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Multiscale Development of Predictive Constitutive Models to Assess Critical Hotspots and Microstructure Sensitivity

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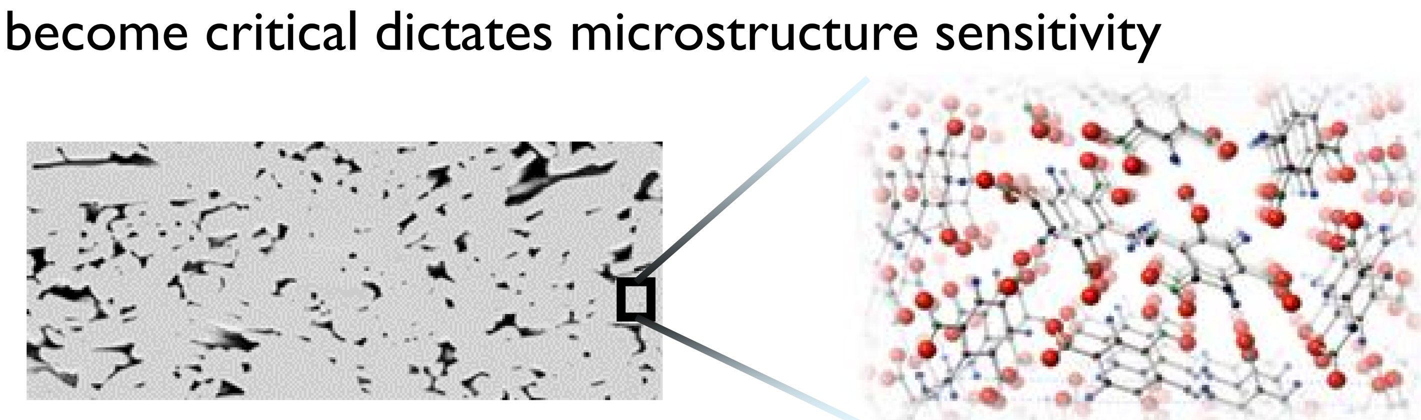
Objective

Connect choices made in model parameters with the microstructure response under non-detonable conditions

Focus

Inherent distribution of defects in non-ideal materials

- Variability of microstructures depend on material choice, sample preparation, and/or experimental/simulation design
- Interactions between hotspots formed at defects can build up and transition from deflagration to detonation
- Formation of hotspots is the precursor observable – how and when they become critical dictates microstructure sensitivity



How do variations in the model parameter values influence the sensitivity of a microstructure?

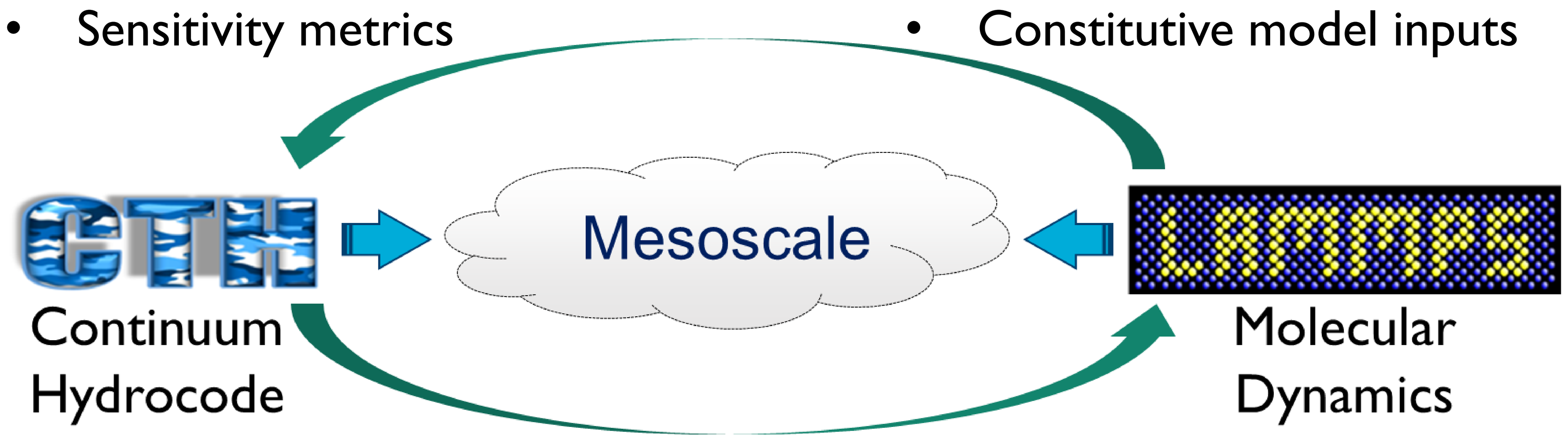
Modeling Framework

Validation

- Microstructure features
- Sensitivity metrics

Training Data

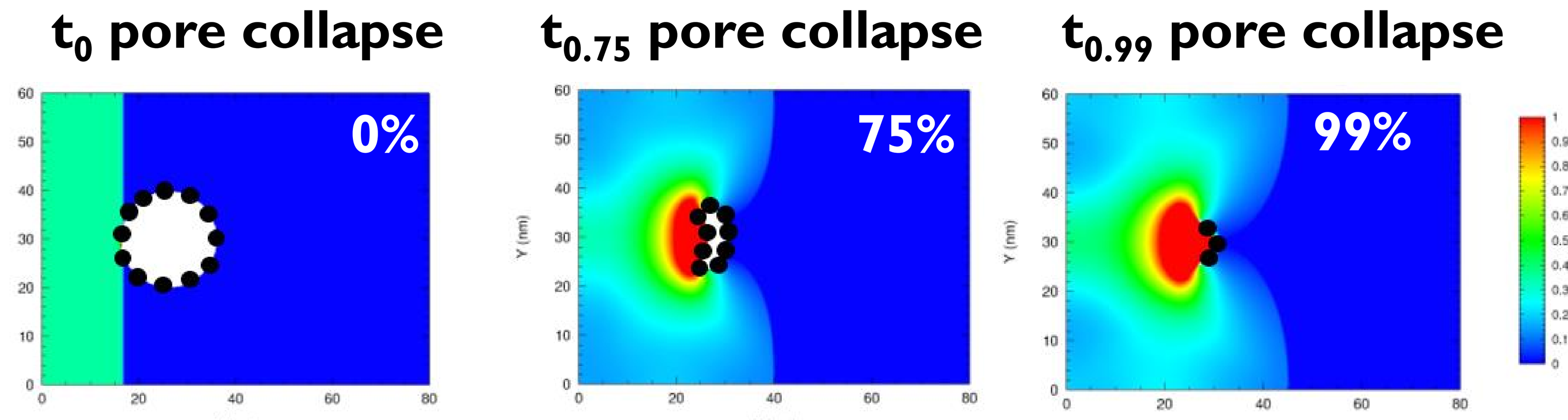
- reaction kinetics
- Constitutive model inputs



Bridging effects of properties across scales

- *Propagate Up* – train phenomenological models with high-fidelity (atomistic) observables
- *Propagate Down* – assess the effects of a given atomistic property on microstructure sensitivity

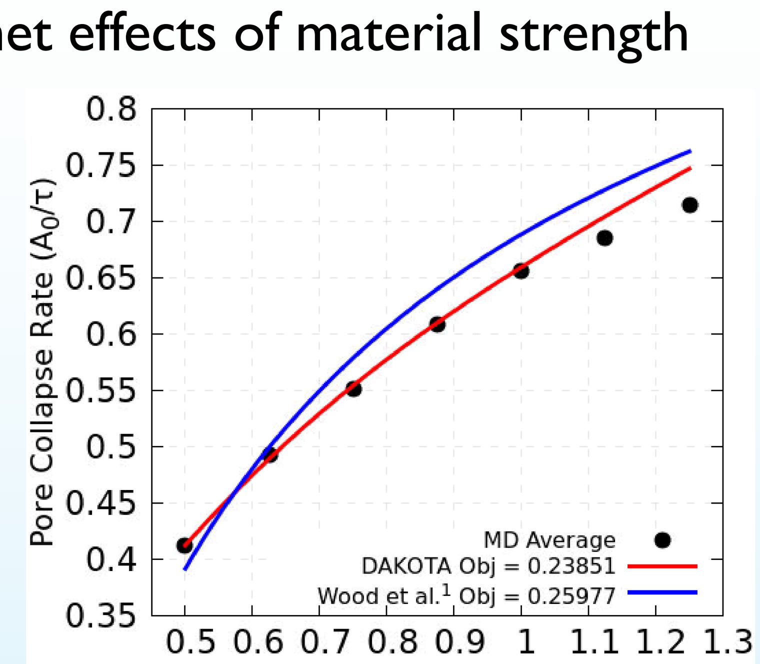
t_0 pore collapse **$t_{0.75}$ pore collapse** **$t_{0.99}$ pore collapse**



(above) Pore collapse can capture the net effects of material strength

Assessing the quality of the DAKOTA optimization

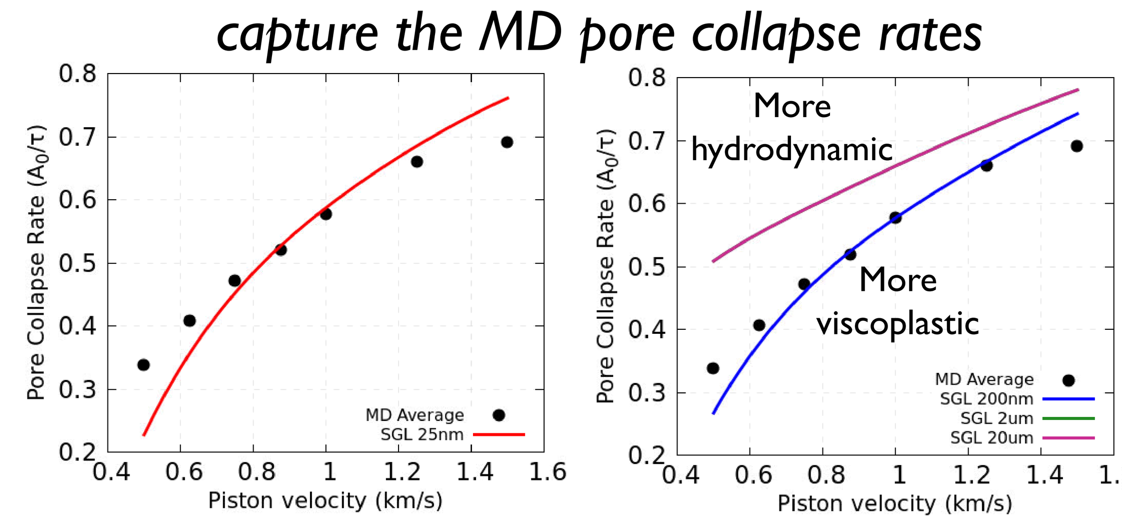
- MD pore collapse rates as the training objective compared to DAKOTA optimization (red) and manual sampling (blue)
- This tool can be used to train any observable obtained from CTH (or any other simulation technique)



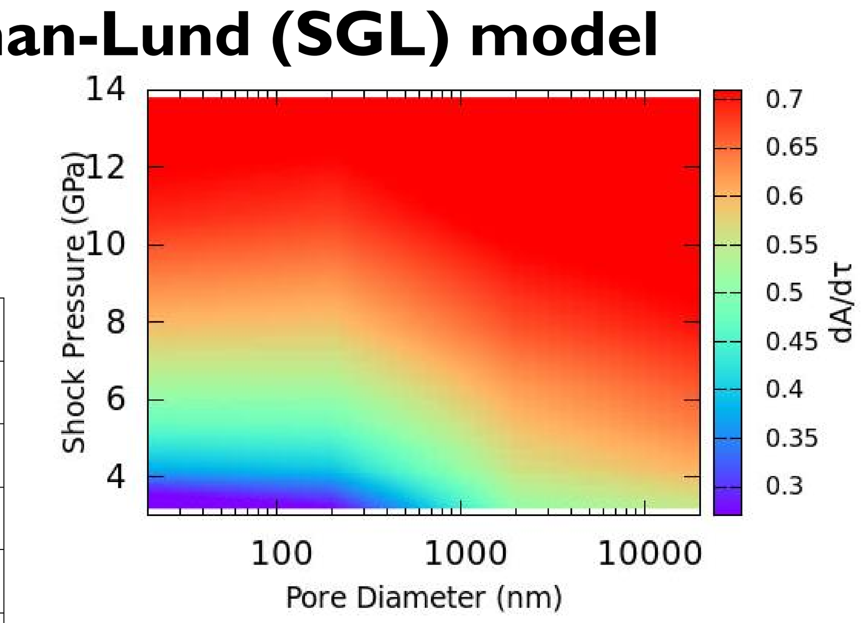
Result

MD-informed Steinberg-Guinan-Lund (SGL) model

We believe a strain-rate dependent strength model (like SGL) is necessary to capture the MD pore collapse rates

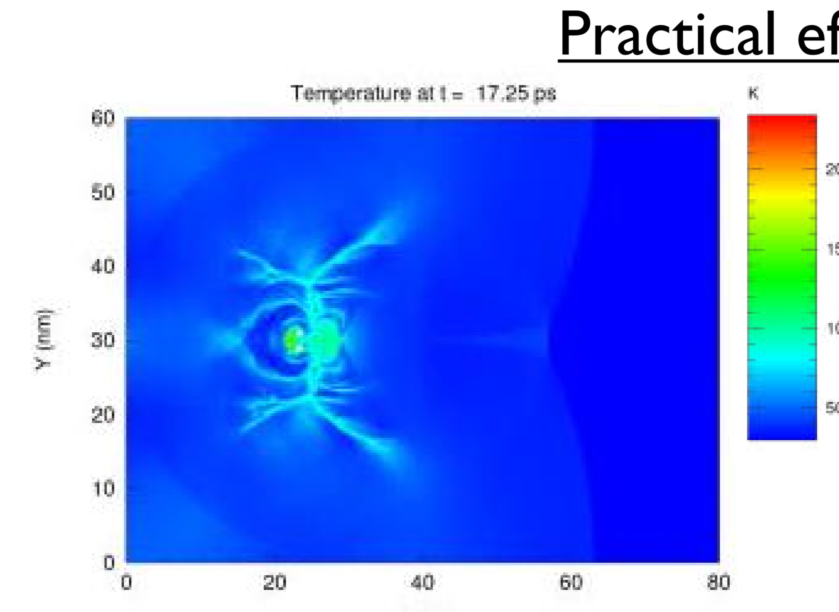


- Trained strength model underpredicts viscoplastic regime and overapproximates hydrodynamic region
- Extrapolation to 200nm appears similar to trained 25nm behavior, while micron sizes are more hydrodynamic-like



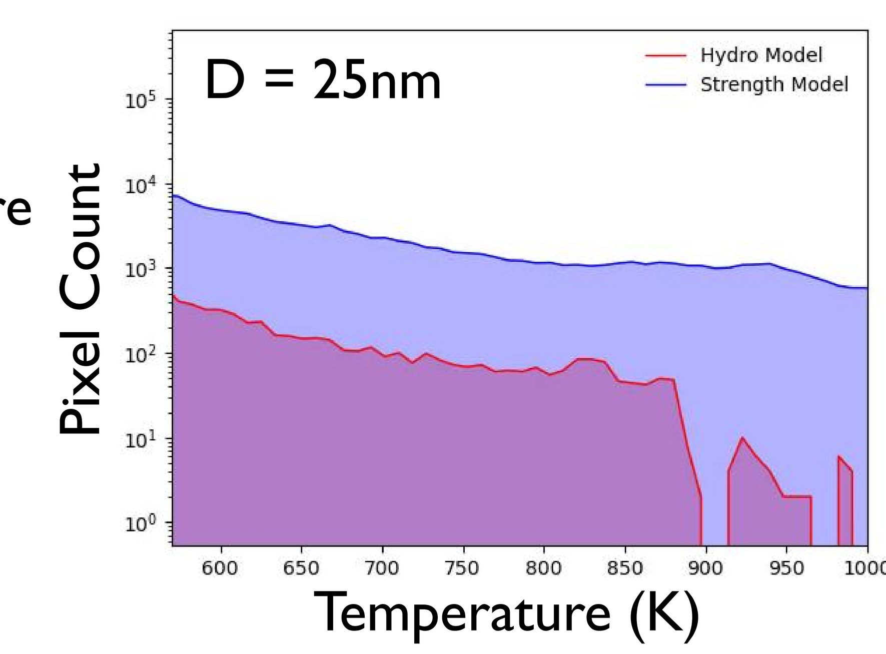
(top) Shock Pressure – Pore Diameter parameter space for pore collapse rate using the MD-informed SGL strength model. Note the relatively larger gradient as a function of shock strength, as compared to pore size

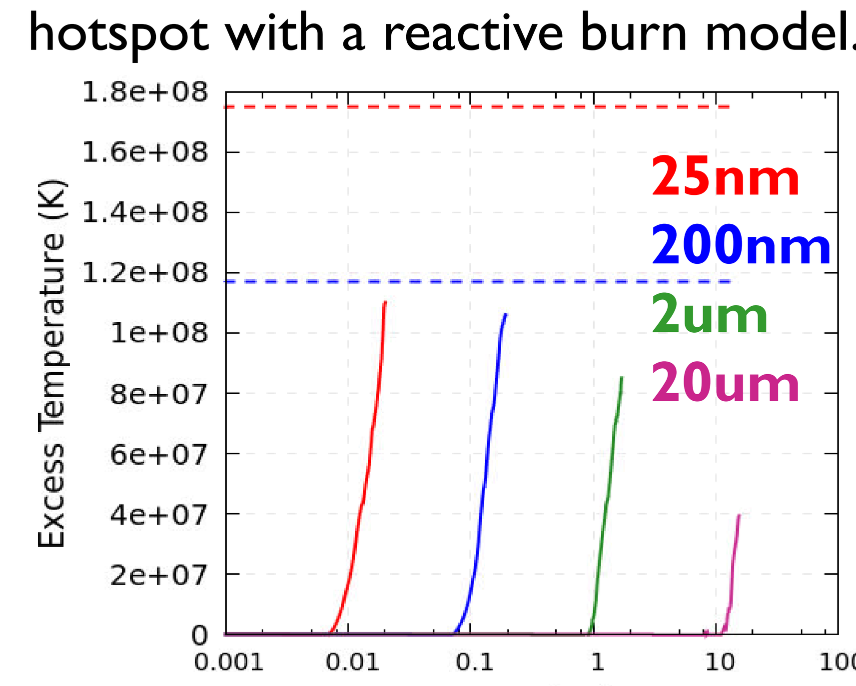
Practical effects on heat generation



(left) Snapshot of U_p = 0.75 km/s at 100% pore collapse for a 25nm diameter pore. Note the existence of localized shear bands with temperatures above the bulk value as a result of modeling with a strain-rate dependent strength model.

(right) Differences in temperature distributions for U_p = 0.75 km/s and pore sizes 25nm and 2um at a time of 100% pore collapse. Excess temperature from SGL strength model over purely hydrodynamic one manifests in viscous (shear) heating. This extra energy could result in a critical hotspot with a reactive burn model.





(left) Temperature difference between the SGL and hydrodynamic model captured over time for different pore sizes (solid). Dashed horizontal lines are predictions using Perry et al.[2] critical hotspot theory, where the same color crossover indicates when the strength model would result in a self-sustained deflagration.

Significance

Applicability of this extensible framework

- Any observable can be transferred from LAMMPS to CTH
- This idea also applies to making connections between any high-fidelity simulations or experiments and other macroscale models

Improvement of explosive component modeling

- Practical effects of a strain-rate dependent strength model arises in shear banding and localized heating
- Quantifying critical hotspots leading to detonation can enhance our understanding of microstructure sensitivity

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[1] M. A. Wood, D. E. Kittell, C. D. Yarrington, A. P. Thompson, *PRB* **2018**
[2] W. L. Perry, A. L. Duque, J. T. Mang, D. B. Culp, *Combustion and Flame* **2021**

Additional program/partner logos can be added here