Top-down versus Bottom-up Multiscale Modeling of Energetic Materials

SAND2019-6903 C

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LAMMPS Users Meeting, Albuquerque, New Mexico (8/14/2019)

The Problem Statement

- Why is the shock initiation to detonation transition a 'multi-scale' problem?
    - What scientific understanding or engineering design is obstructed by this problem? *(condensed phase chemistry, non-equilibrium processes, inverse performance design, etc.)*
    - Are the approximations in our modeling & simulation tools too prohibitive?

    Remember that these approximations are most often computational conveniences.

- What do Sandia's shock mod/sim capabilities look like? What are the goals?

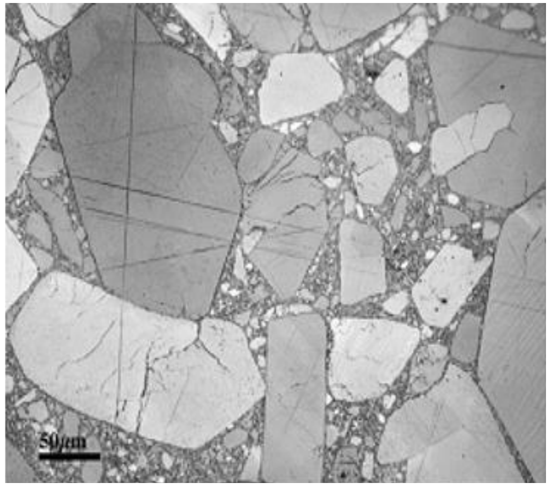
Shock Waves and Energetic Materials

Lets talk critical length and timescales

- Macro-scale Detonation

Run to detonation ~mm, ~µs

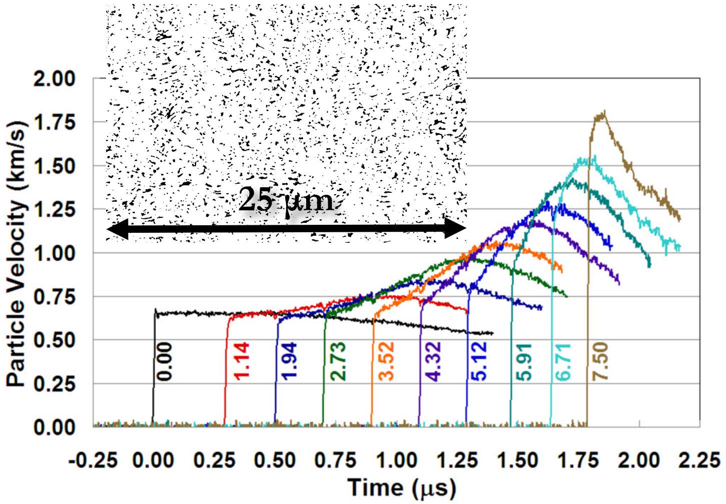
Grain/particle sizes ~10-100µm



- Shock wave rise, width

Particle, shock and detonation velocities ~µm/ns

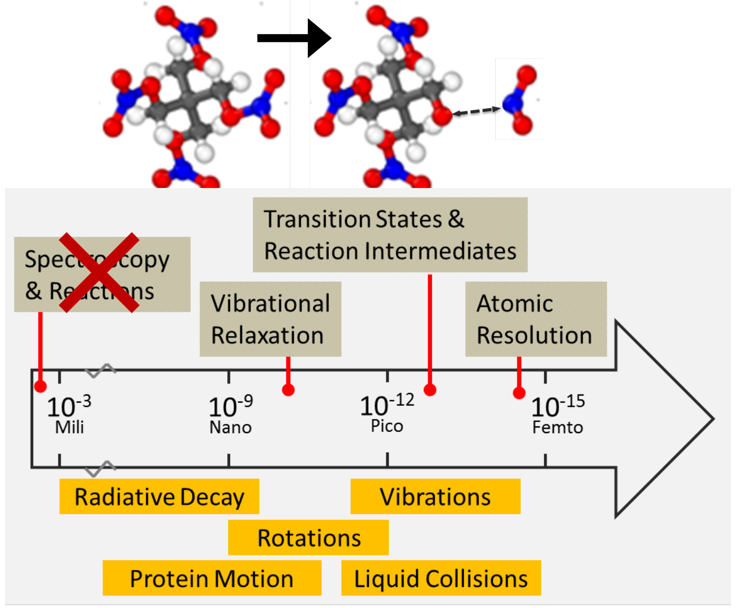
Defect sizes ~10nm-1µm



- Chemical Reactions

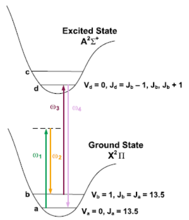
Unit cell of EM ~1nm

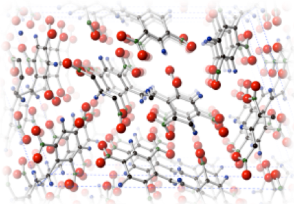
Period of CH stretch ~10fs



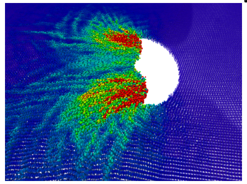
Shock Initiation of Explosives at Sandia

Quantum / MD Large Scalable Codes



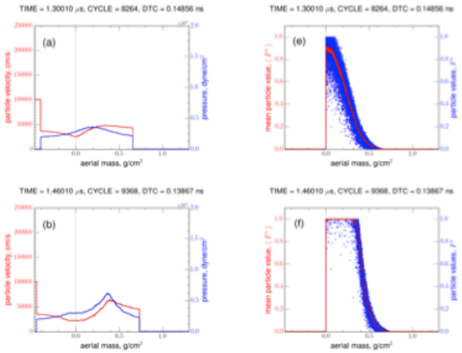


HNS crystal structure



LAMMPS + Kokkos

New Continuum Codes



Stochastic reactive shock waves

Formation Modeling

-poured
-pressed
-deposited
-AM of EM

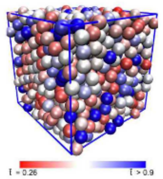
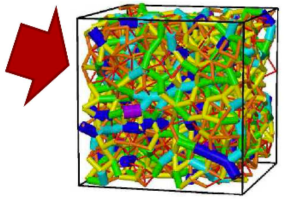


Image stack, or simulated µstructure



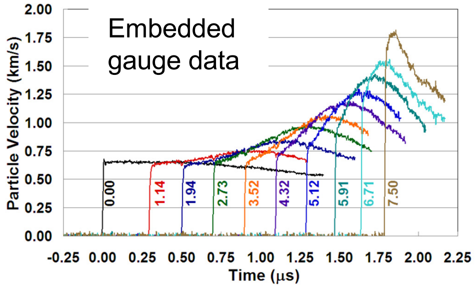
Graph of contact network

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

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

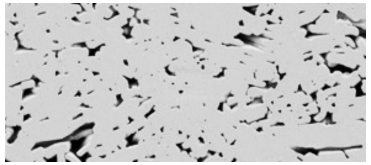
Tests and Experiments

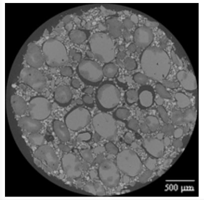
- Performance
- Sensitivity
- Threshold and UQ



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

Microstructural Analysis

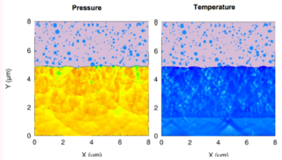


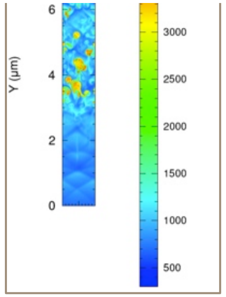


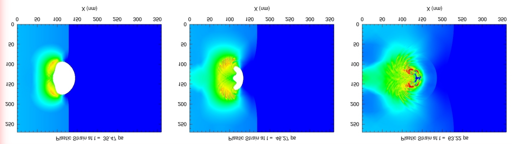
X-section of HNS pellet (top) and CT scan courtesy of Andres Chavez (left)

Mesoscale Simulations

Reactive shock waves in hexanitrostilbene (HNS) explosive





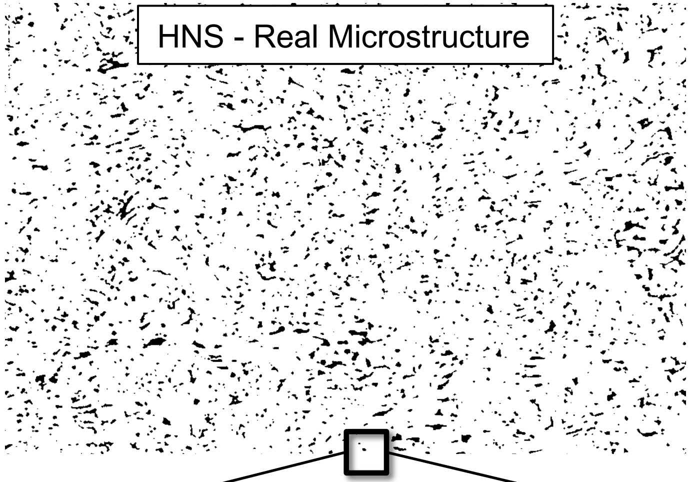


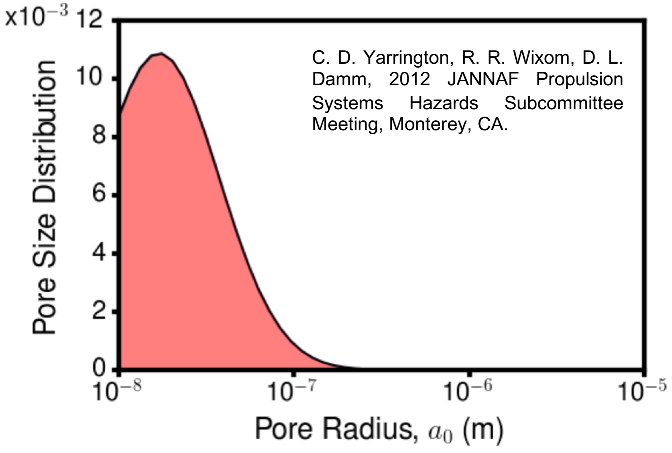
Microstructure Matters

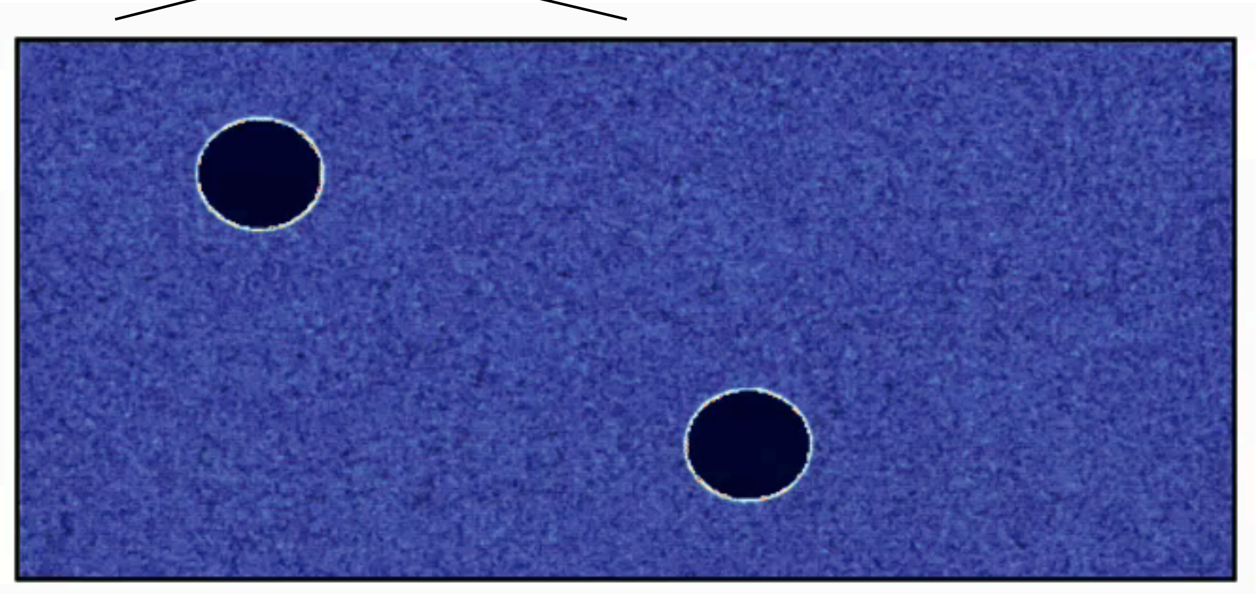
- Shock wave dissipates at defects, lost as heat
- Chemical reactions produce more heat and over pressure due to expanding gasses
- What defects lead to ignition?

Length (nm) and time (ps) scales make experiments extremely challenging

Need a model to capture both mechanical and chemical response



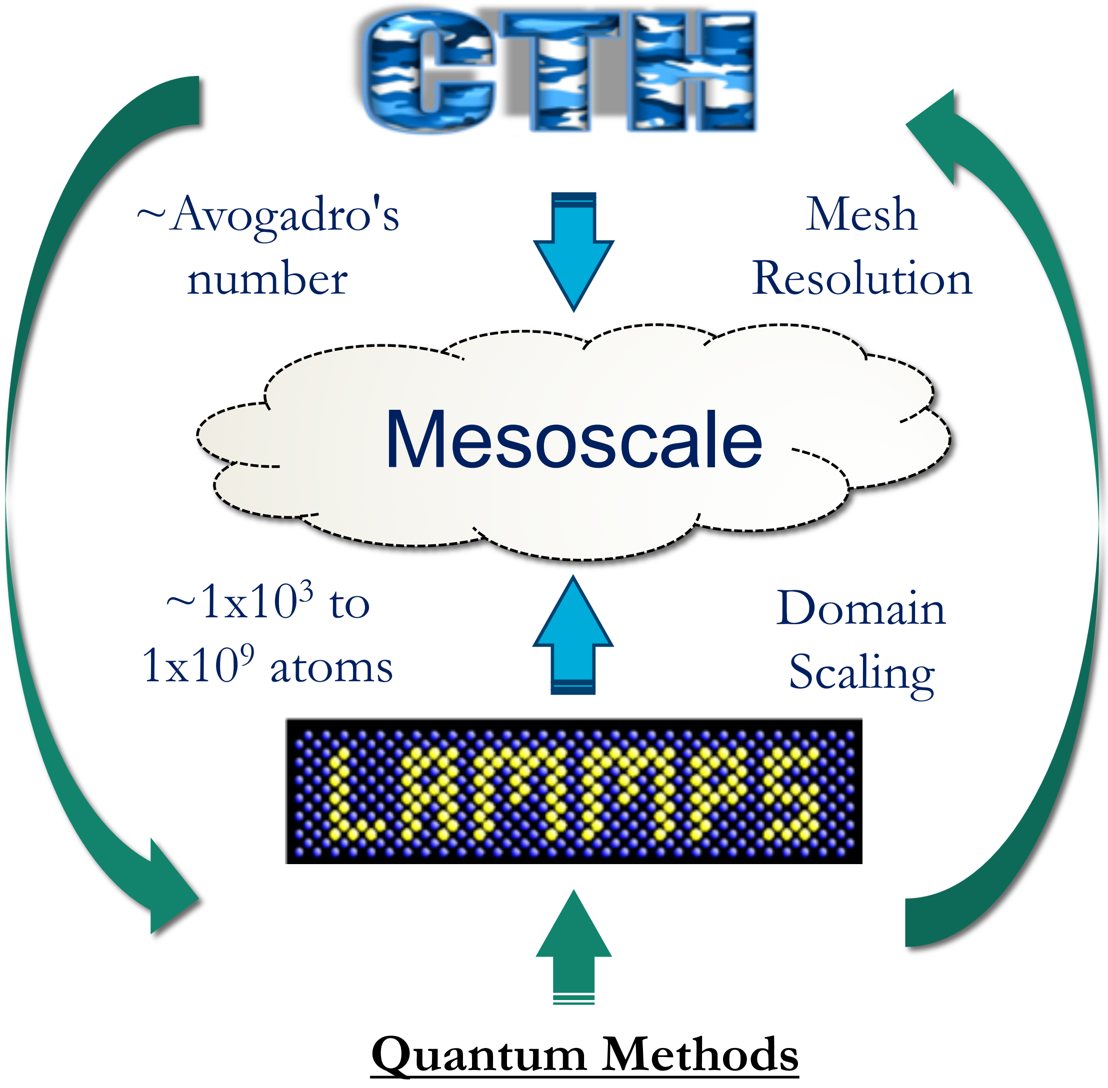




Sandia Mesoscale Modelling of Explosives

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

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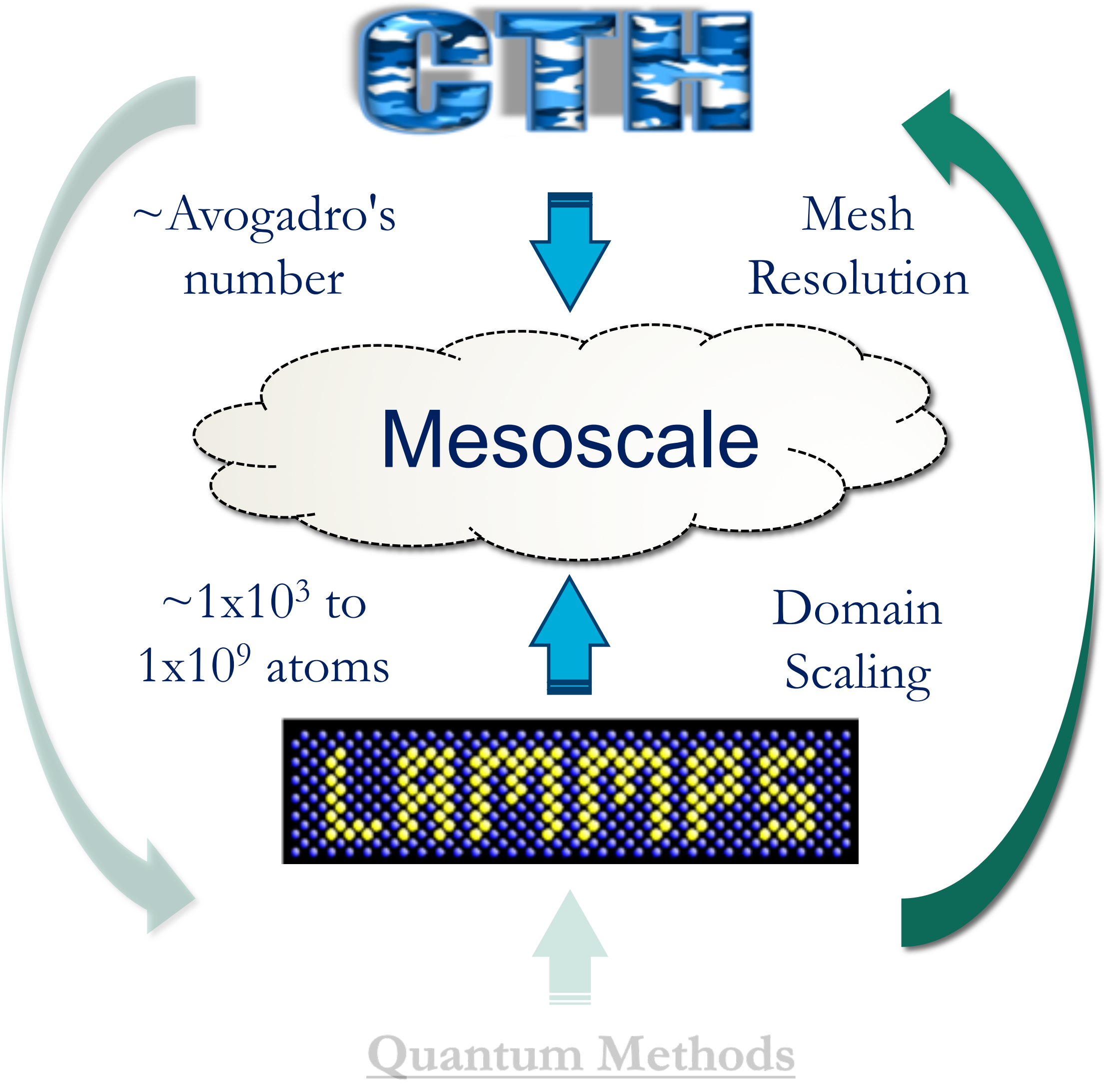

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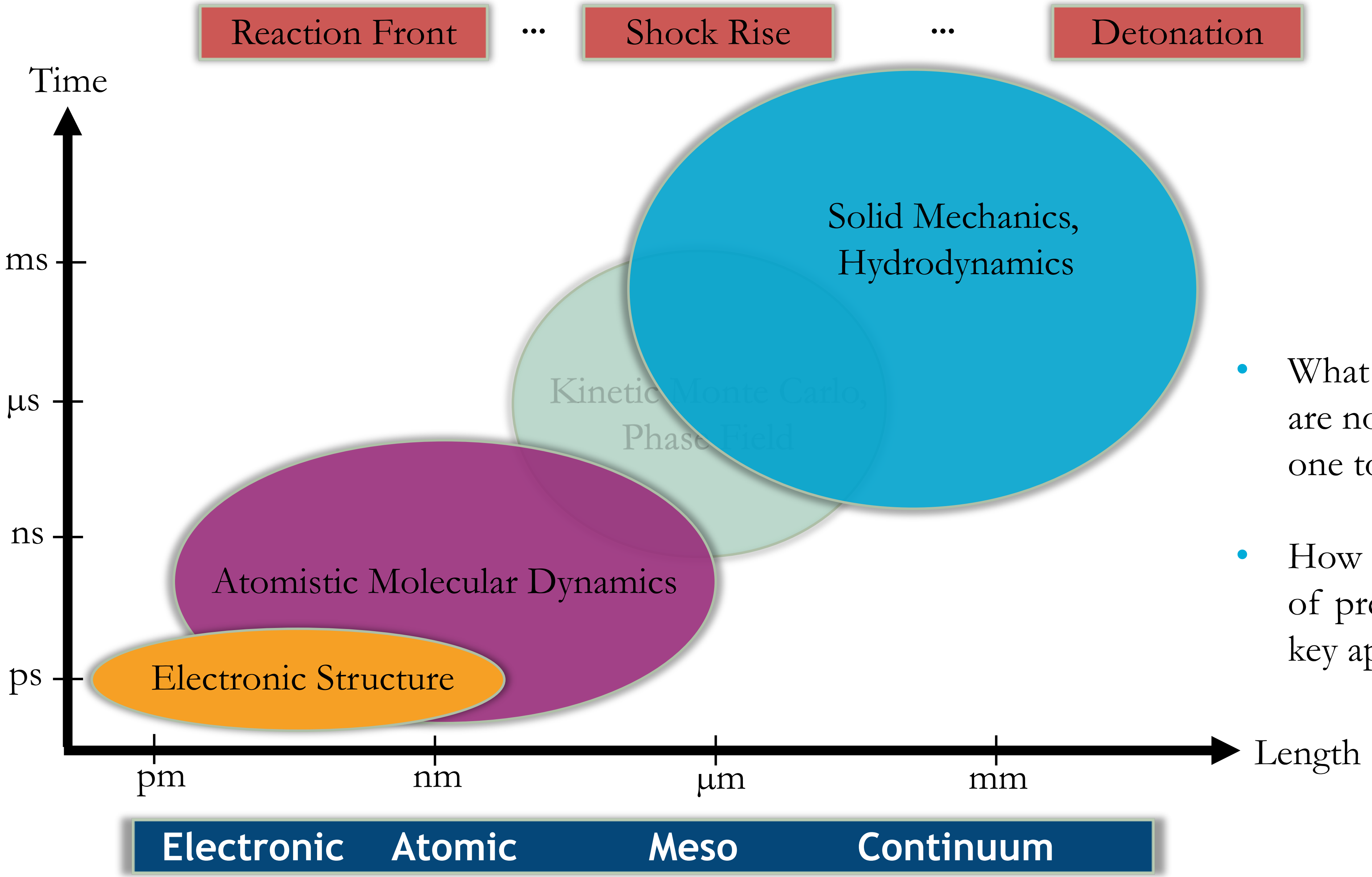
Identifying Vastly Different Approximations



- What to do for problems that are not well posed within any one tool?
- How can we preserve accuracy of predictions where multiple key approximations are made?

Strength Models in Hydrodynamics (the approximation)

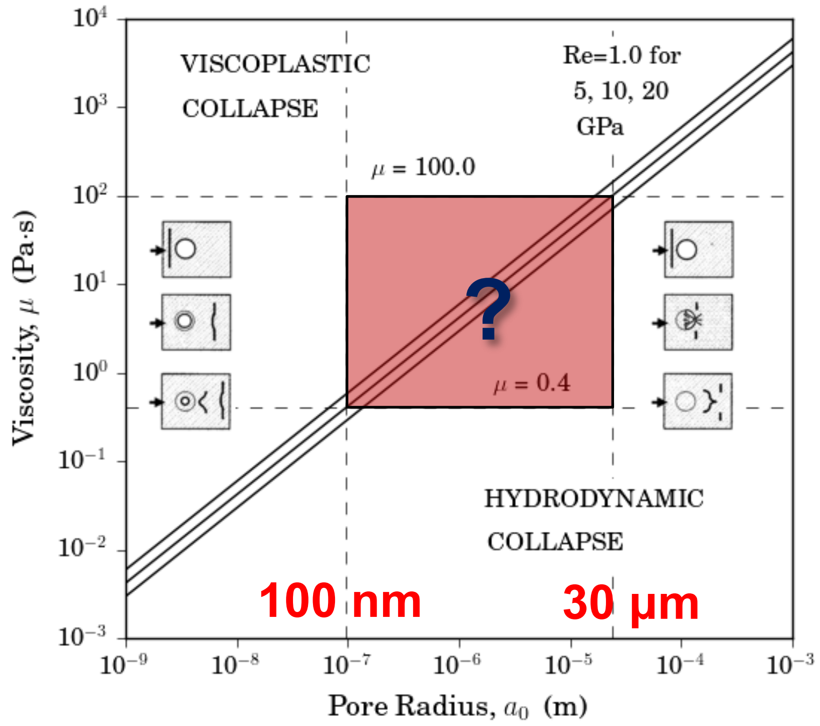
- A hydrodynamics code approximates a solid as a viscous liquid
  - Solves Navier-Stokes equations on a grid preserving mass and energy through grid
- But what about heterogenous materials? Or where material strength matters?

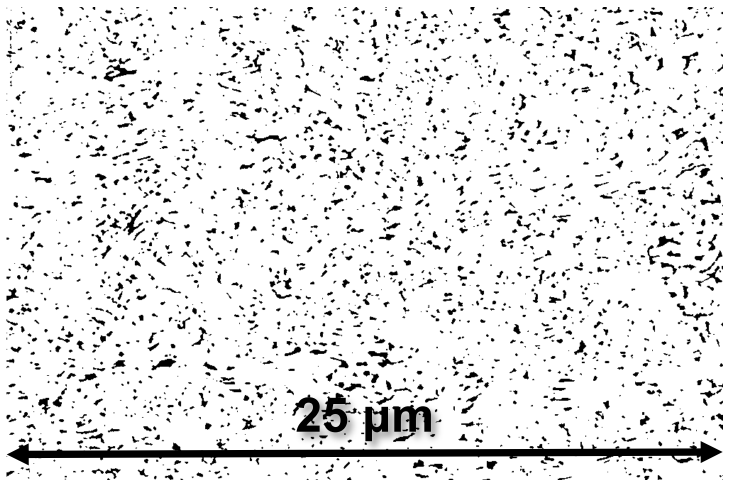
$$Re = \frac{Inertial\ Forces}{Viscous\ Forces} \sim \frac{a_0\sqrt{\rho P}}{\mu}$$

Pore Radius, a_0
(Shock) Density, ρ
(Shock) Pressure, P
(Shock) Viscosity, μ

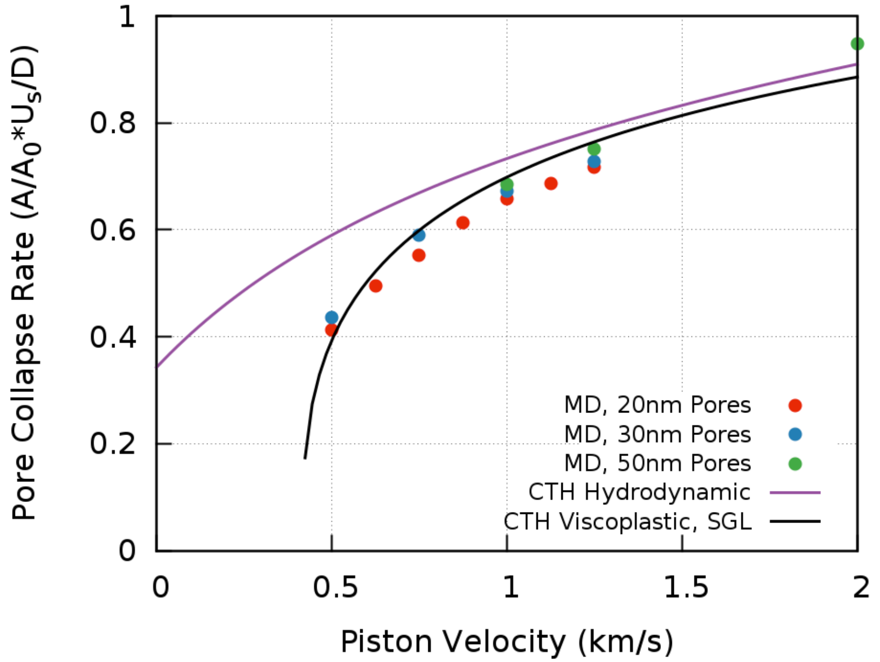
$$\mu = a_0\sqrt{\rho P}$$

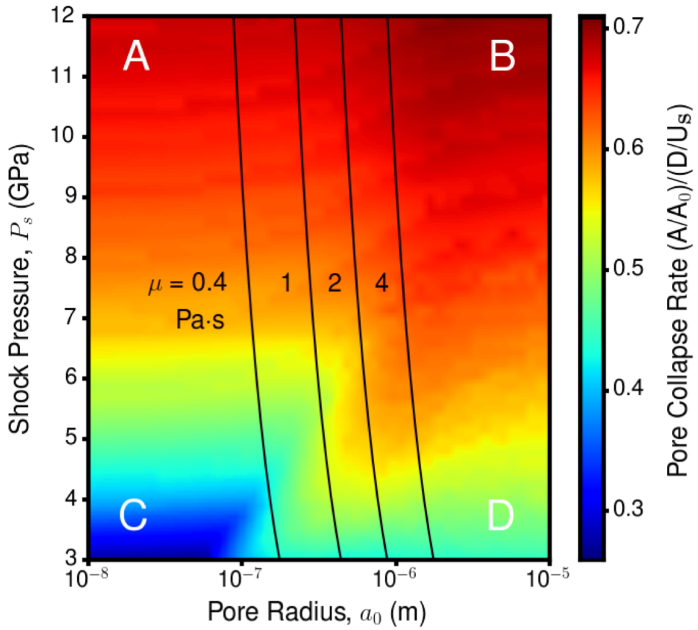
$$P = \frac{1}{\rho}\left(\frac{\mu}{a_0}\right)^2$$

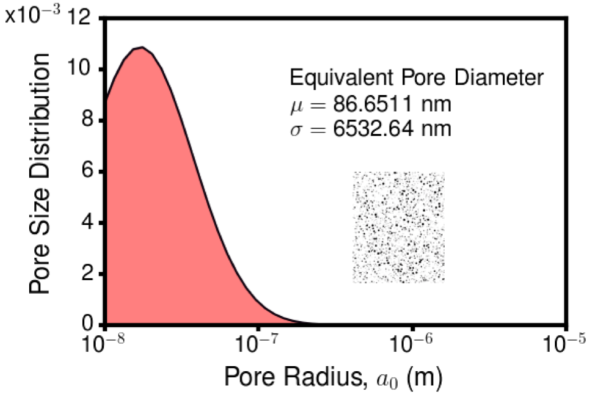


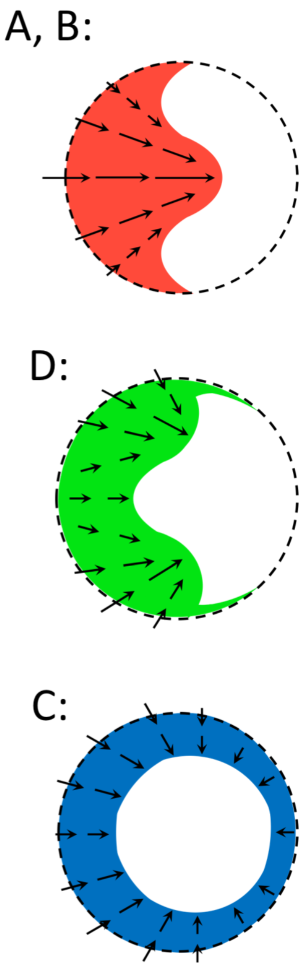


Moving Beyond the MD Scale



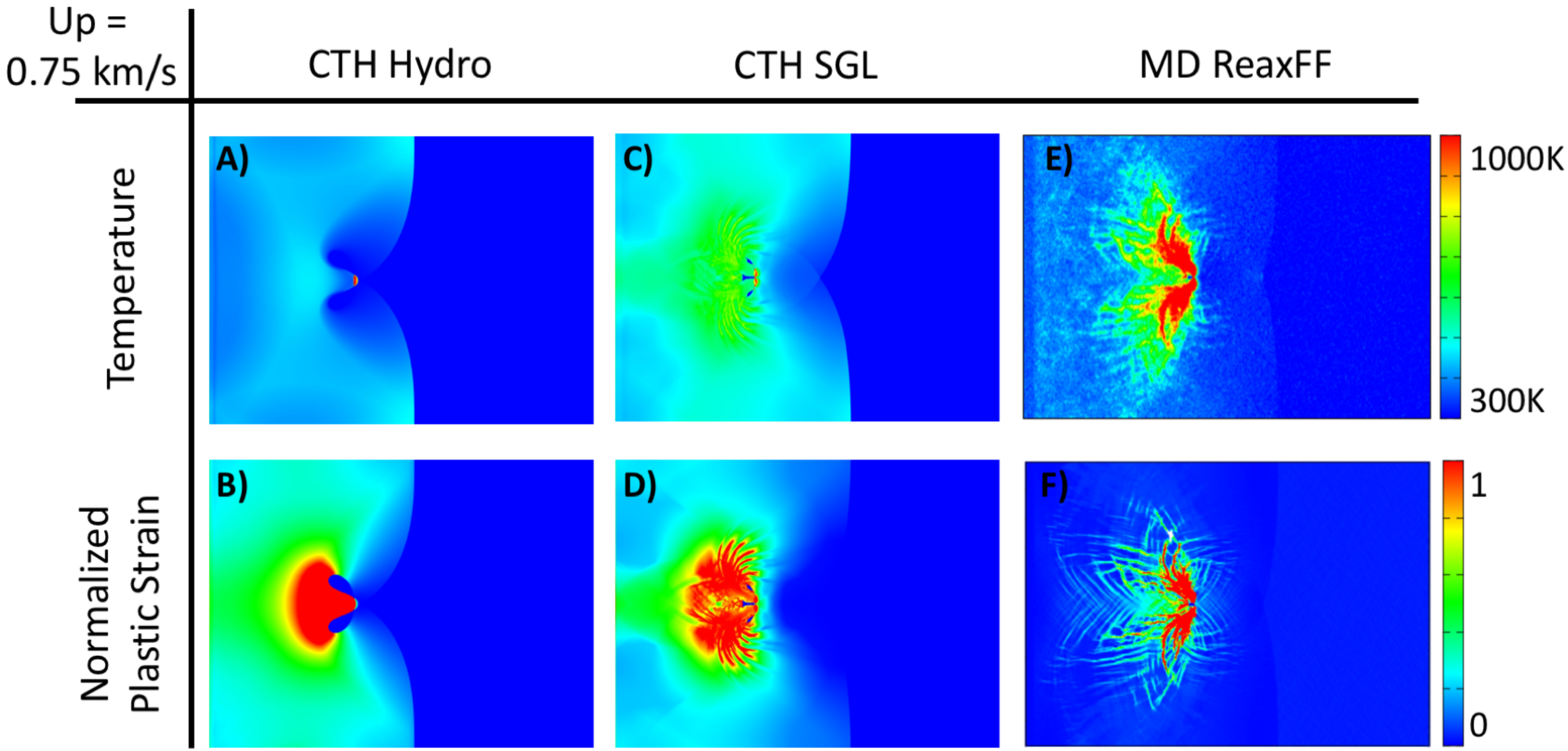






- Training data of collapsing pores from MD sent to CTH for strength model parameterization

Much Better Mechanical Agreement



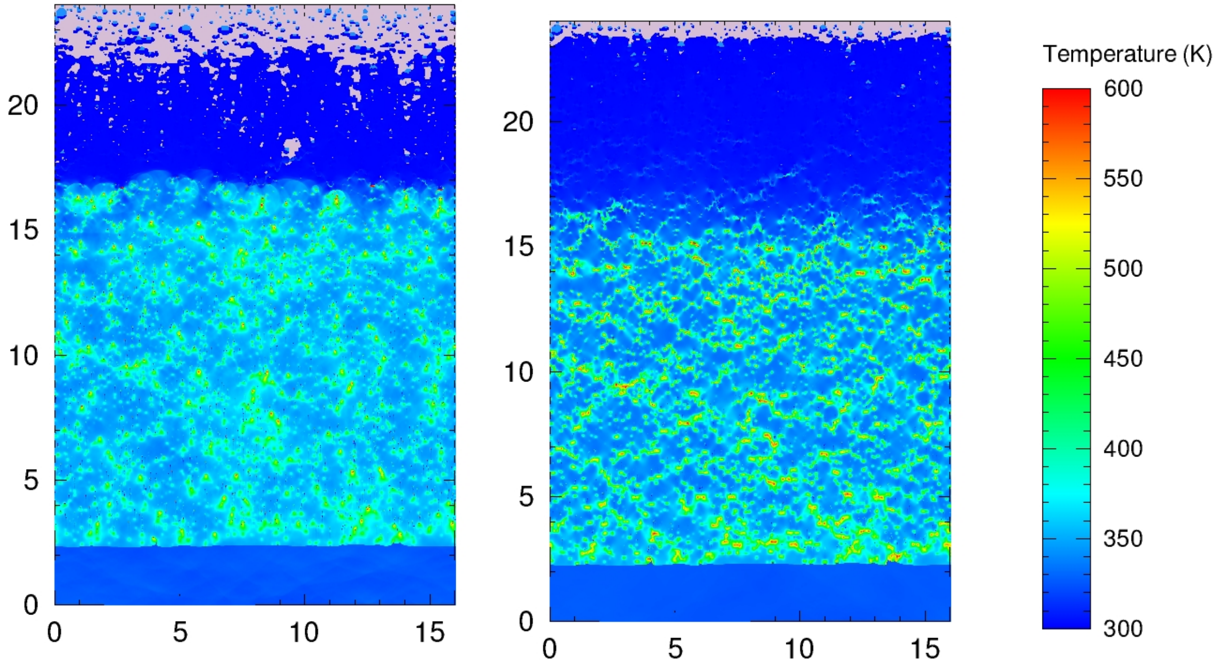
CTH now predicts:

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

Practical Effects of Strength Models

$$\sigma_{ij} = \bar{P}\delta_{ij}$$

$$\sigma_{ij} = \bar{P}\delta_{ij} + S_{ij}$$



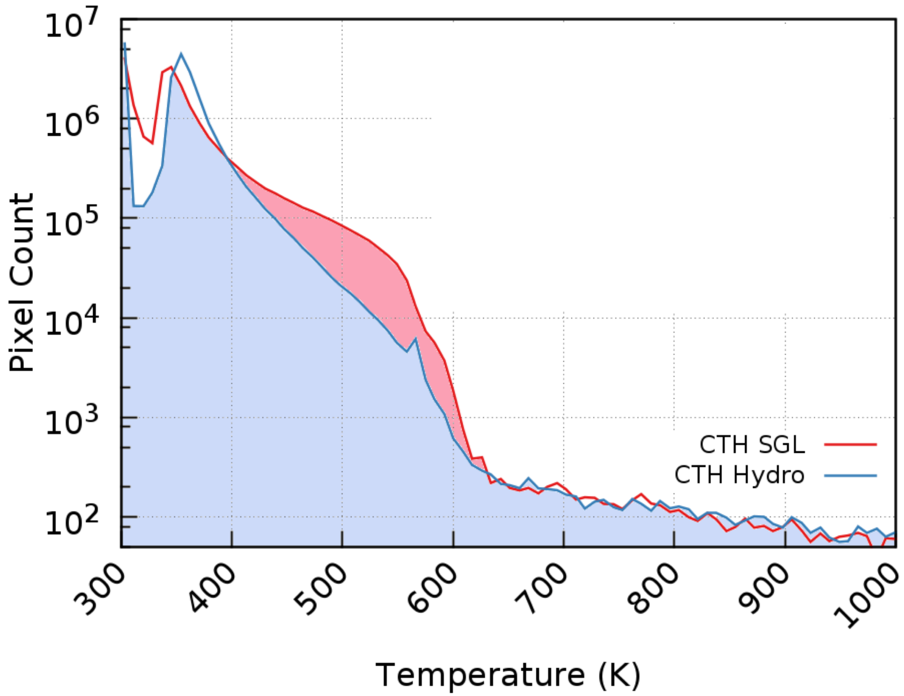
Hydrodynamic

- Higher average temperatures
- More dispersion of leading shock

Current SGL model

- Higher local temperatures
- Similar "collapse" times

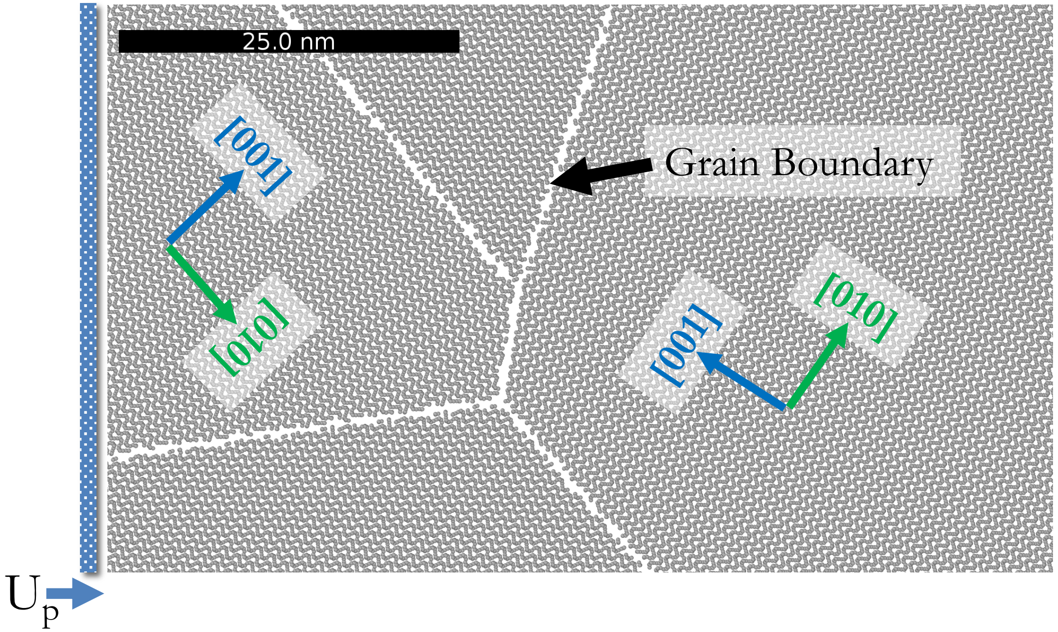
- Microstructure generated using experimental pore size distribution
- Piston impact at 0.6 km/s



What are we missing?

Crystallographic Orientation

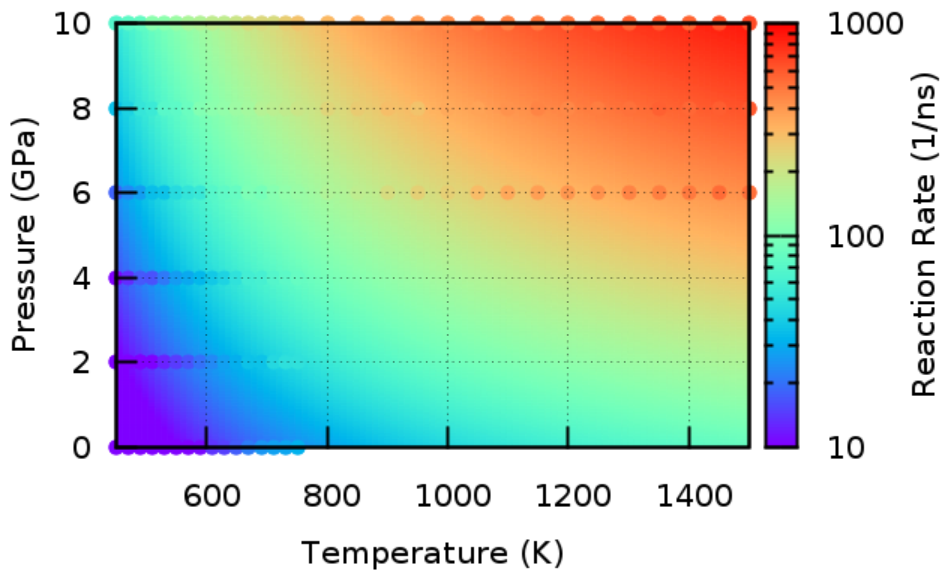
- Single crystal shock response is clearly an approximation at the mesoscale, grain boundaries and orientation effects need to be considered.
- Is a full crystal plasticity model needed?



Reaction Kinetic Terms

- CTH burn models are parameterized to experiments with limited data, reactive MD can fill this gap by providing burn rates: $\dot{\lambda} = f(\lambda, P, T)$
- The challenge is accessible timescales, not length scale as in pore collapse

Stretched Arrhenius: $\dot{\lambda} = (P - P_0)^n e^{-\Delta G / k_b T}$



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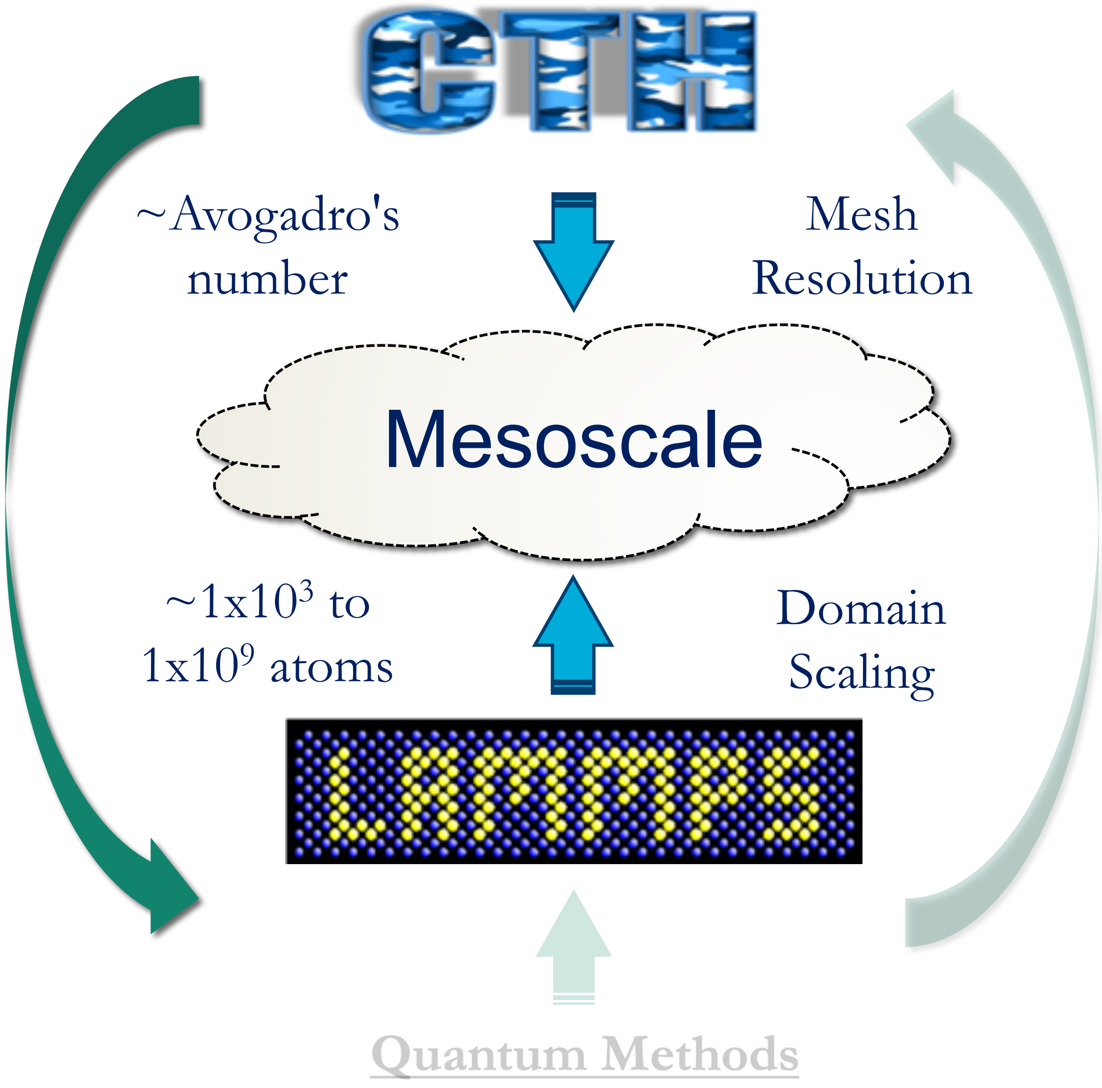

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Modeling Ignition and Growth

Beyond Heuristics

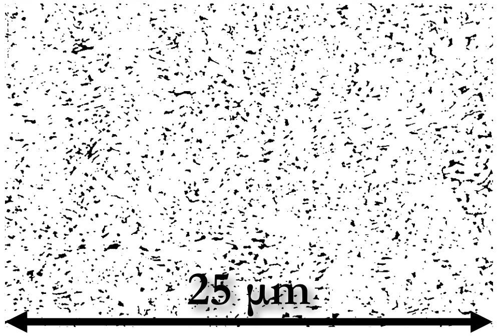
- Energy content is a matter of chemical composition, energy release rate is a function of the microstructure
- Quantifying sensitivity has been an outstanding problem
- Relative measures at best TATB<RDX<TATP etc.

HNS-IV Lot 1

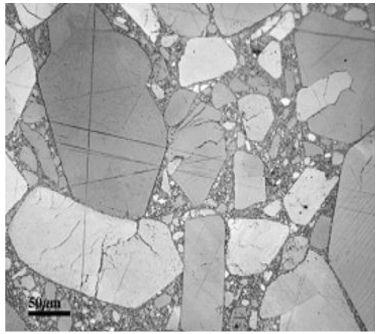
HNS-IV Lot 2

HNS-I

Pressed powders



Plastically bonded



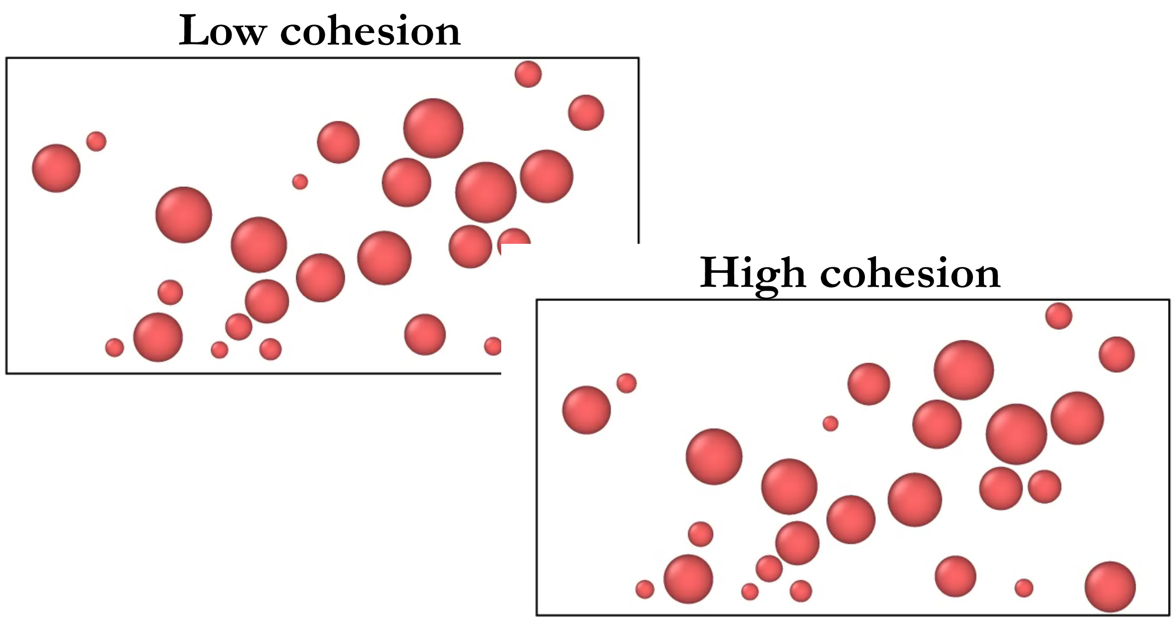
- Isolated hot-spots are unlikely to cause detonation, the entire material acts as a thermal bath
- We assume extended defects, or interacting clusters of hot-spots are responsible for I&G
- Looking at a micrograph, can we make estimates of shock sensitivity?

Synthetic Microstructure Generation

Discrete Element Method

- Experimental micrographs are hard to come by, need an alternative for input geometries
- A pore is now a particle, take snapshots from this coarse grained simulation.

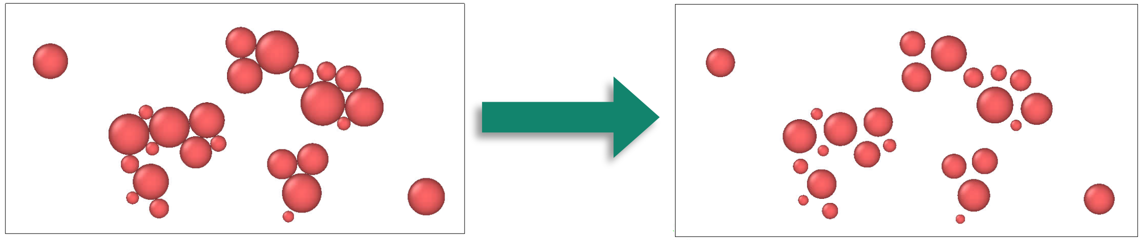
Langevin dynamics with range of contact cohesion values:



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

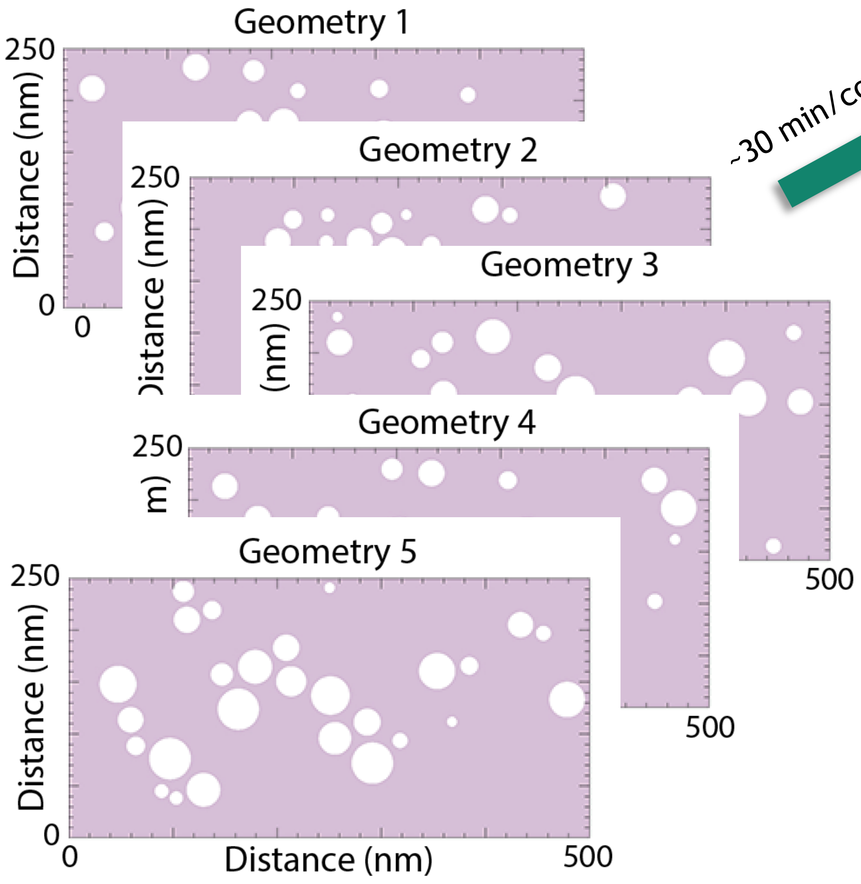
Variations: Particle size distribution, TMD, cohesion, friction, random seed

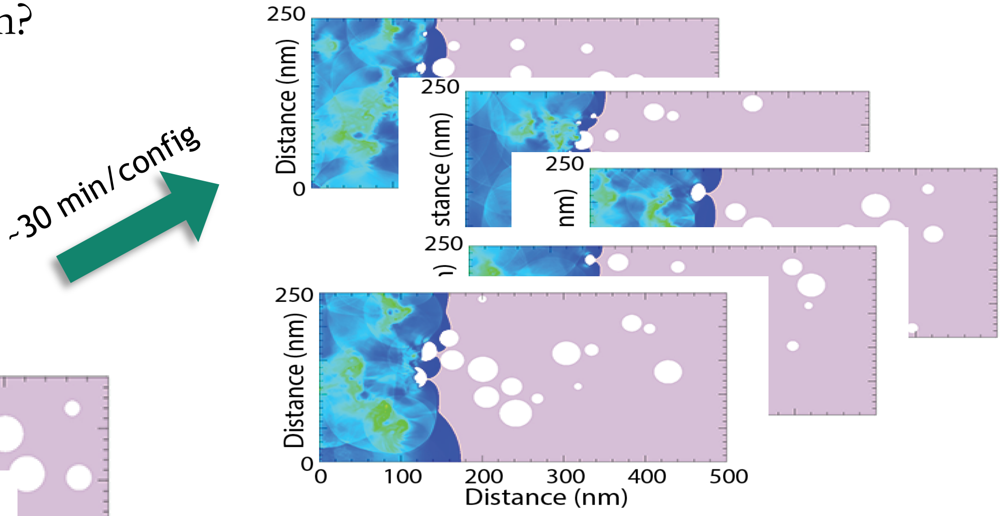
Final step: shrink particles uniformly to generate final configuration



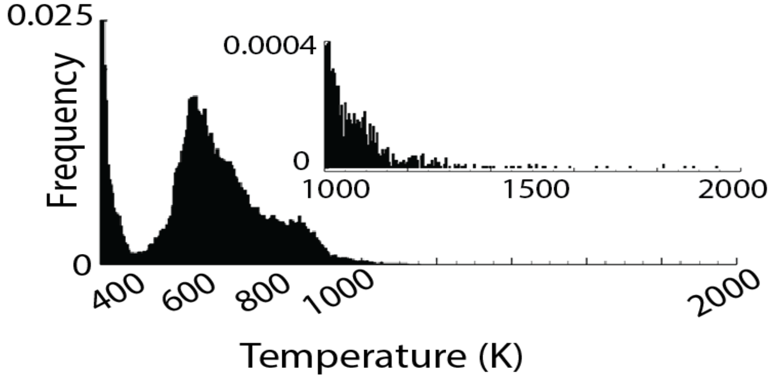
Proxy Measure of Sensitivity

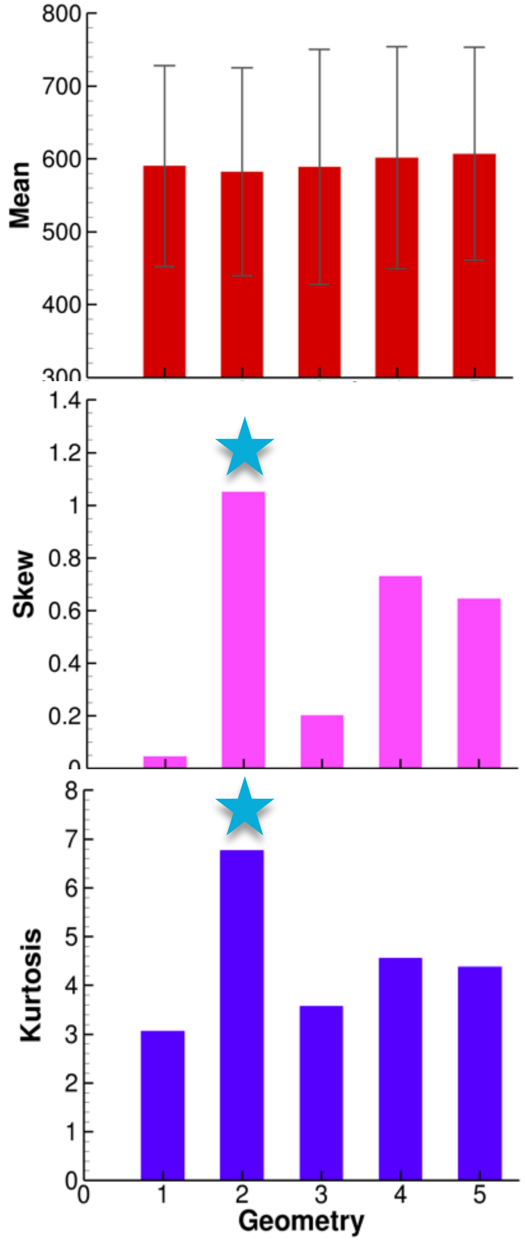
- Which pore clusters lead to ignition?





- Ignition probability ~ Temperature Distribution





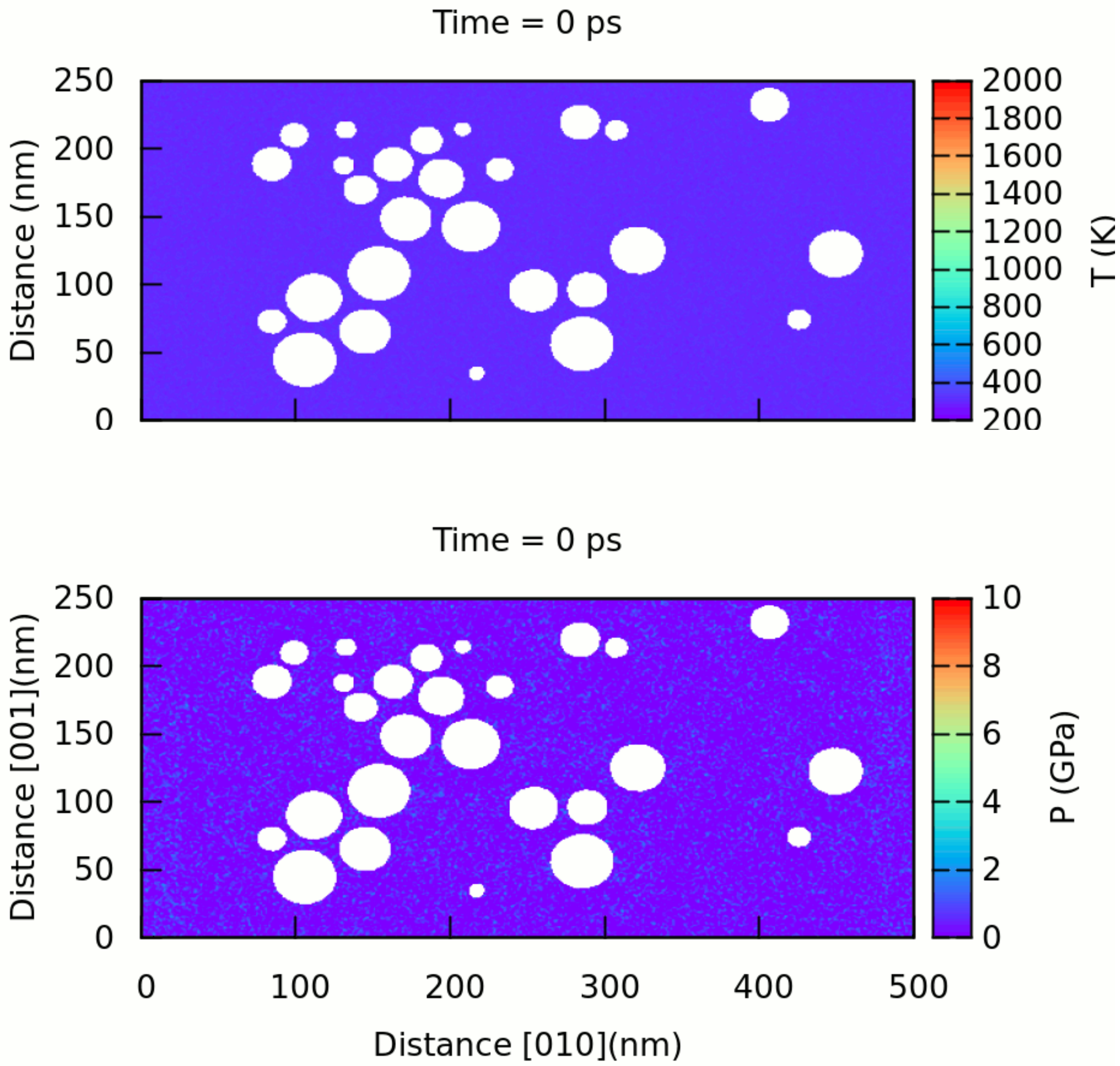
CTH Exploration, Return to MD

Limiting the computational cost

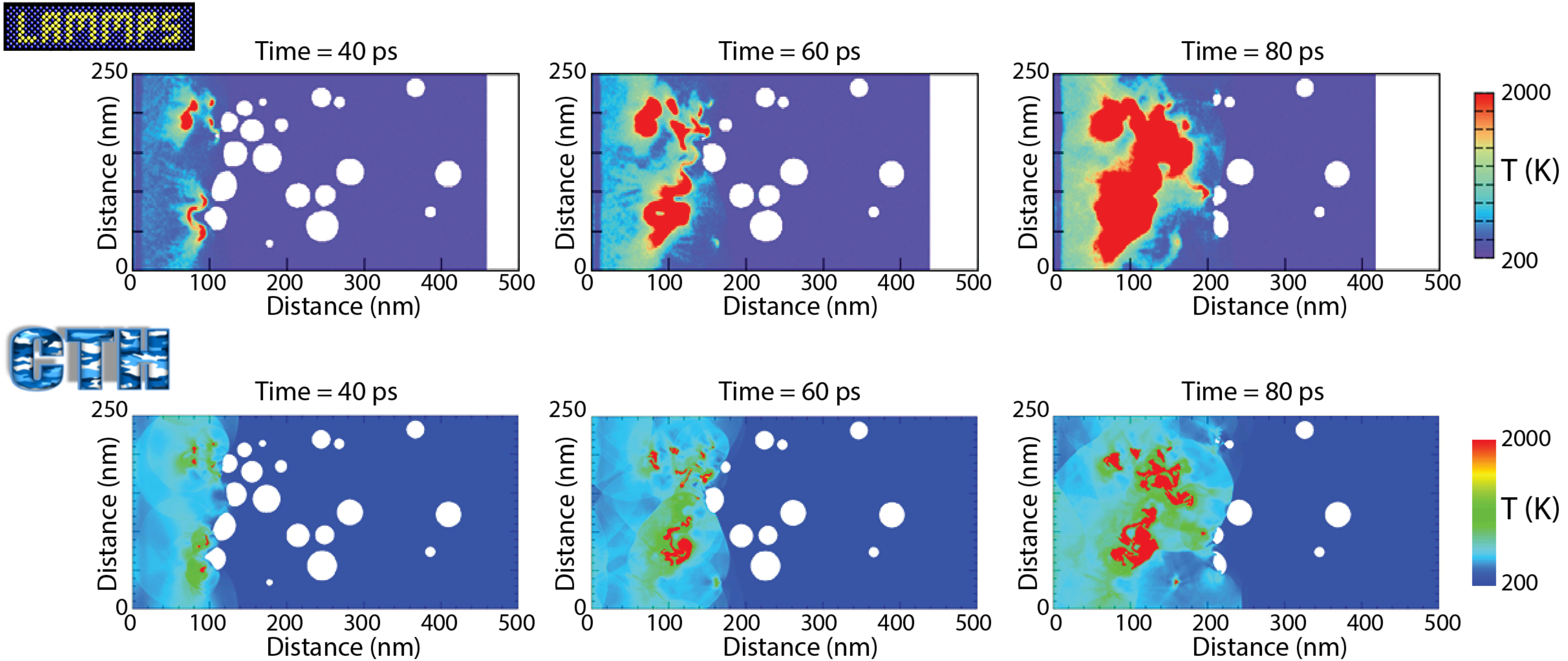
- Generated synthetic microstructures can still be directly simulated in MD (~22M atoms, ~3.3M cpu*hours)
- Detailed chemistry for 'free' with ReaxFF, can capture ignition → deflagration with realistic hot spots

Scale-free observations

- Still working with very small pore sizes, these are still proof-of-concept simulations of the CTH → MD coupling
- With more pores, more rarefactions and shock reflections.



Chemical Agreement Needs Some Work



Conclusions and Outlook

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- The interesting physics/chemistry of shock waves in energetic materials span many length and time domains, necessitates a merger of computational tools

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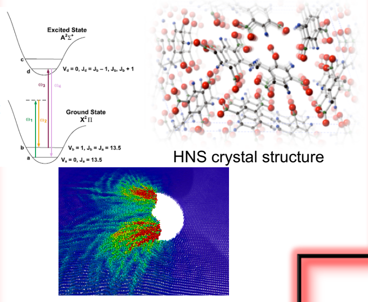

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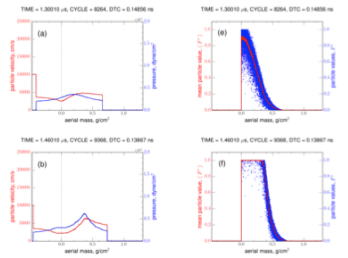

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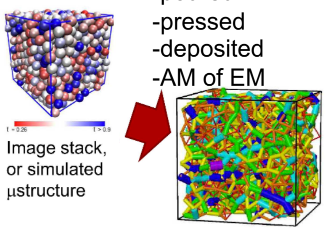

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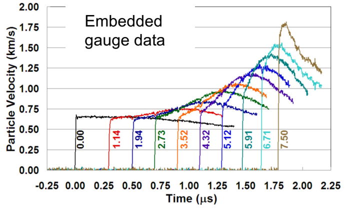

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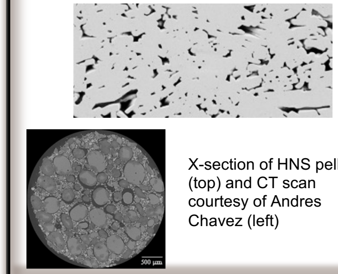

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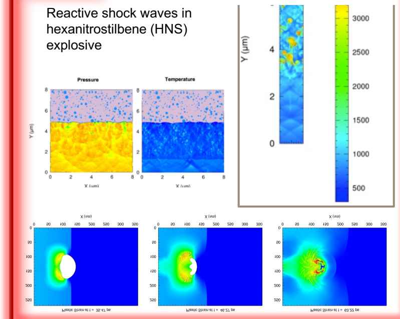

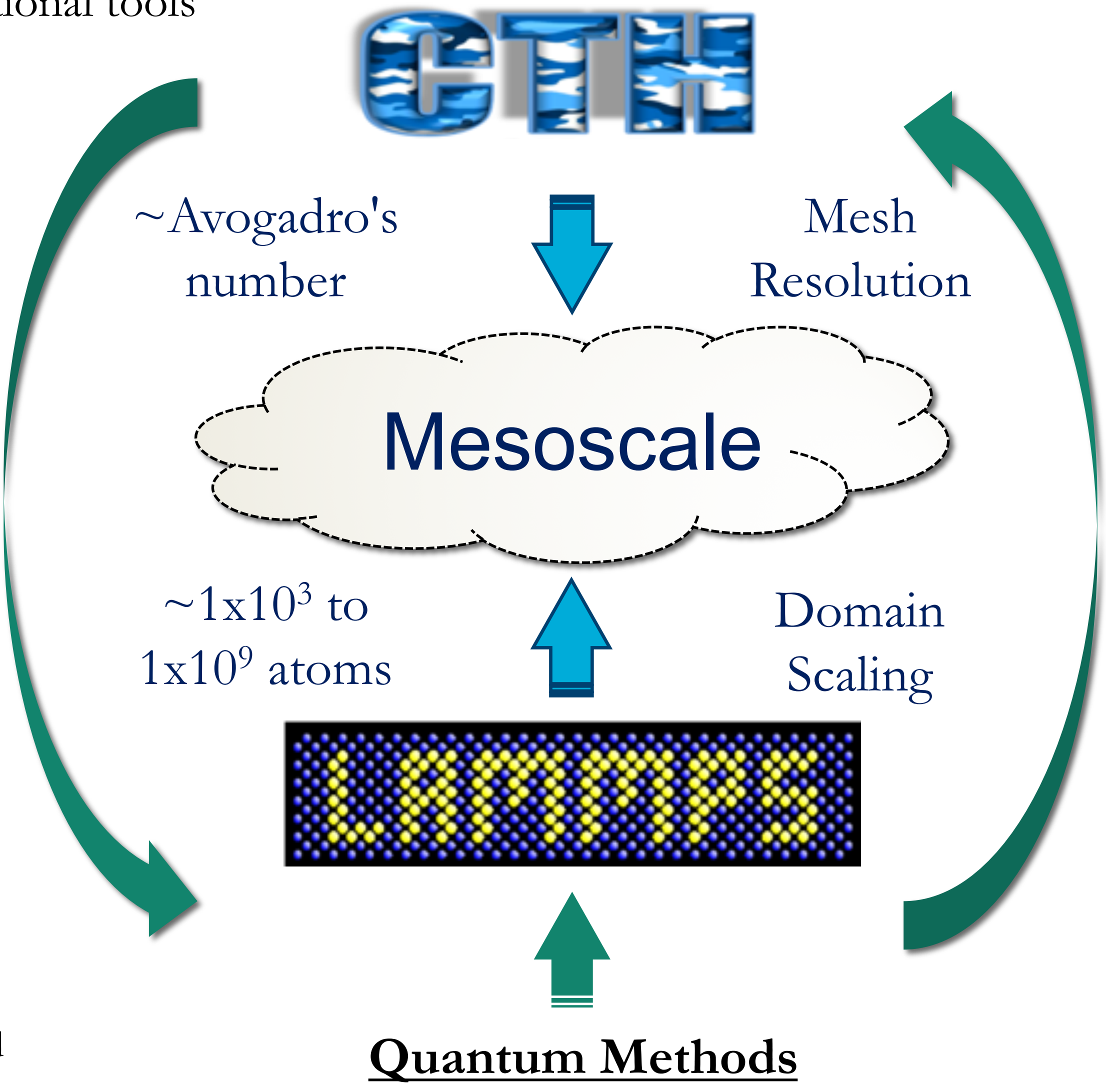

Advanced Scientific Computing: Physics and Engineering Models

Lab Directed Research and Development