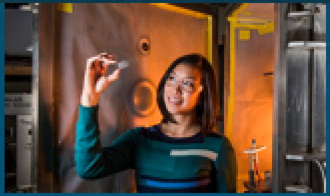
SAND2022-2766C

Sandia National Laboratories

Data Mining the Mesoscale to Study Shock Ignition and Reaction Growth in Pressed Energetic Materials



TMS 2022 Annual Meeting and Exhibition

Anaheim, CA

Feb 27 – March 3, 2022

PRESENTED BY

Judith Brown, Julia Hartig, Michael Sakano, Dan Bolintineanu, Mitch Wood

March 14, 2022

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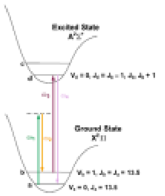
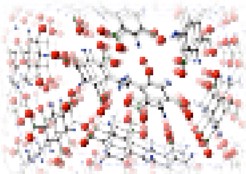
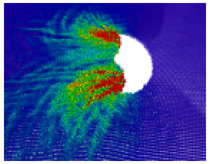
Shock Initiation of Explosives at Sandia

Quantum / MD Large Scalable Codes



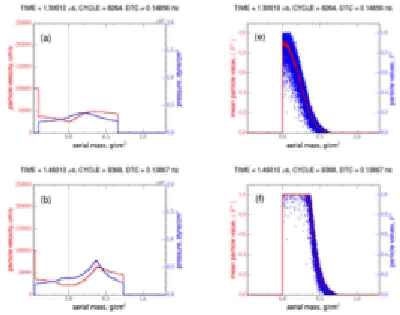


crystal structure



LAMMPS + Kokkos

New Continuum Codes



Stochastic reactive shock waves

Formation Modeling

-poured
-pressed
-deposited
-AM of EM

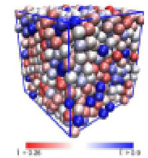
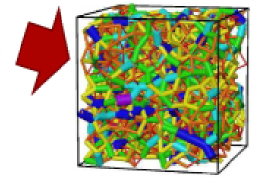


Image stack, or simulated μstructure



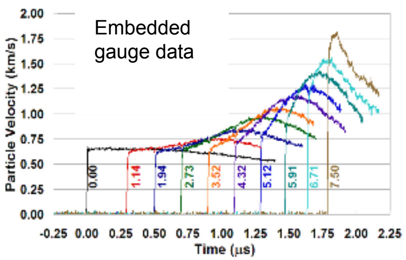
Graph of contact network

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

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

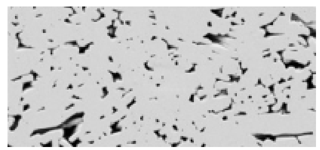
Tests and Experiments

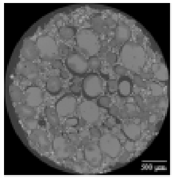
- Performance
- Sensitivity
- Threshold and UQ



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

Microstructural Analysis

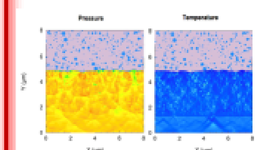


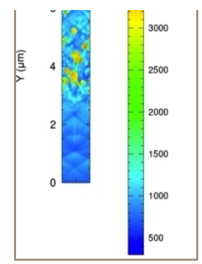


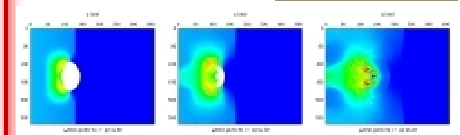
X-section of pressed pellet (top) and CT scan courtesy of Andres Chavez (left)

Mesoscale Simulations

Reactive shock waves in pressed explosive



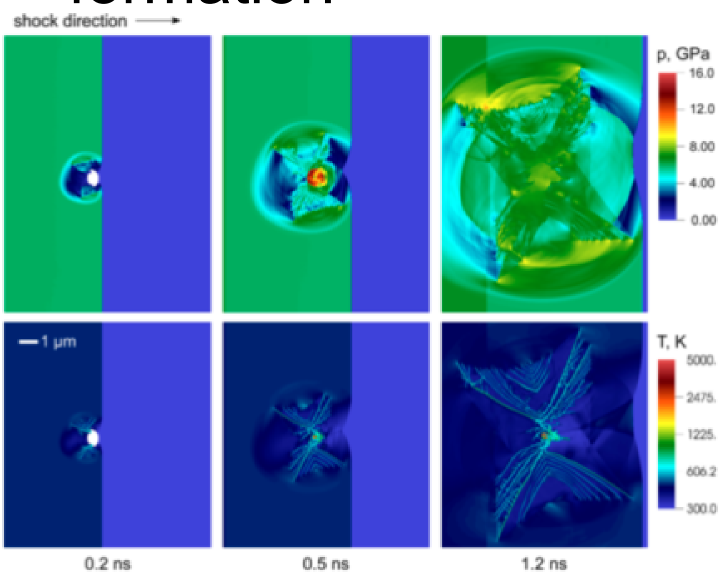




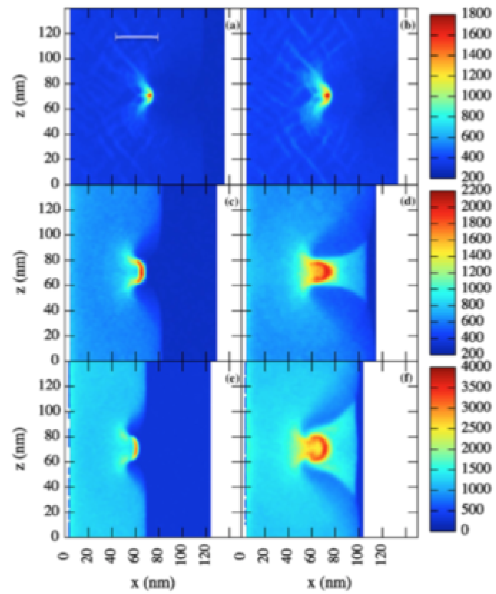
Role of Porosity in Shock Initiation

- Some degree of porosity present in almost all energetic materials
- Pore collapse can be key mechanism for hot spot formation

Many Single-Pore Collapse Studies



Austin et. al, J. App. Phys. 117 (2015), 185902



Eason and Sewell, J. Dynamic Behavior Mater. 1 (2015), 423-438

- What about pore interactions?
- Can we link particular porosity configuration with some metric of sensitivity to detonation?

Microstructure of Pressed Energetics

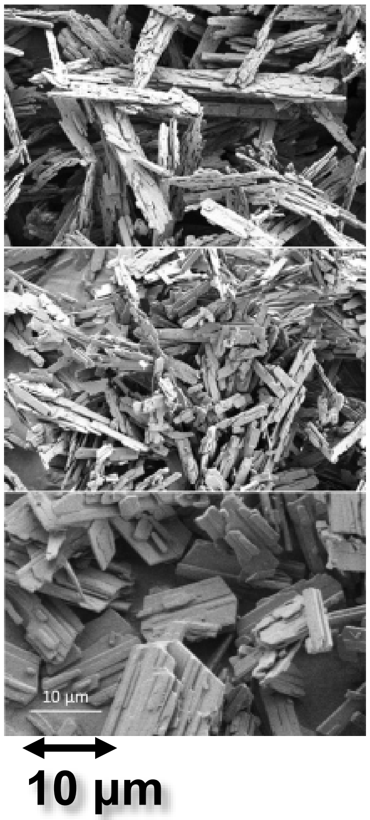
- Energetic material powder pressed to ~90% TMD

Loose Energetic Crystals

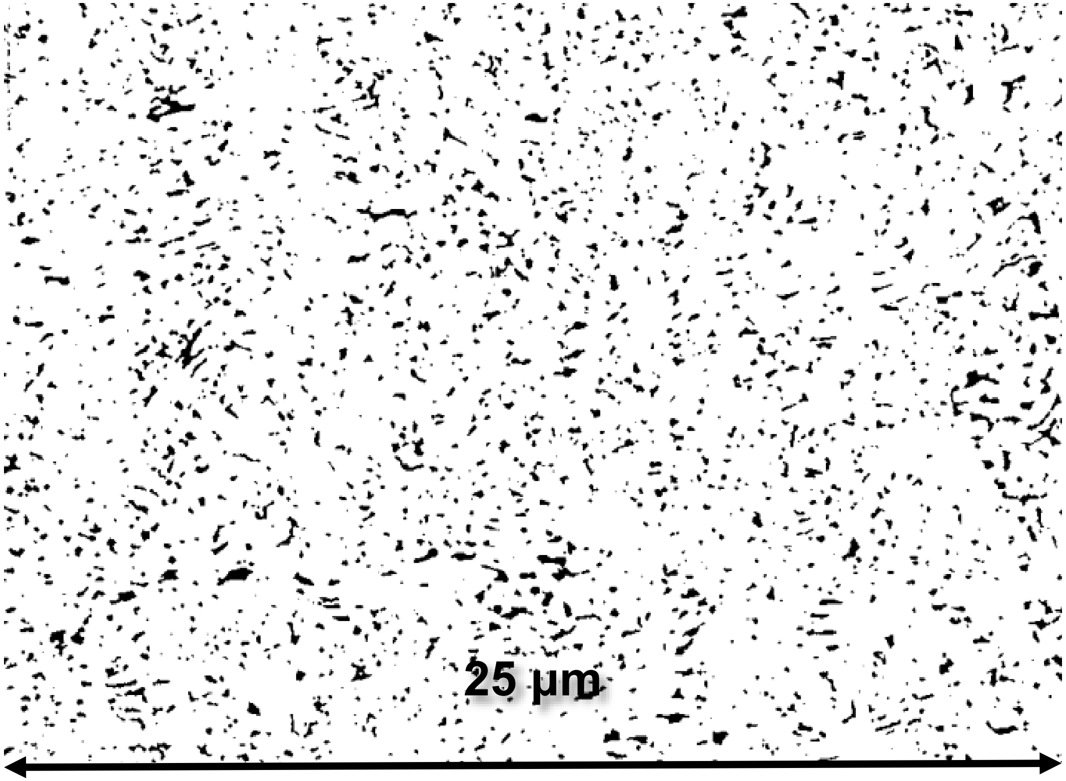
Lot 1

Lot 2

Lot 3



Thresholded SEM image of pressed microstructure



C.D. Yarrington, R.R. Wixom, D.L. Damm, J. App. Phys. 123 (2018) 105901

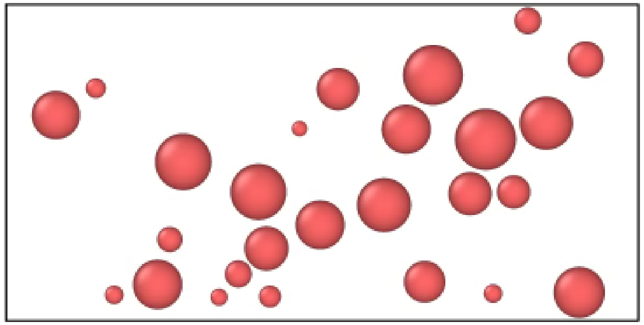
Synthetic Microstructure Generation

- 2D Discrete Element Method (DEM) simulations used to generate many microstructures with different porosity configurations

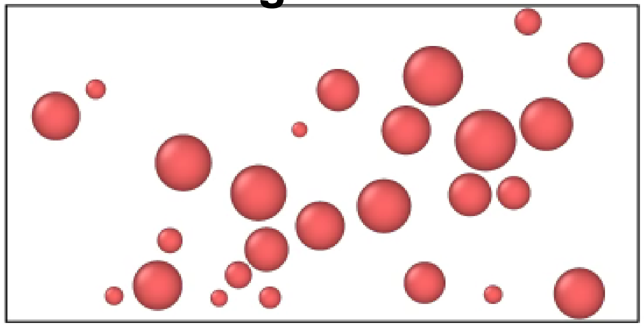
Initial state: spheres placed at random in 250 X 500 nm domain, no overlaps

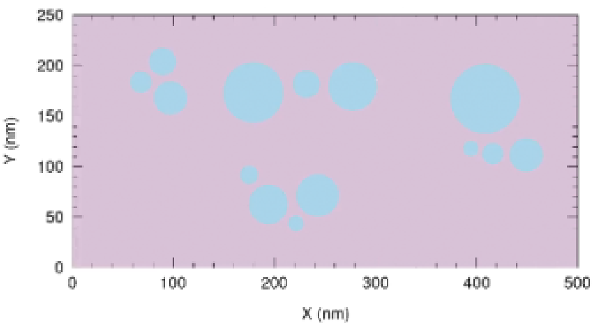
Langevin dynamics with range of contact cohesion values:

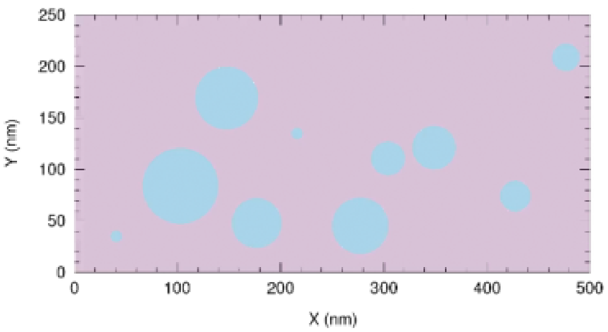
Low cohesion

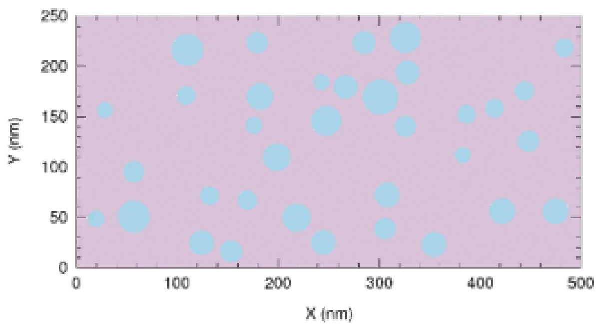


High cohesion



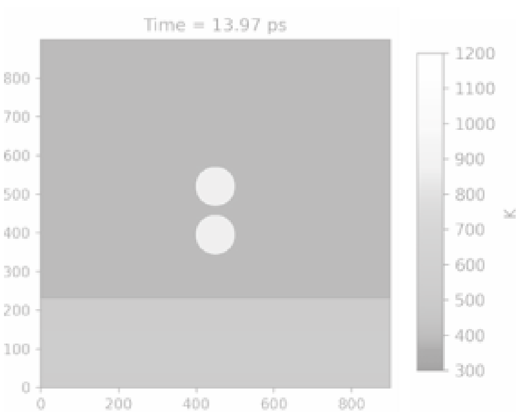




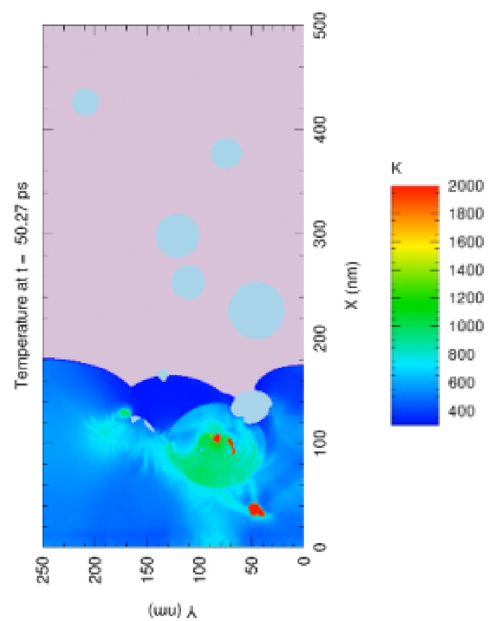


Hierarchical Length Scales in SDT

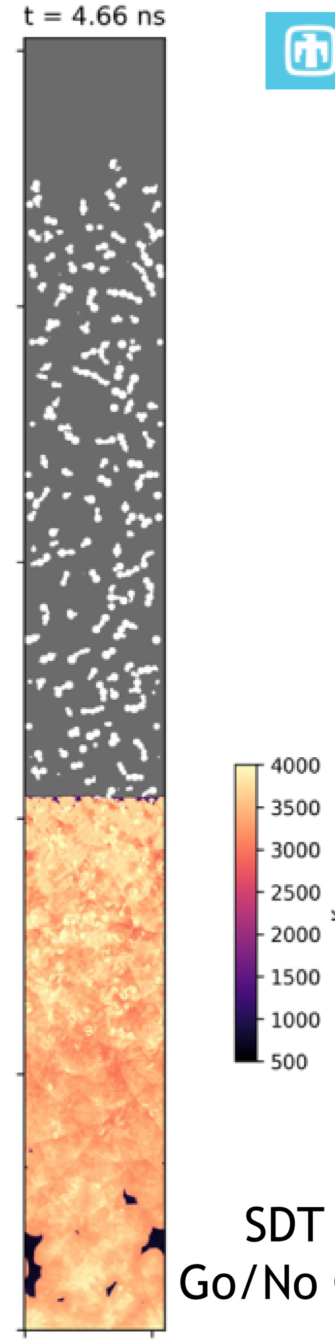
- Two-pore collapse studies
- Small microstructure subset studies
- Full run to detonation distance



Hot spot ignition



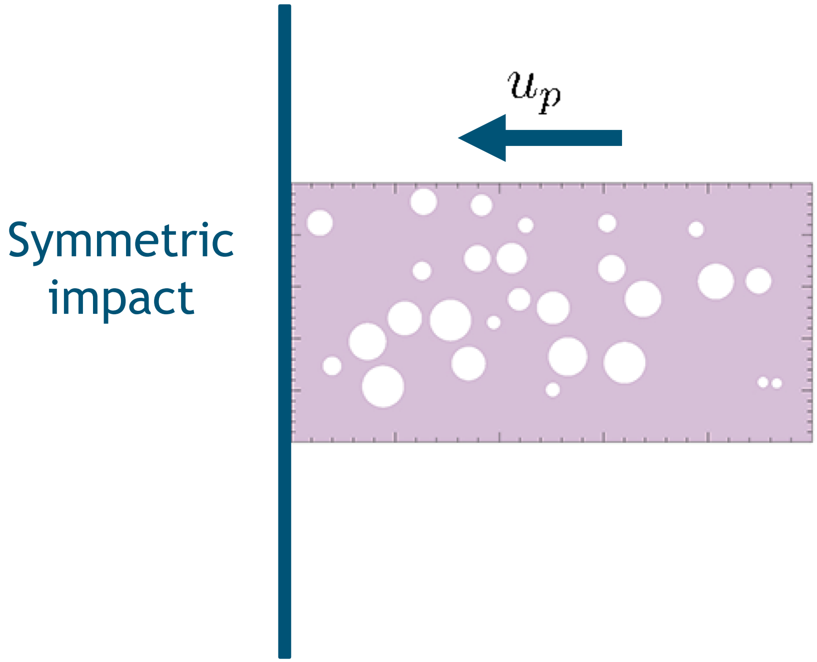
Early sensitivity metrics (??)



SDT
Go/No Go

Continuum Hydrocode Simulations—CTH

- Reverse ballistic impact calculation
- Evaluate many microstructures to elucidate geometries that show higher propensity for hot spot formation



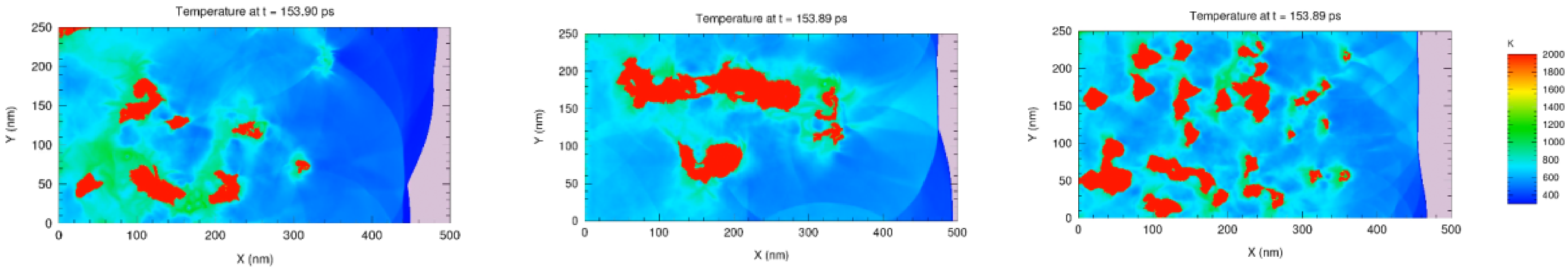
Material Models

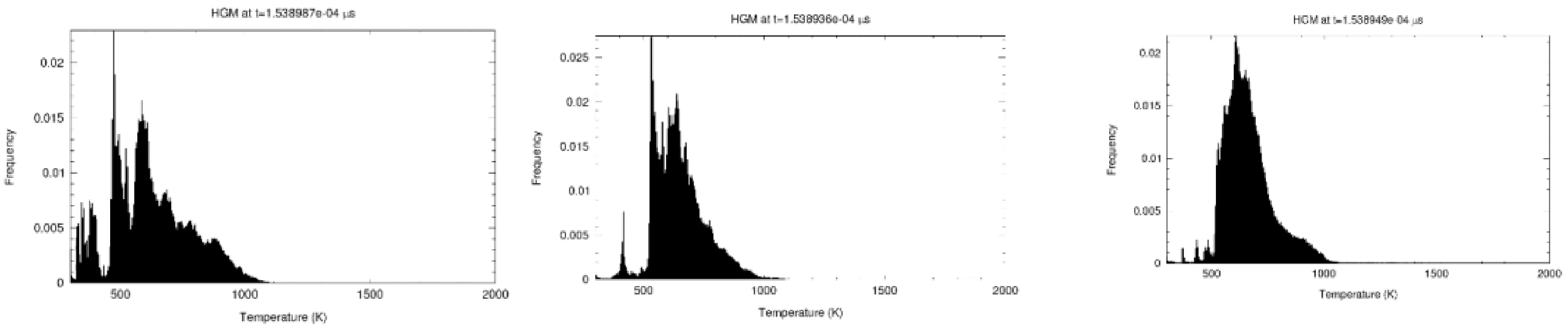
- Pores filled with air
- Energetic matrix:
  - Mie-Grüneisen equation of state
  - Stienberg-Guinan-Lund viscoplastic strength model
  - Arrhenius burn model

Single-pore collapse rate was used to calibrate SGL model from MD simulations

Mine Temperature Field Data for Sensitivity Indicators

- Temperature histograms provide fingerprint for each microstructure and its hot-spot evolution---note these change over time and include both ignition and growth information



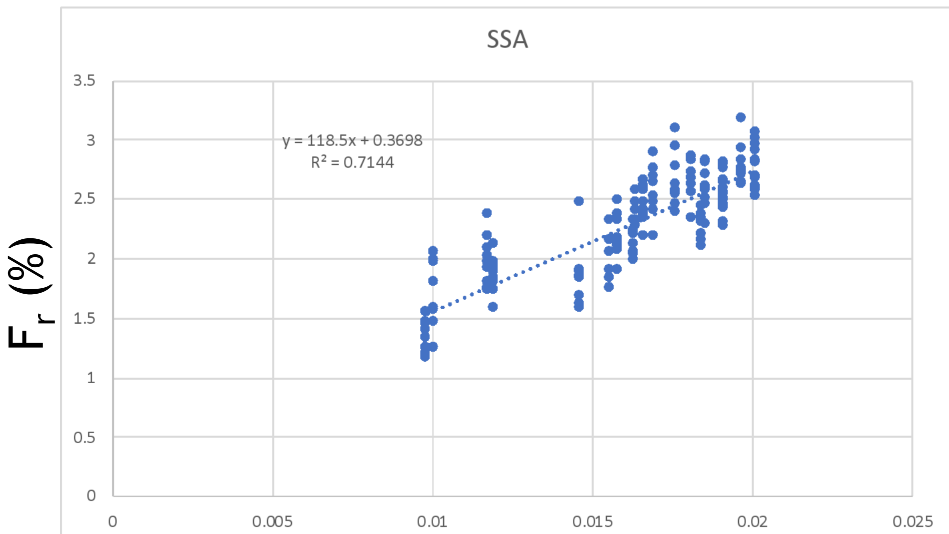


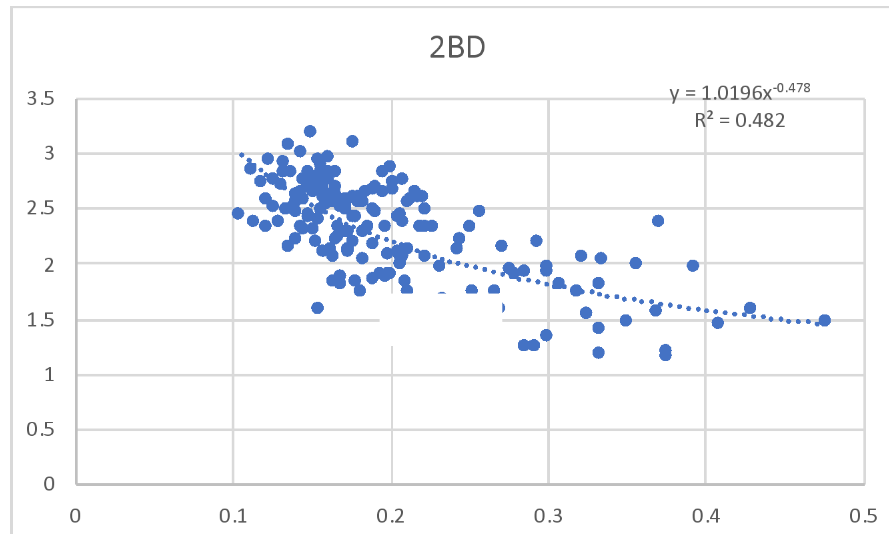
- Area fraction of reacted material, F_r provides information about reaction growth

$$F_r = \frac{\Sigma area(\lambda > 0)}{totalarea}$$

Area Fraction of Reacted Material Across Many Different Microstructures

- F_r calculated at fixed time (150ps) when shock has traversed ~450 nm

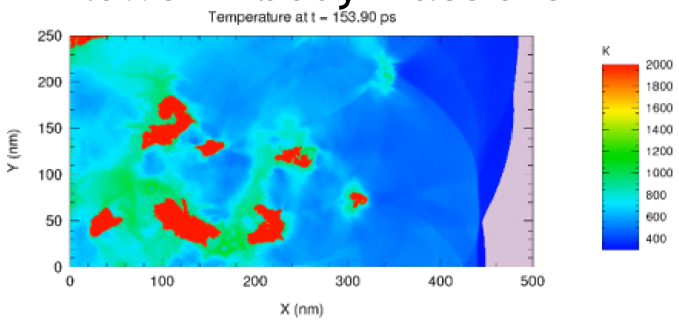




Length Scales, Time History, and Appropriate RVE size

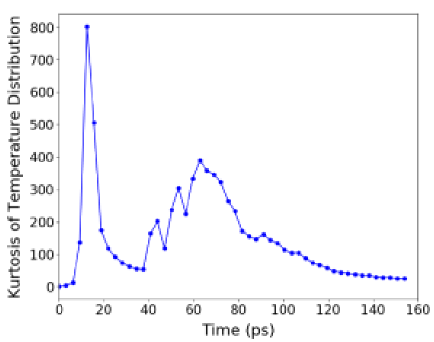
- Consider kurtosis of temperature distribution

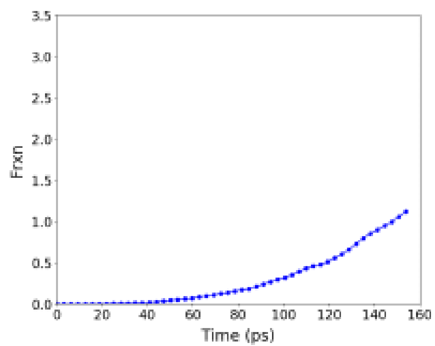
Larger pores, lower SSA, lower 2-body fractions



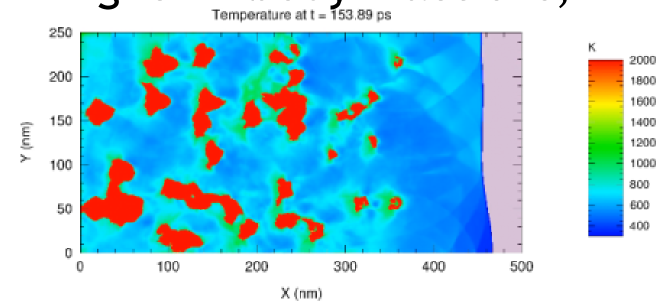
Lower initial peak

Longer time to plateau

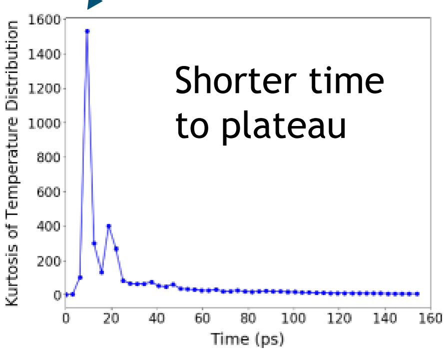




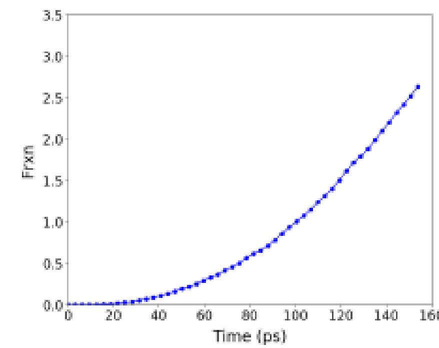
Smaller pores, lower SSA, higher 2-body fractions,



Higher initial peak



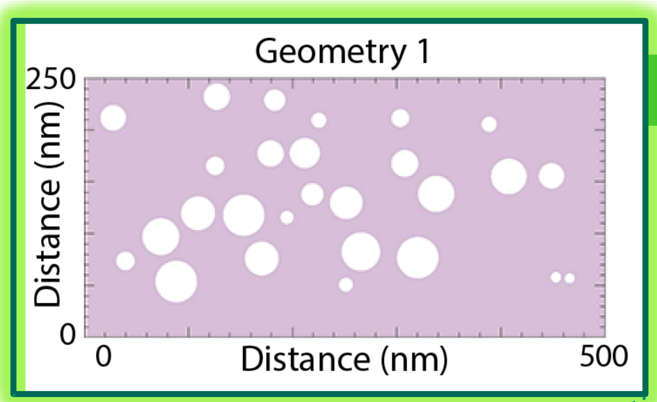
Shorter time to plateau



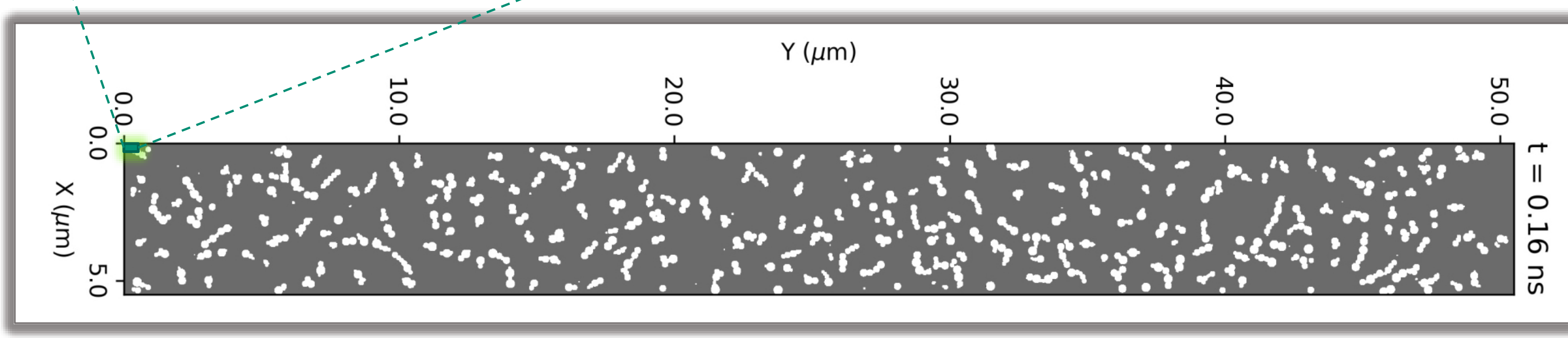
Large Multipore Simulations

Need larger microstructures to see run-to-detonation behavior

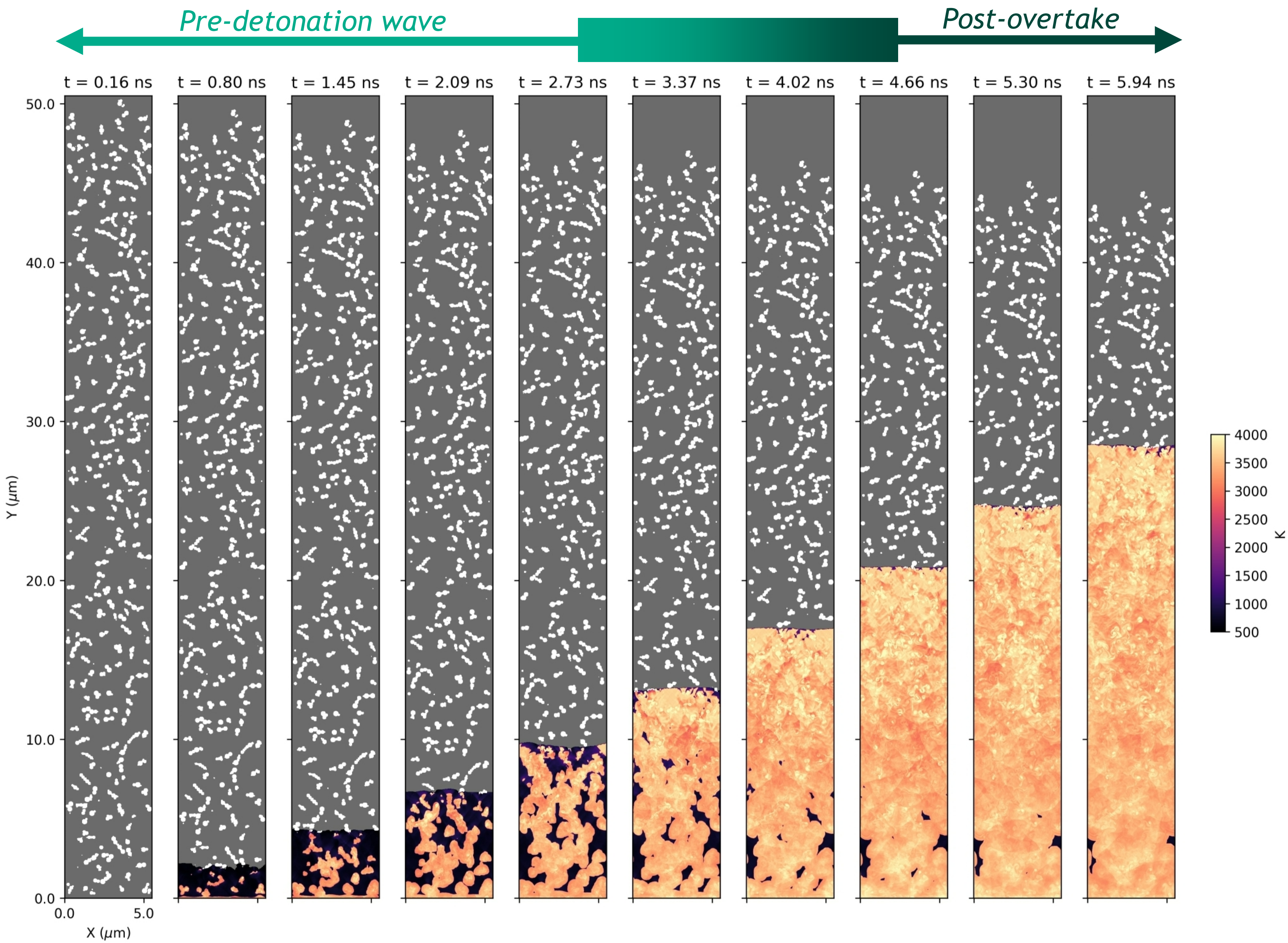
"Small" Multipore



"Large" Multipore

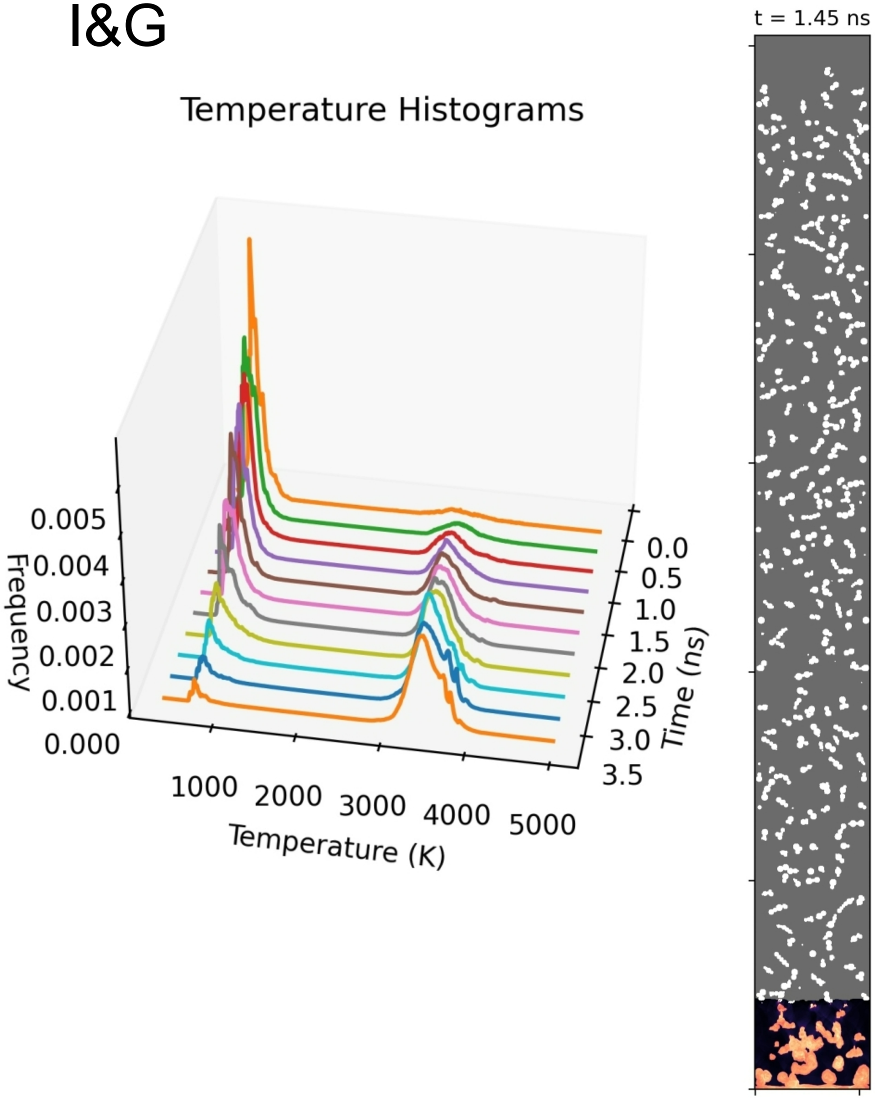


Large Multipore Simulations

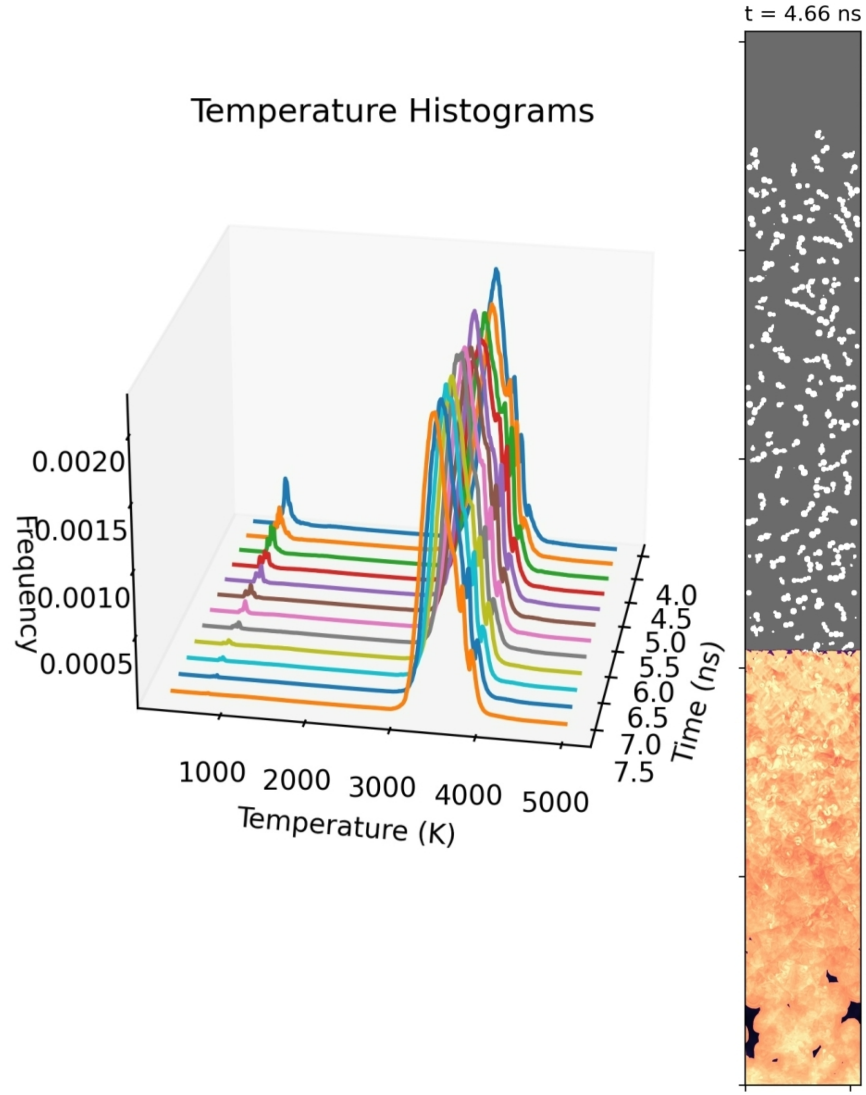


Temperature Histograms

- Pre-detonation hot spot I&G

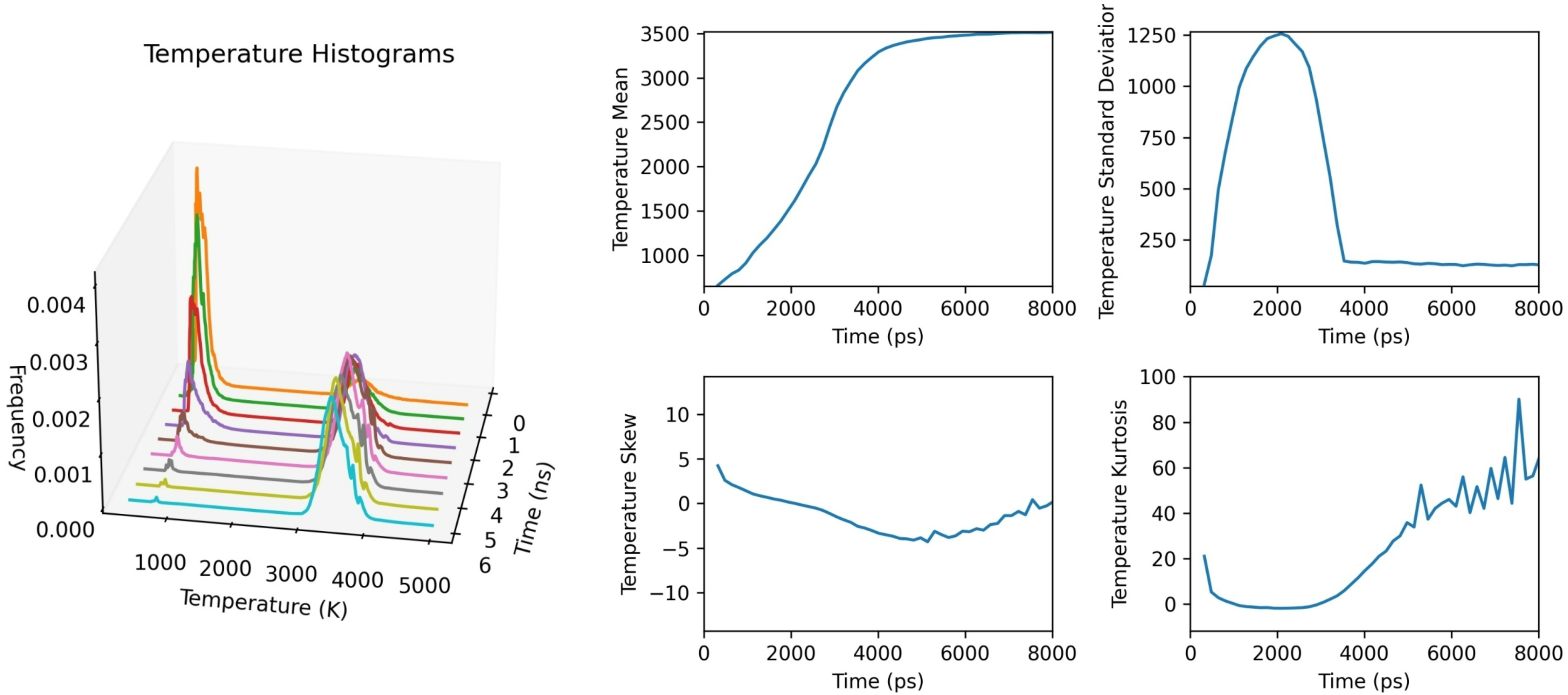


- Detonation



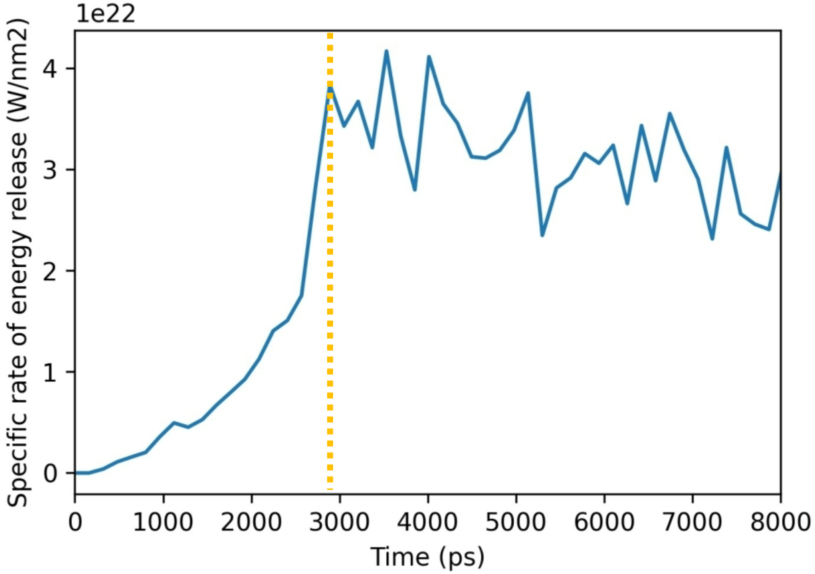
Large Multipore Temperature Statistics

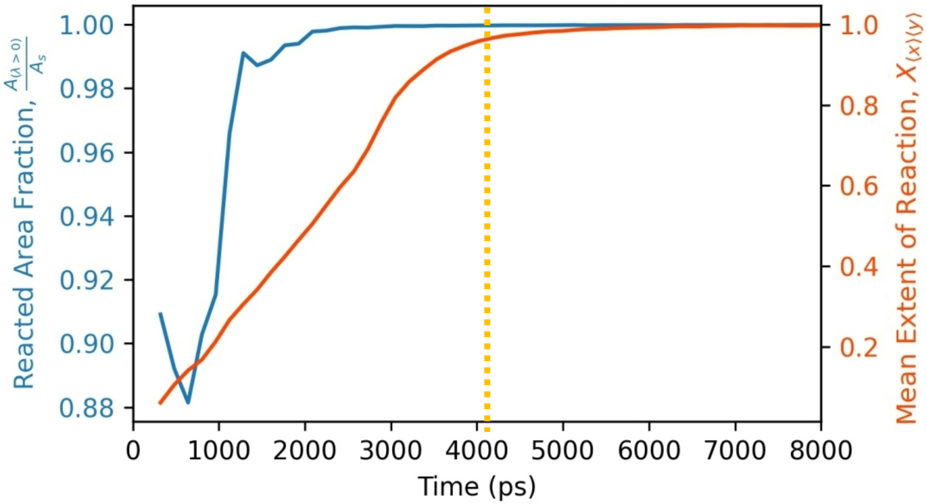
- New trends in temperature statistics appear at detonation transition
- Mean and σ level out, but kurtosis continues climbing

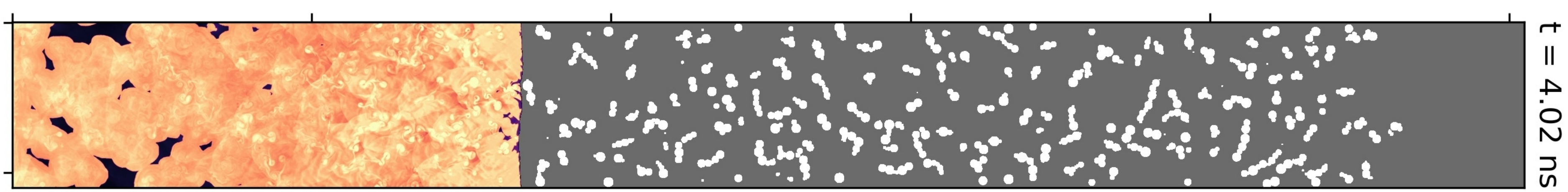


Other Detonation Indicators

- Extent of reaction in shocked zone → 1 post-overtake
- Specific rate of energy release plateau

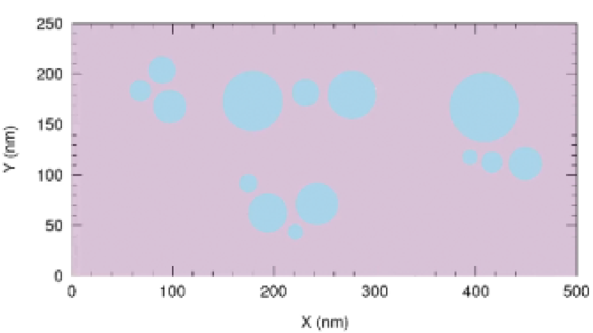


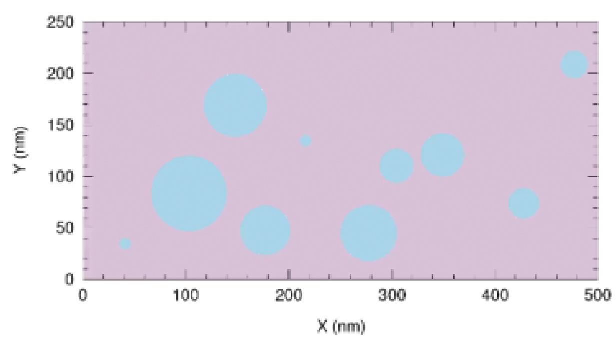


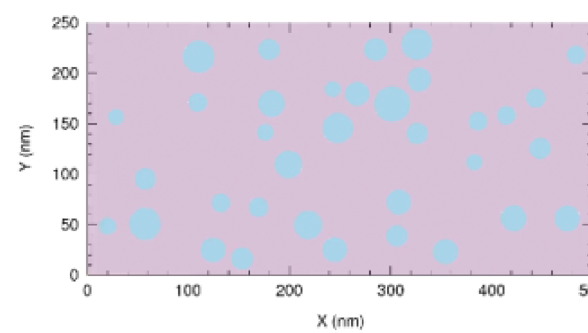


Conclusions

- Evolution of temperature distribution with time and shock run distance is a complex function of chemistry and microstructure features
  - Pre-detonation vs post-detonation
  - shock propagation & chemical reactions introduce different length and time scales
  - Different "sensitivity" indicators for hot spot ignition, growth, and coalescence phases
- Specific surface area and pore 2-body fraction are leading geometric indicators of sensitivity







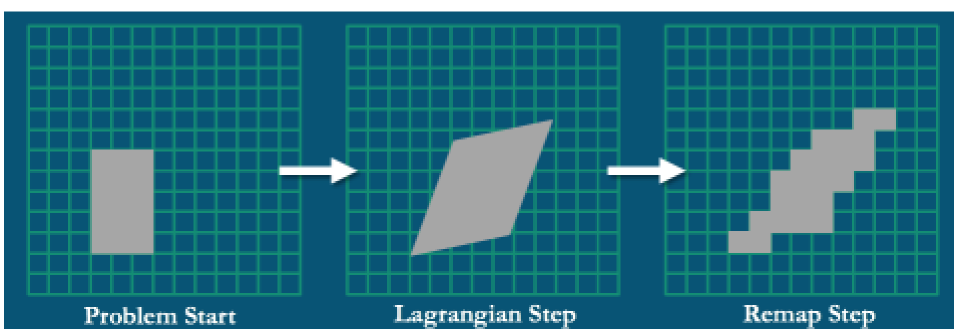
Thank You!

Continuum Hydrocode Simulations—CTH

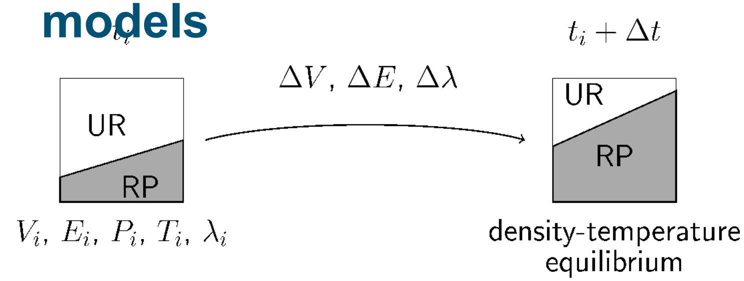
- CTH—3D, large deformation, multi-material shock physics hydrocode developed at Sandia National Laboratories

Mass	$\frac{d\rho}{dt} = -\rho\nabla \bullet \vec{V}$
Momentum	$\rho\frac{d\vec{V}}{dt} = -\nabla P - \nabla \bullet \left[\boldsymbol{\sigma} + \mathbf{Q}\left(\vec{V}, c_s\right)\right]$
Energy	$\rho\frac{dE}{dt} = -P\nabla \bullet \vec{V} - \left[\boldsymbol{\sigma} + \mathbf{Q}\left(\vec{V}, c_s\right)\right] \bullet \nabla\vec{V}$

Lagrangian and remap solution steps as they appear in CTH



Density-temperature equilibrium for reactive burn models



McGlaun, J. M., Thompson, S. L., and Elrick, M. G., *Int. J. Impact Engng.*, 10 (1990) 351-360.

CTH Strain Rate Dependent Model – Steinberg, Guinan and Lund (1988)

- Assume a constant shear modulus
- Neglect work hardening
- Assume linear variation of the Grüneisen parameter

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