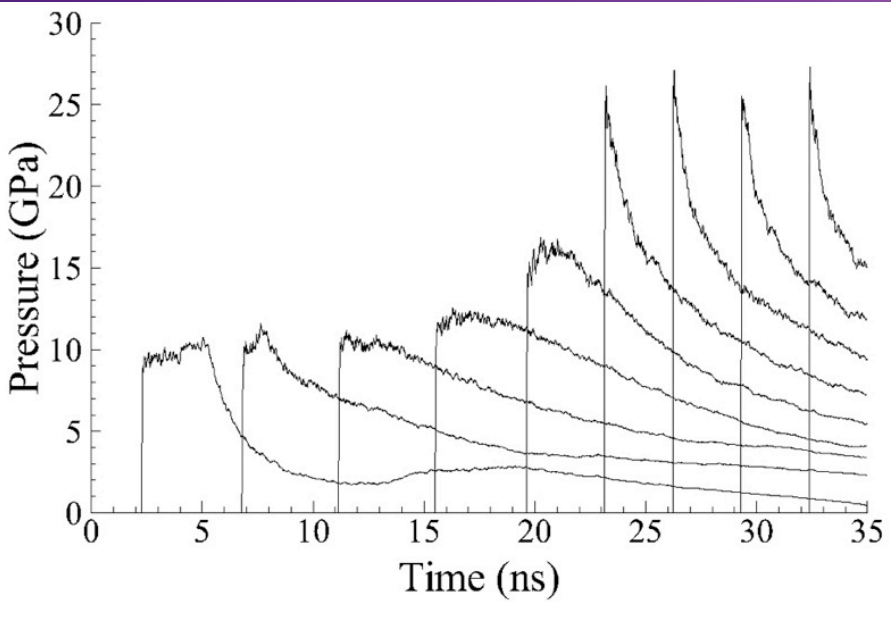
2.5 km/s impact



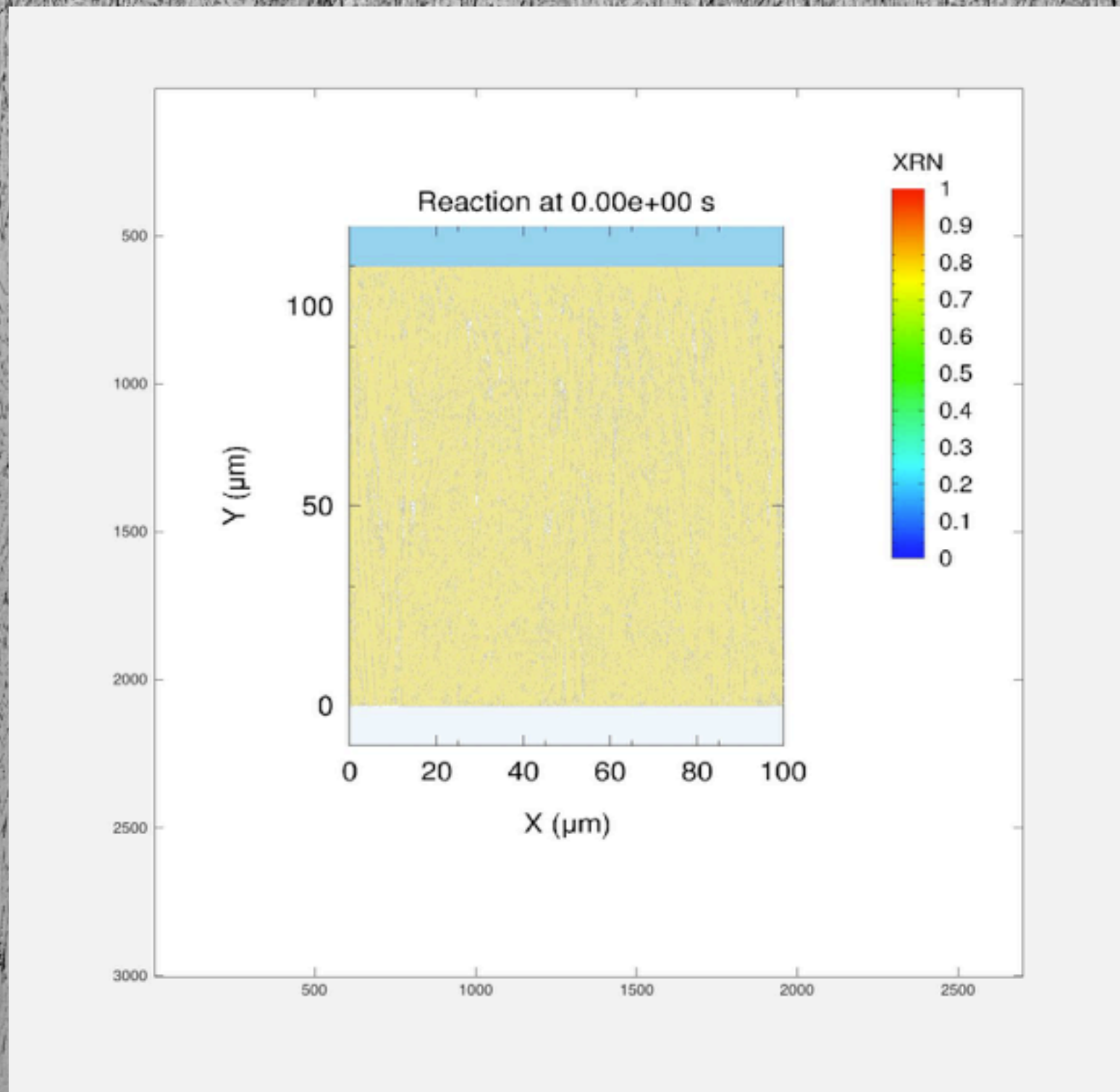
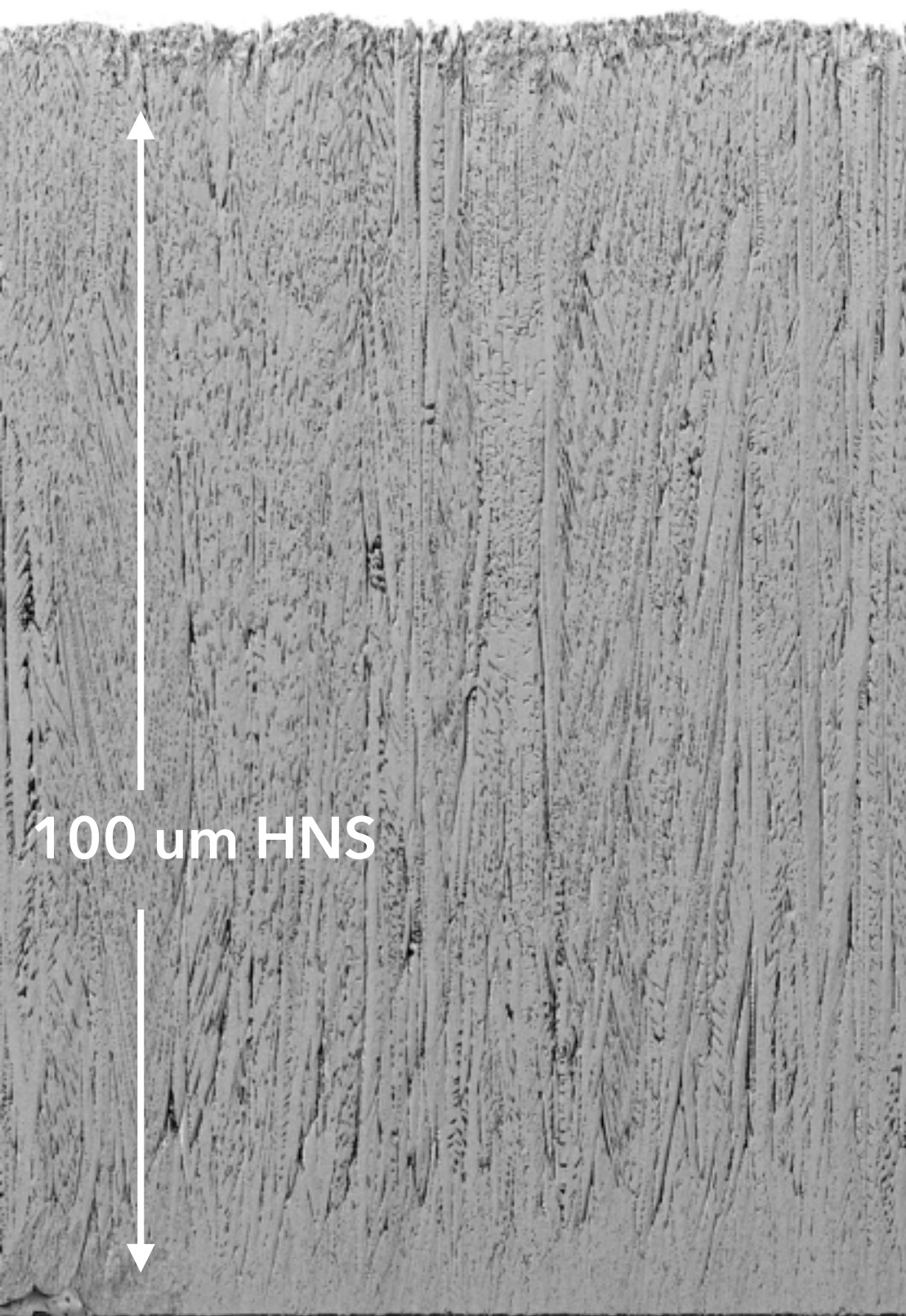
25 μm











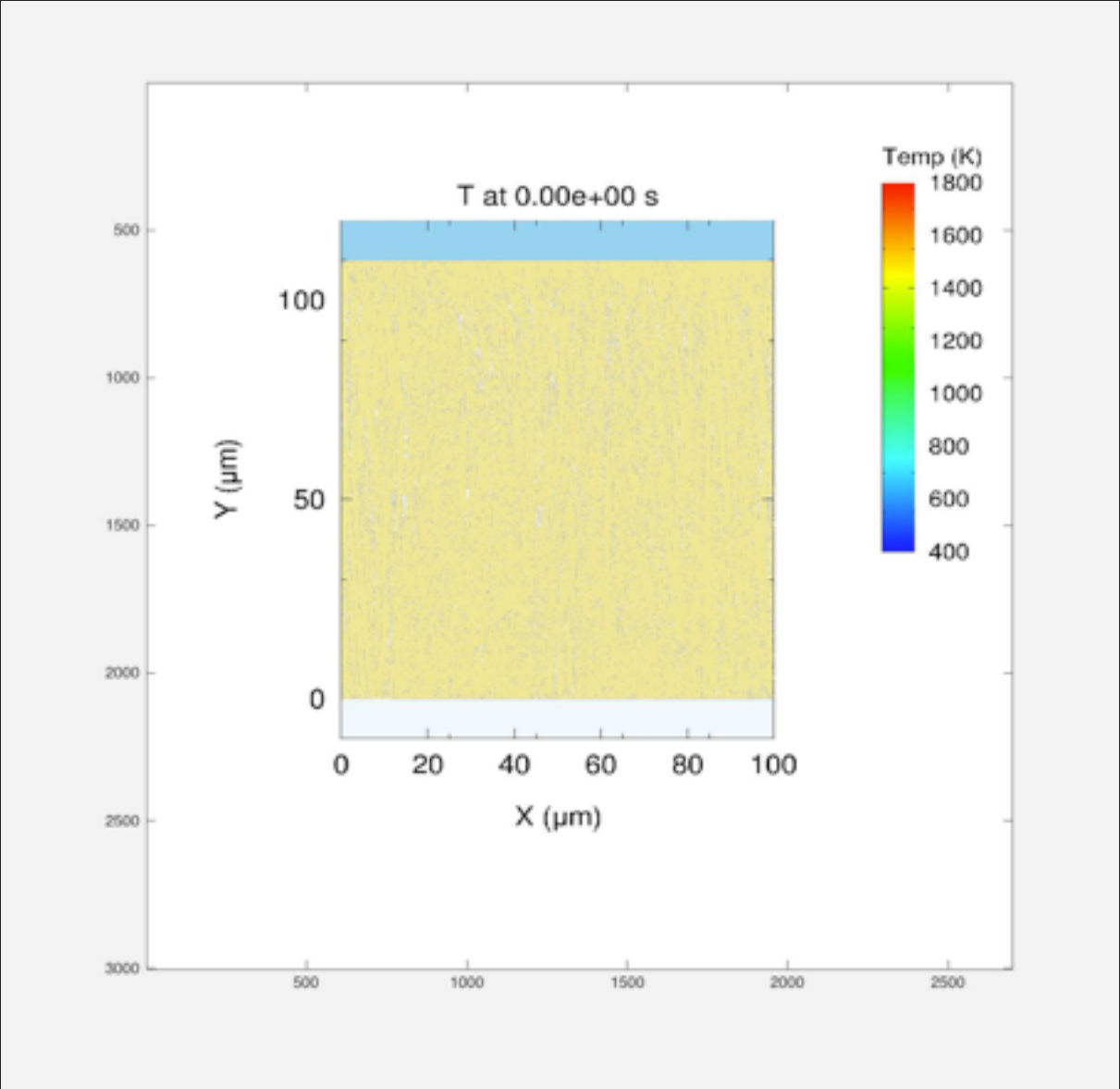
PMMA SUBSTRATE



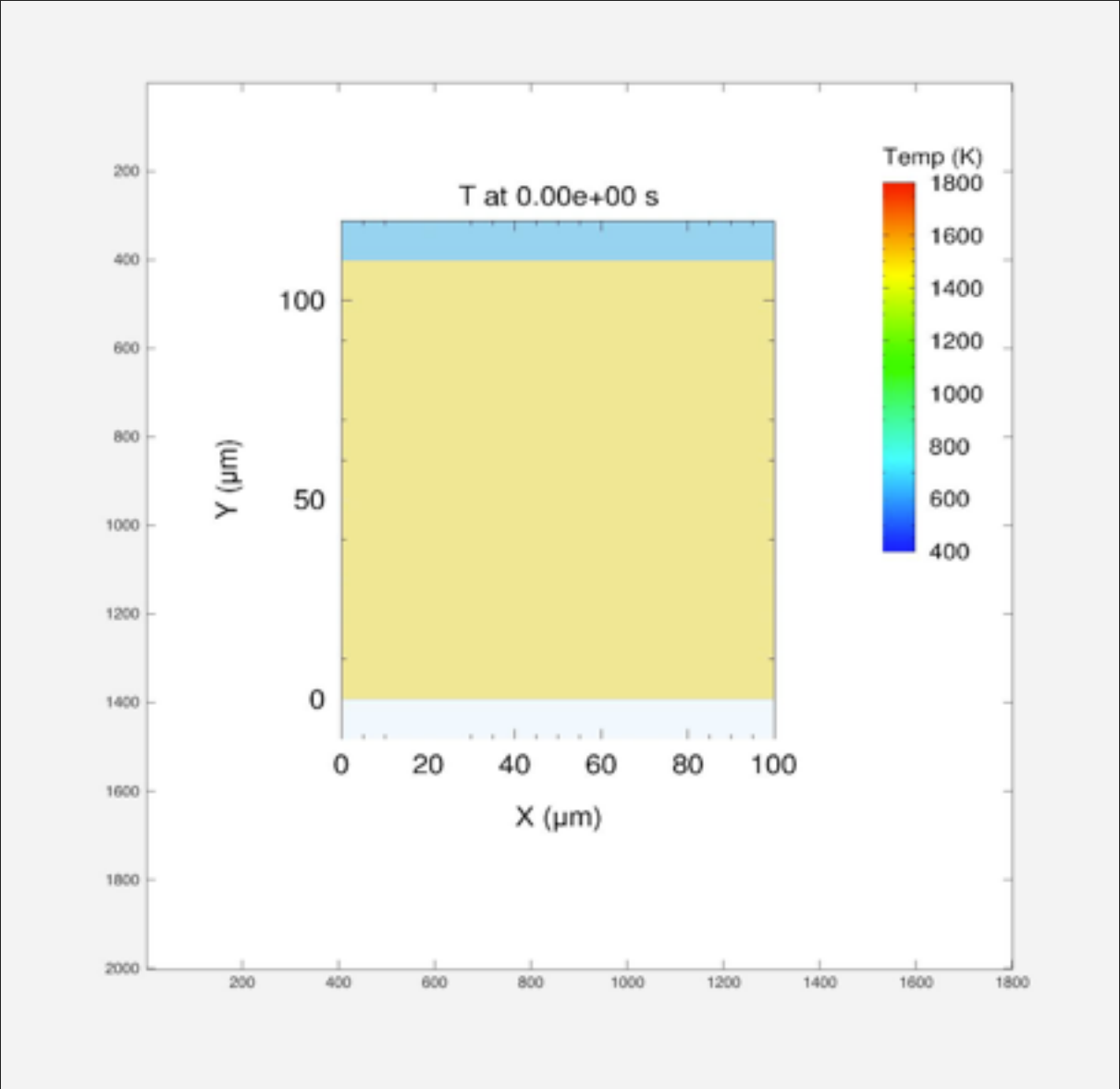


# Can a continuum model ever retain the accuracy of smaller scales?

Grain-scale



Continuum



# THE END. ANY QUESTIONS? ... I HAVE SOME.

---

- ▶ Is a truly predictive model in our future?
  - ▶ DFT-MD
  - ▶ Reactive MD
  - ▶ Course Grained MD
  - ▶ Grain scale hydrocode simulation
  - ▶ Continuum scale hydrocode simulation
- ▶ Grain-scale vs Continuum: Do we gain anything?
- ▶ MD to hydrodynamics: Which constitutive relationships matter?
- ▶ Can we use these simulations to predict failure / performance?
- ▶ Can we design an optimal microstructure for a specific application?



