SAND2022-17103C

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Microscale Modeling of Energetic Materials – Strength & Plasticity Informed by Molecular Dynamics

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International Conference on Plasticity, Strength, and Damage 2023

January 2-9, 2023

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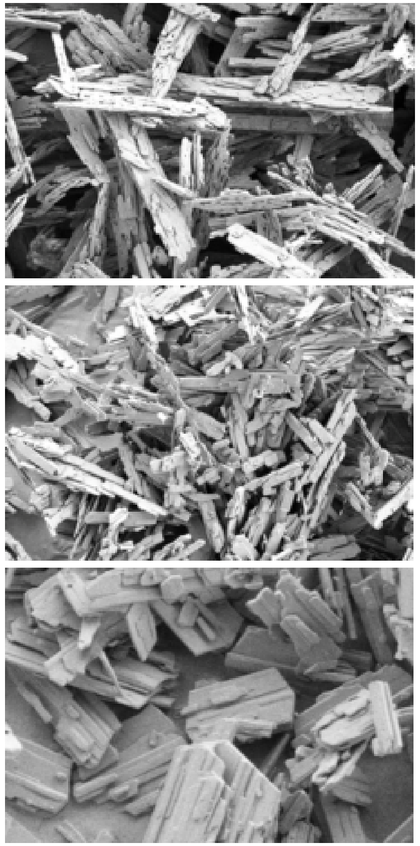
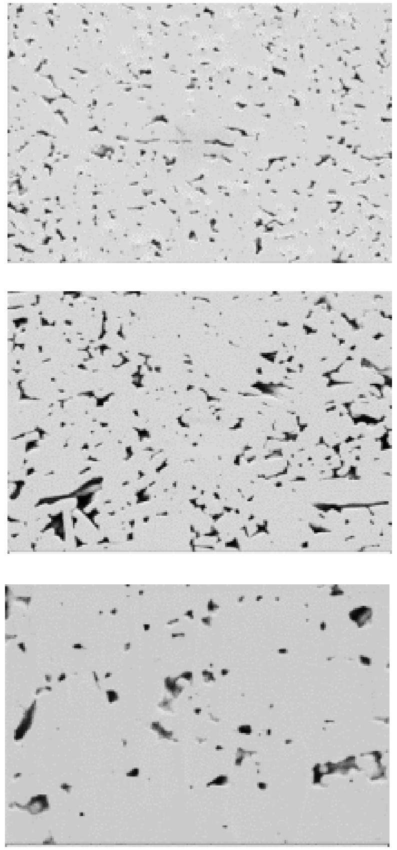
Property-Performance Relationships in Energetic Materials

Various batches of explosive powder (HNS) → Microstructures of pressed pellets → Import microstructures to hydrocode for simulation of run-to-detonation

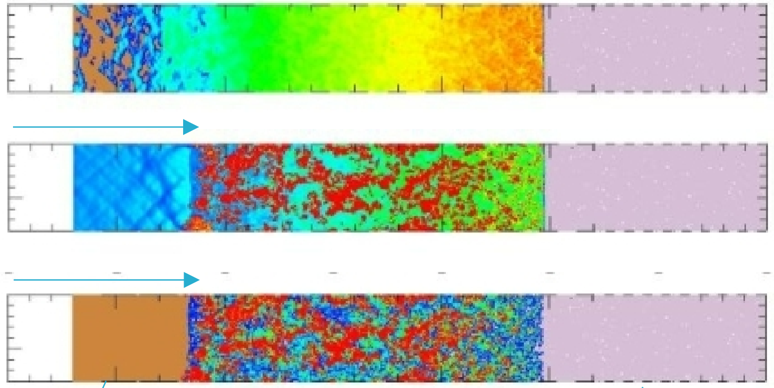


50 µm

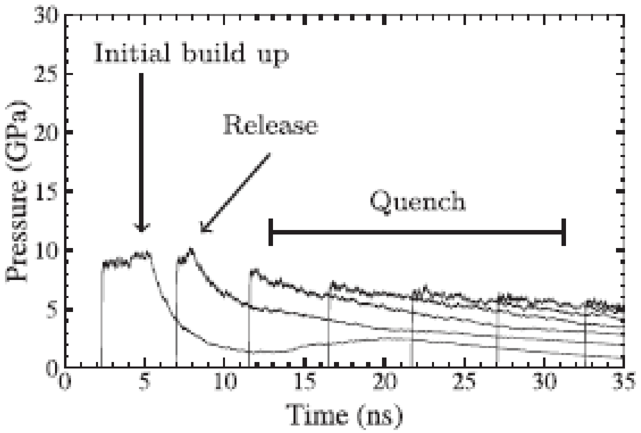


10 µm

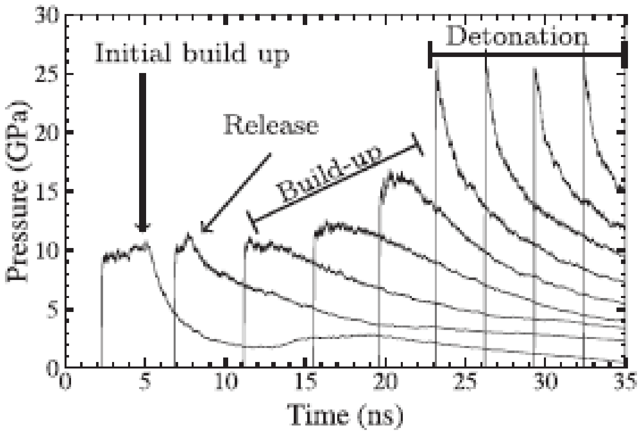
70 µm



Flyer velocity below threshold (no-go)



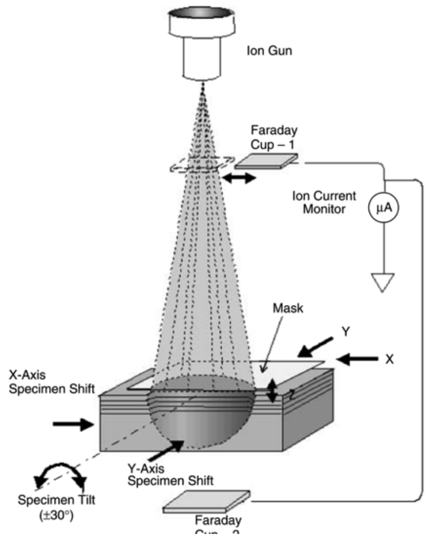
Flyer velocity above threshold (go)



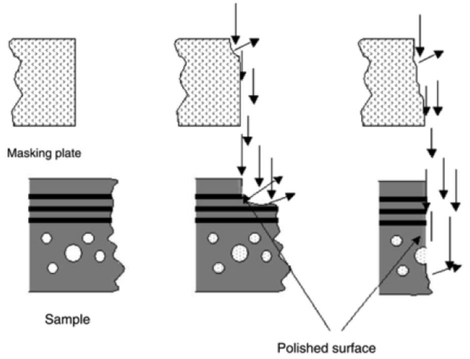
Direct numerical simulations of energetic material microstructures predict the material's response

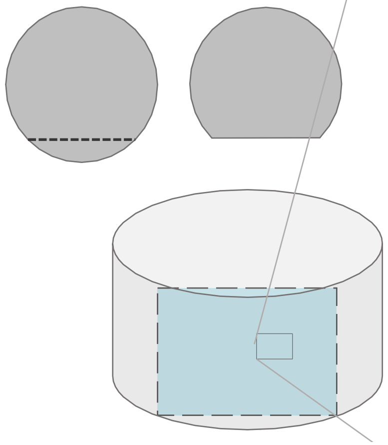
Cole D. Yarrington, Ryan R. Wixom, and David L. Damm , "Shock interactions with heterogeneous energetic materials", Journal of Applied Physics 123, 105901 (2018)

Microstructure Characterization

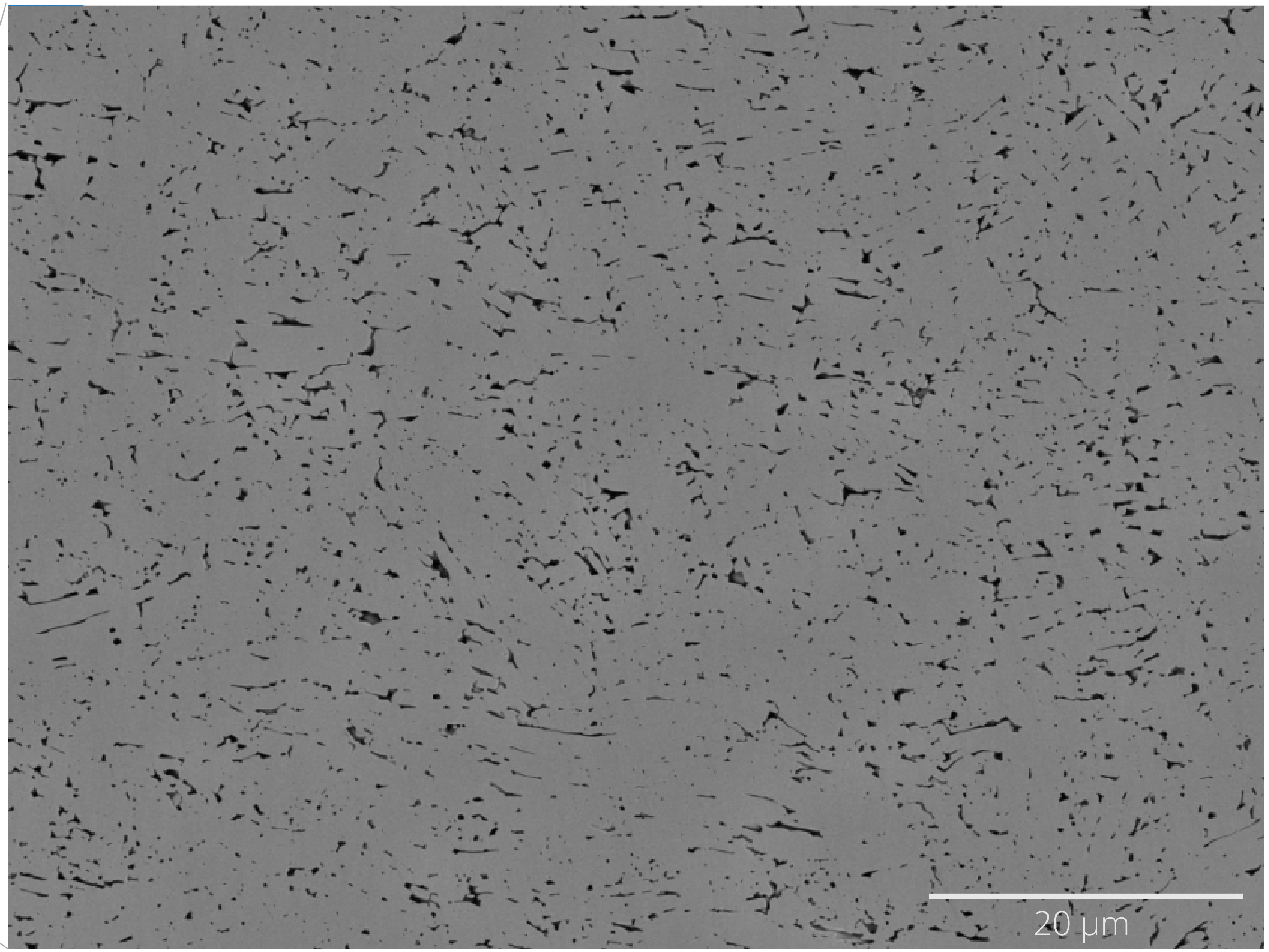


Argon ion cross-section polishing





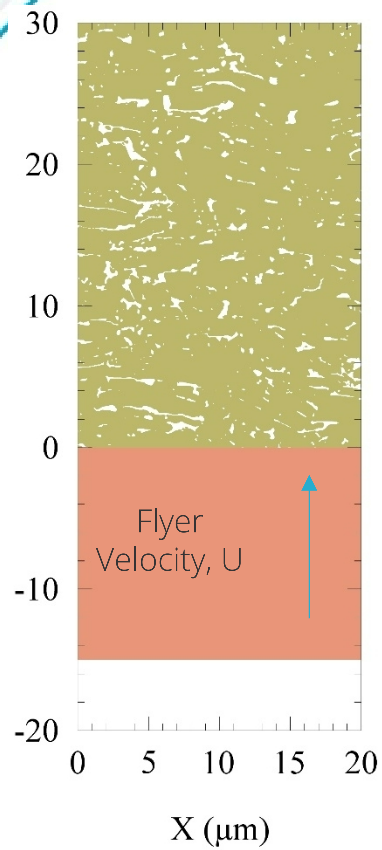
Pressed pellets

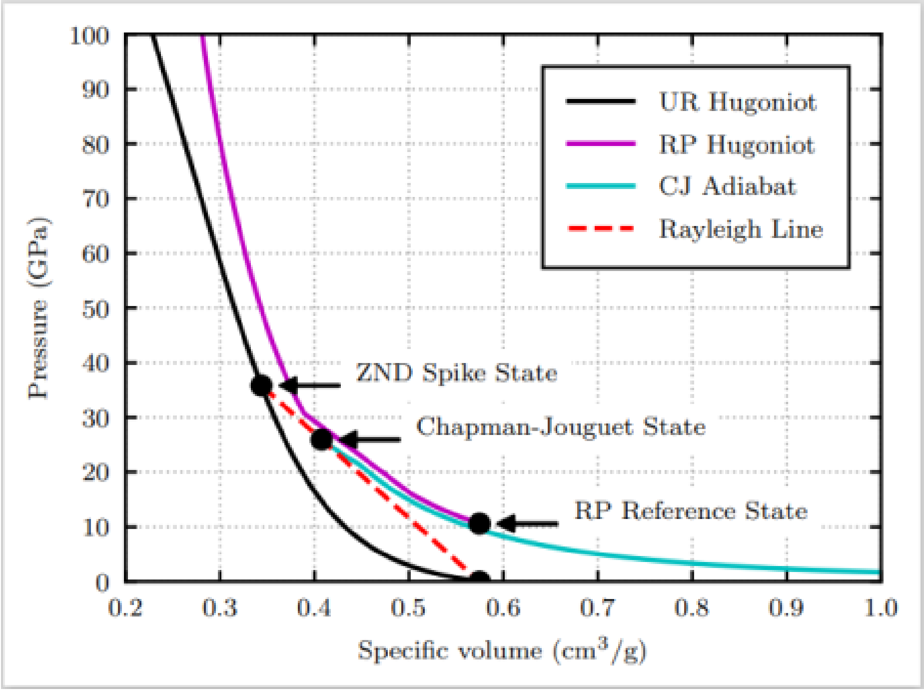


Wixom et al. J. Mater. Res. 25 1362 (2010).

High resolution SEM image (10 nm/pixel) [Credit: Rob Knepper, SNL]

Model Description – EOS, Strength, and Reactive Burn Model





Unreacted (UR) and reaction products (RP) Hugoniots for fully dense (solid) HNS.

- Reaction products EOS uses a SESAME table which includes states off the CJ adiabat (accessed during hotspot formation)

- Plastic deformation of the solid crystal at voids and defects generates heat and increases the local temperature (hot spots)
- Reaction rate depends on local temperature in the solid

$$k = A \exp(-E/RT)$$

- We use the activation energy, *E*, based on thermal decomposition data
- Frequency factor, *A*, is adjusted (calibrated) so that flyer impact simulations match experimental data

Constitutive models for strength and plasticity determine the amount of heat generated by viscous heating and ejecta impact during pore collapse

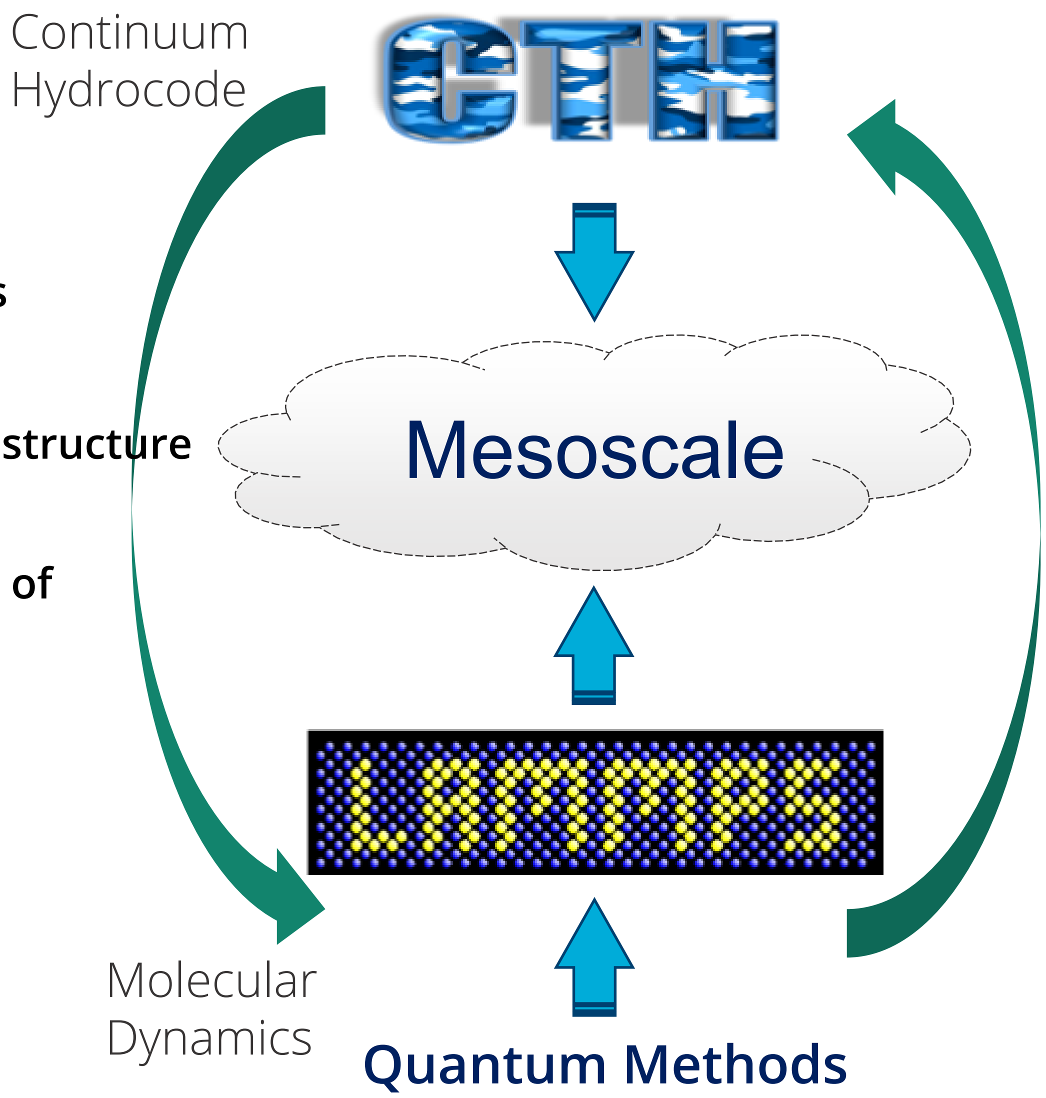
→These models are a **major source of uncertainty in hydrocode simulations**

Problem: Strength and plasticity of energetic molecular crystals at high strain rates & sub-micron length scales

Coupling Continuum Hydrocode and MD Simulations

Continuum Properties Propagated Down:

- ‘Critical’ local microstructure features
- Evaluate measures of sensitivity

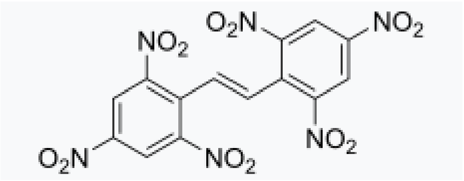


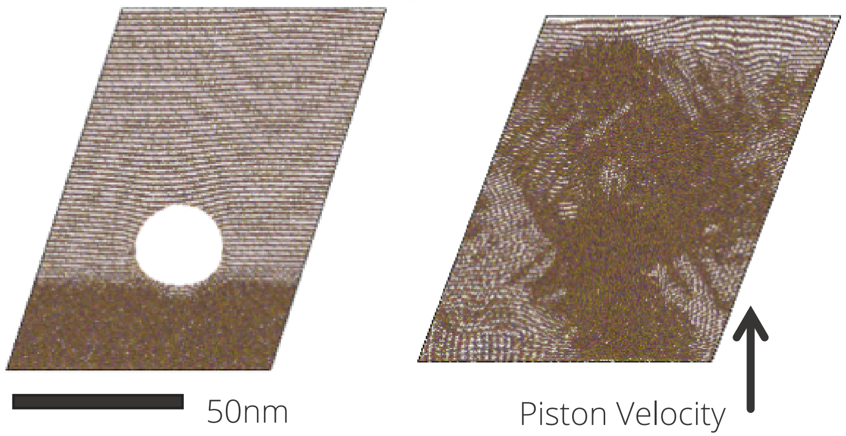
Atomistic Properties Propagated Up:

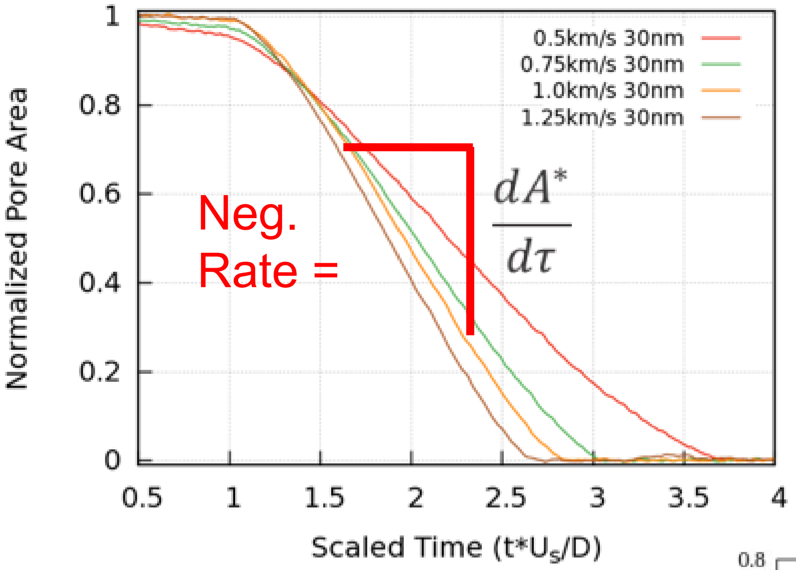
- Global reaction kinetics
- Strength model parameters
- Effects of anisotropy in strength, EOS
- Validate ‘sensitive’ microstructures

M Wood et al. Phys Rev B. 97 014109 (2018).

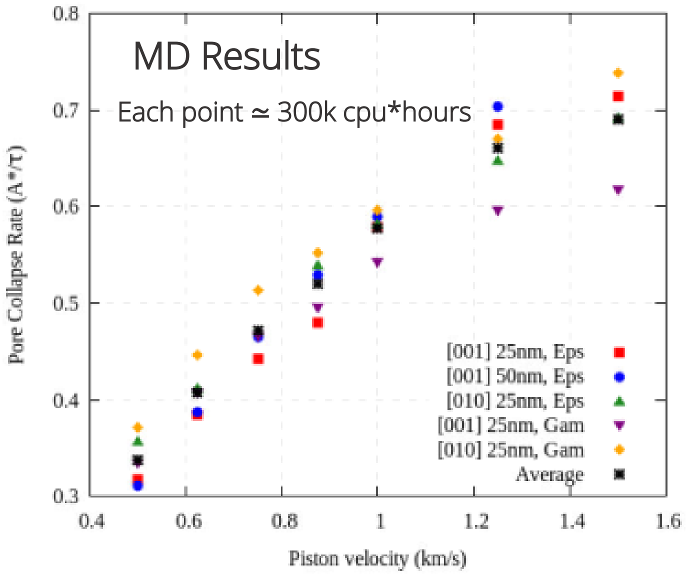
Training Data - Material Strength Measures from MD







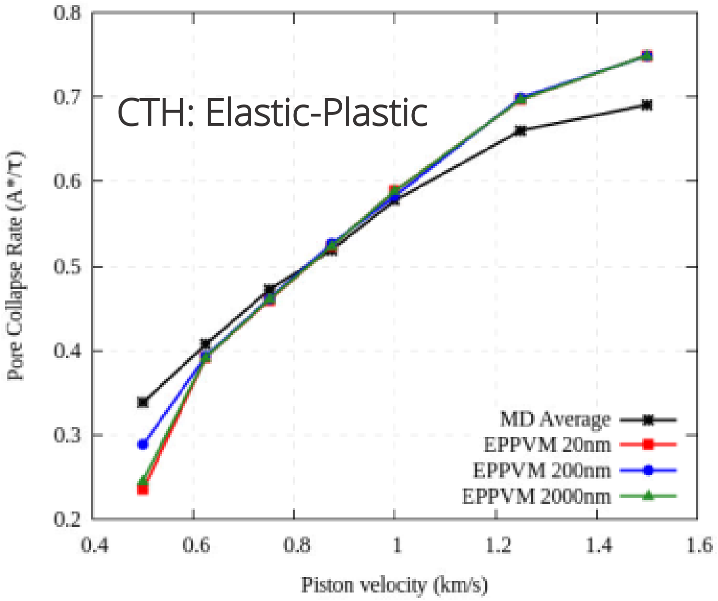
A pore collapse rate of 0.5 means the pore is half closed in the time it takes the shock to travel the diameter of the pore



Viscoplastic: Low U_P, or large pores

Hydrodynamic: High U_P, or small pores

How does one accurately model this response in continuum hydrocodes?



J Brown, M Wood, M Sakano, J Hartig; "Multiscale Development of Predictive Constitutive Models to Resolve the Shock to Detonation Transition," APS SCCM 2022

Automated Continuum Strength Model Calibration

Steinberg Guinan Lund[1] strength model

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)	$\dot{\varepsilon}_p = \left\{\frac{1}{\mathbf{C_1}} exp\left[\frac{2\mathbf{U_K}}{kT}\left(1-\frac{Y_T}{\mathbf{Y_P}}\right)^2\right] + \frac{\mathbf{C_2}}{Y_T}\right\}^{-1}$
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:	$\gamma = \gamma_0/(1+\mu)$

Bolded inputs were trained

$$Y_T \leq \mathbf{Y_P}$$

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

$$argmin\left|CTH\left(\frac{dA^*}{d\tau}\right) - \mathrm{MD}\left(\frac{dA^*}{d\tau}\right)\right|$$

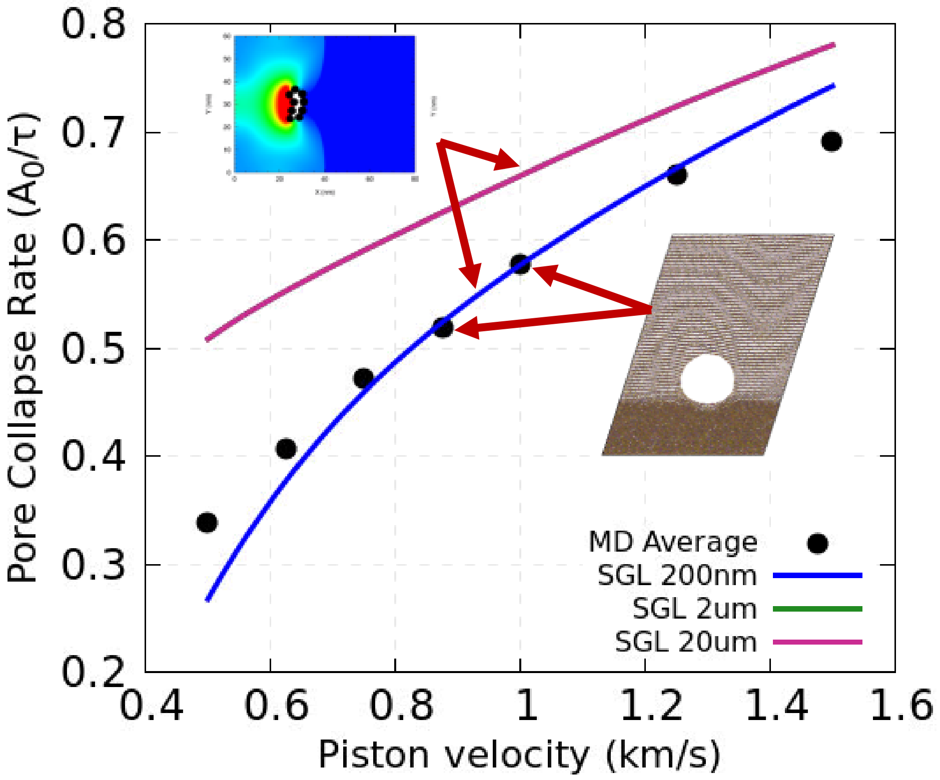
- Iteratively runs CTH calculations for each parameter set in real time
- DAKOTA workflow is automated

[1]D.J. Steinberg, C.M. Lund, JAP, 65, 1528, (1989)

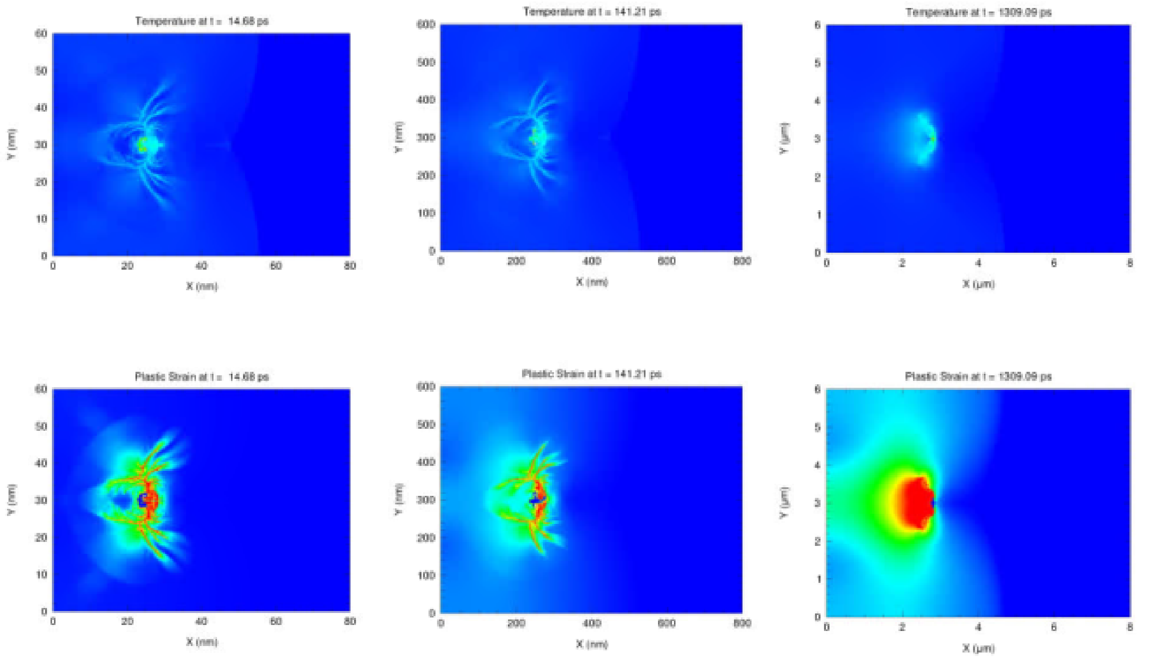
https://dakota.sandia.gov/

Optimization Delivered a Strength Model Calibrated to MD

Calibrated Results



Pore Collapse is size-dependent



25nm

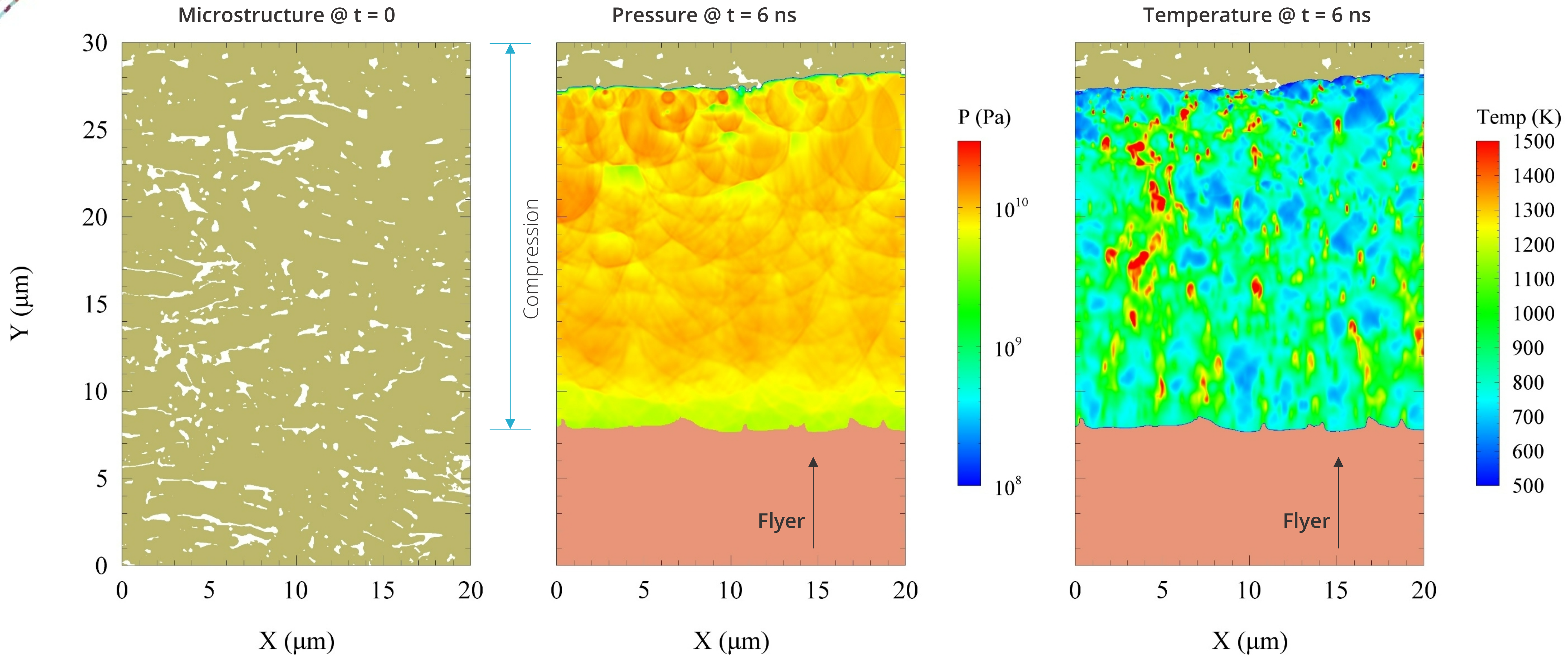
200nm

2μm

Continuum hydrocode (CTH) strength models were trained using results from MD

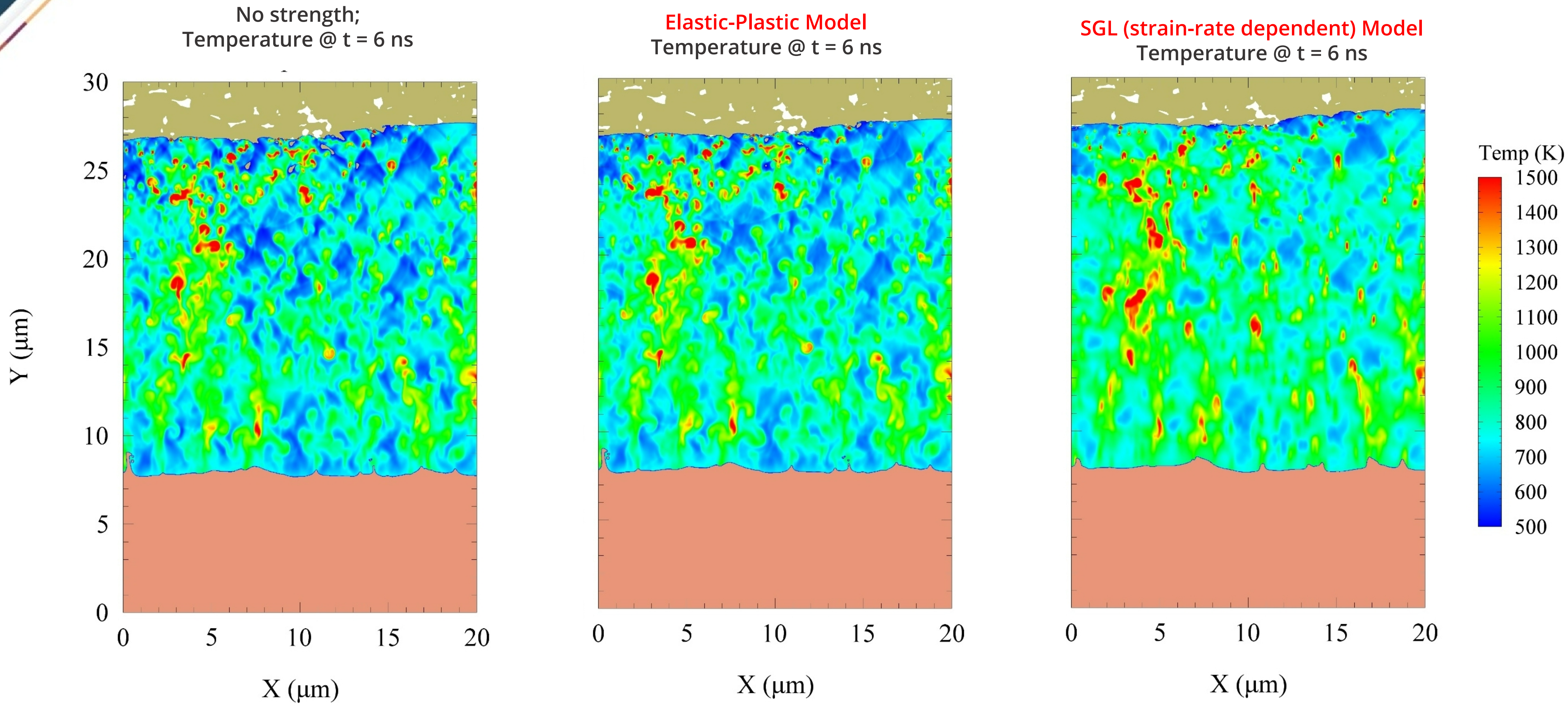
J Brown, M Wood, M Sakano, J Hartig; "Multiscale Development of Predictive Constitutive Models to Resolve the Shock to Detonation Transition," APS SCCM 2022

Hydrocode Simulations - Hotspot Formation



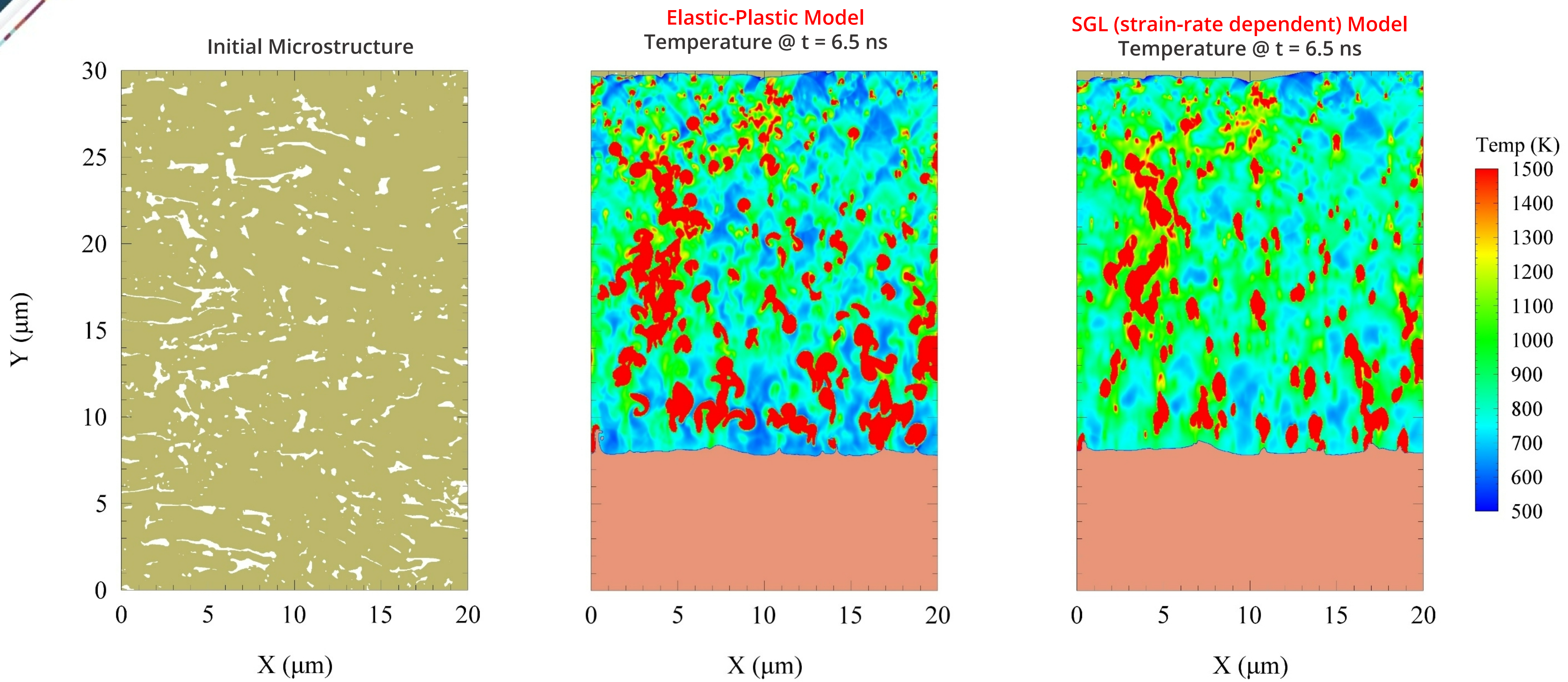
Inert simulation (no reaction) of hotspots, with pressure and temperature fields at time = 6 ns after impact.

Effects of strength model



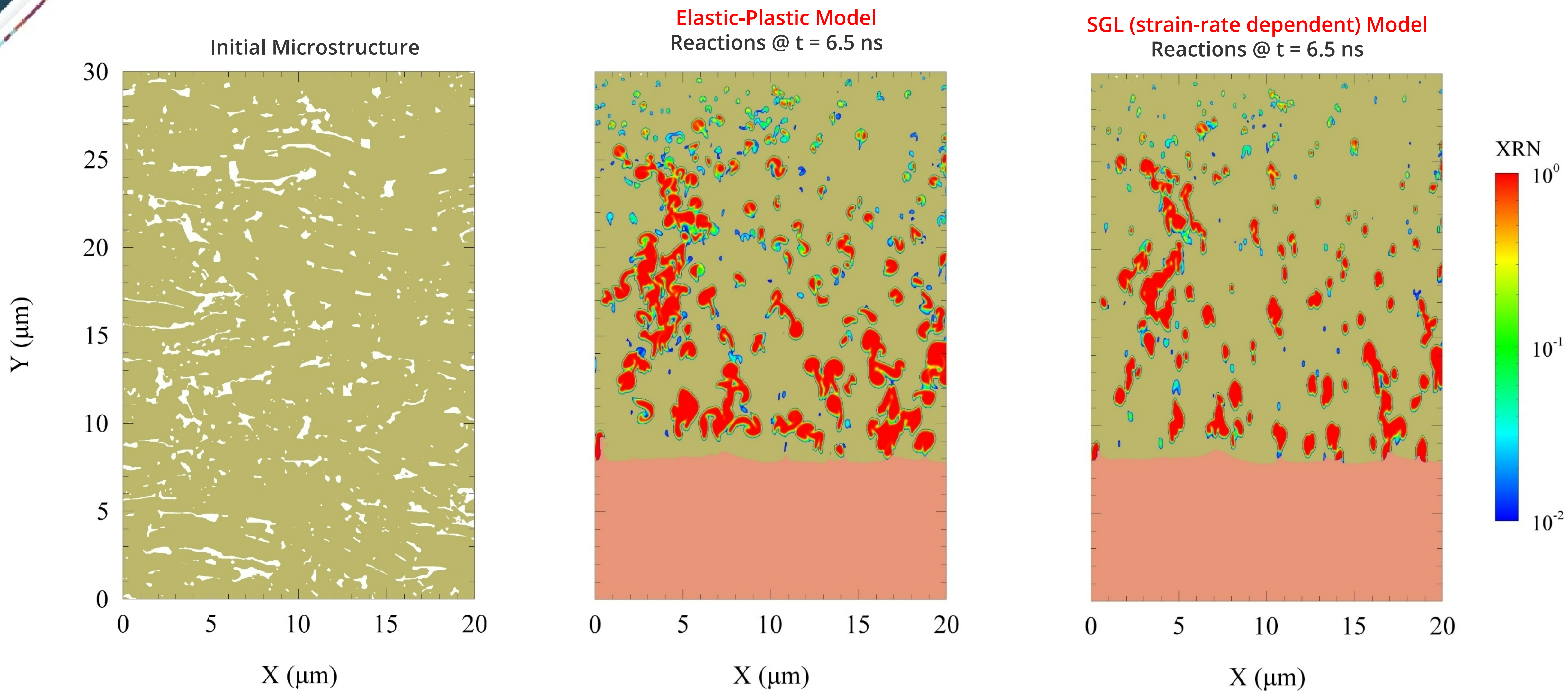
Inert simulation (no reaction) of hotspots due to void collapse and viscous heating;
(Impact pressure ~12 GPa)

Hotspot Temperature (with Reactions)



Simulations including reactions show the effects of strength model on the number, size, and shape of hotspots.

Effects of strength on hotspot reaction

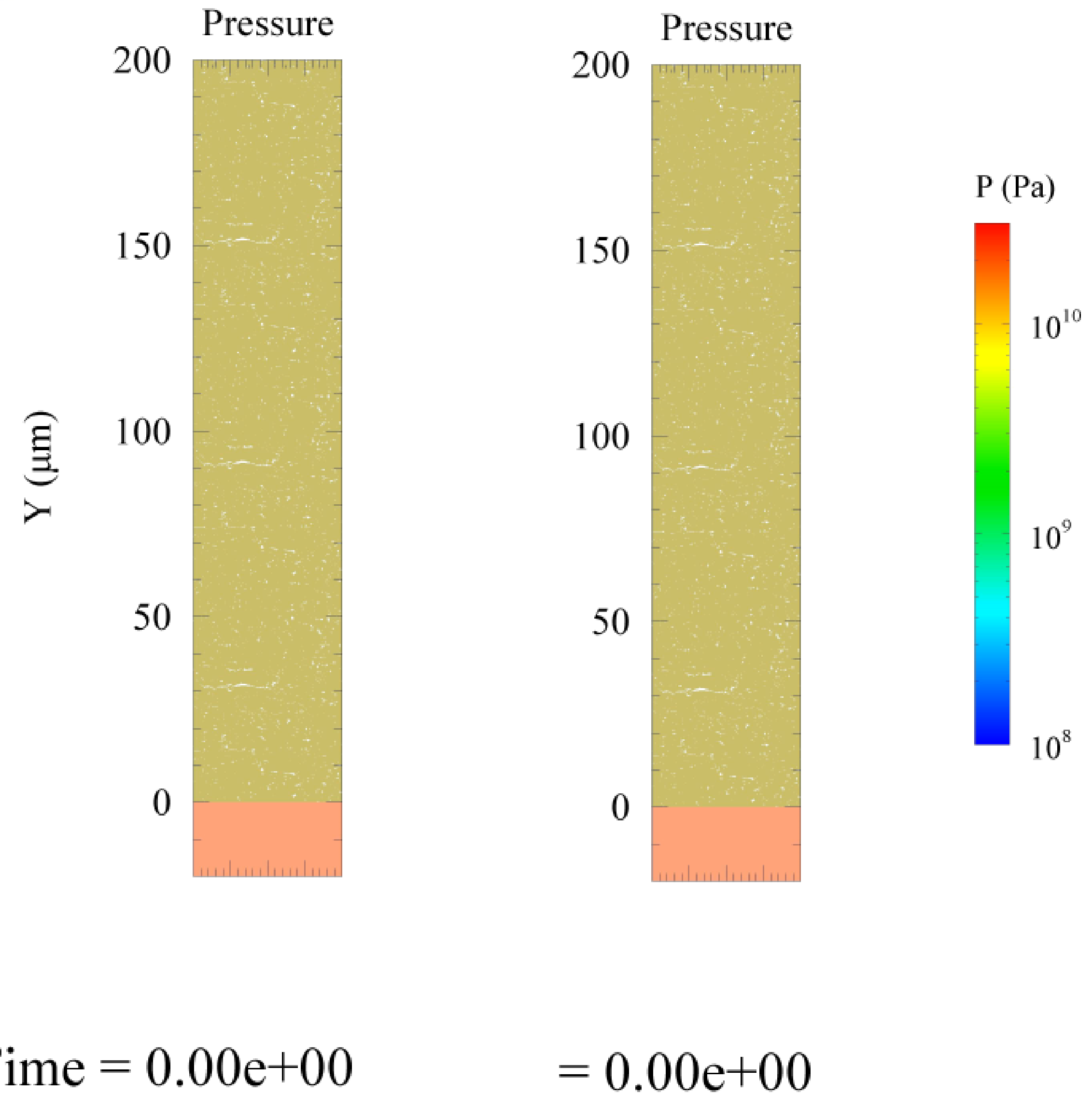


“Extent of reaction” variable (varies between 0-1), illustrates the location of burning hotspots relative to the location of defects in the initial microstructure.

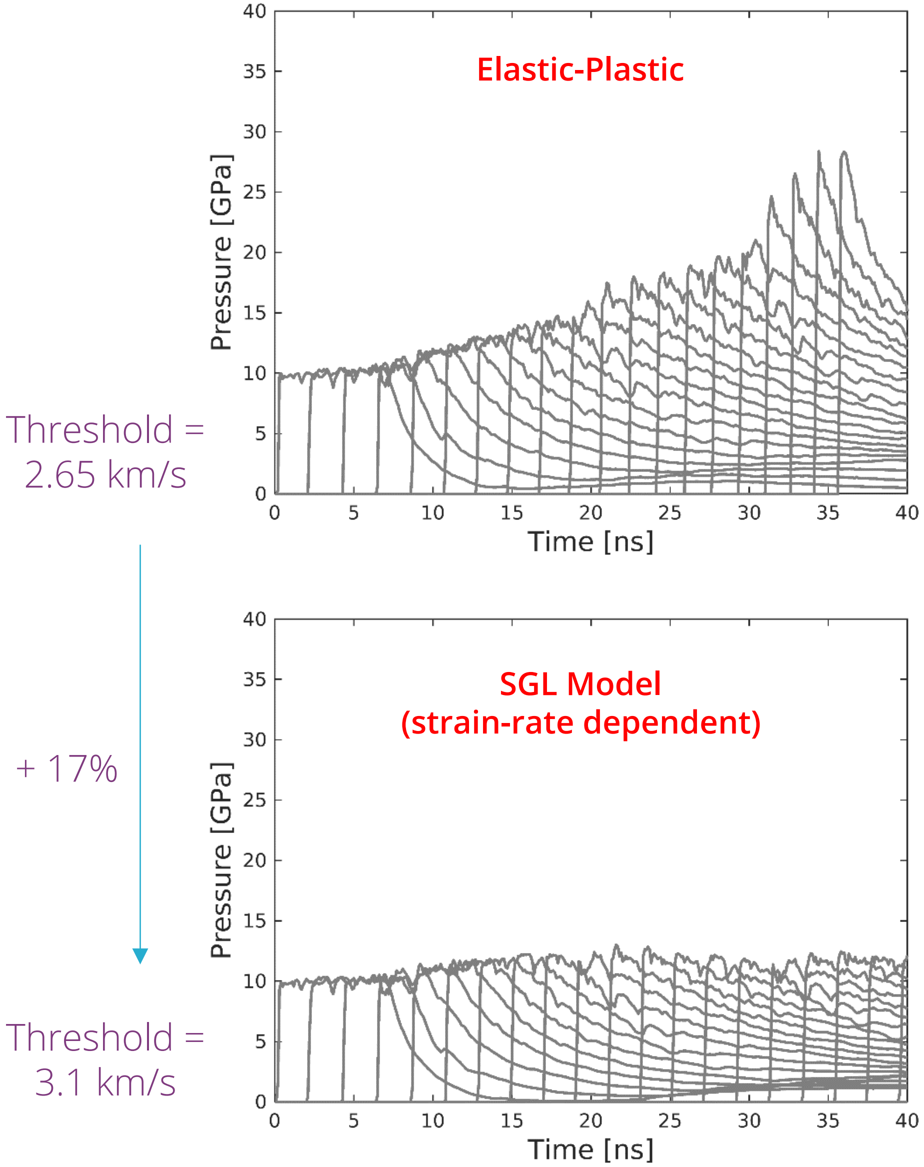
Full-scale, Direct Numerical Simulations of Detonation

Elastic-Plastic Model

SGL Model (strain-rate dependent)



Pressure Profiles (3 km/s)



Concluding Remarks

Multi-scale modeling of energetic materials is rapidly advancing and enabling predictions of microstructure-performance relationships

- SNL has active research programs in Atomistic / Molecular Dynamics and Mesoscale Modeling of HE
- Our objective is to develop *predictive* models of energetic material response (Models that are right, for the right reasons)

Material strength and plasticity play a crucial role in the formation of hotspots

- Models are difficult to validate experimentally at < *μm* length scales
- A strain-rate dependent strength model (SGL) was trained using MD results
- The new model significantly influences the details of hotspot formation and run-to-detonation (vs. naïve approaches such as no strength or elastic-plastic)
- This multi-scale approach has added credibility to mesoscale simulations of shock initiation

Acknowledgements

Explosive Technologies Group

- James Stewart
- Robert Knepper

Engineering Sciences Center

- Judith Brown
- Michael Sakano
- Julia Hartig

Computational Sciences & Math Dept.

- Mitch Wood

Development of a predictive capability for Energetic Materials is a collaborative effort across multiple centers at Sandia