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Grain Scale Modeling – Impact of Constitutive Models

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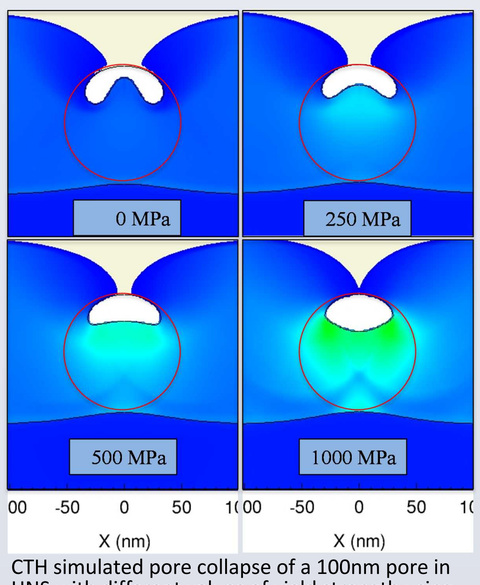
Abstract

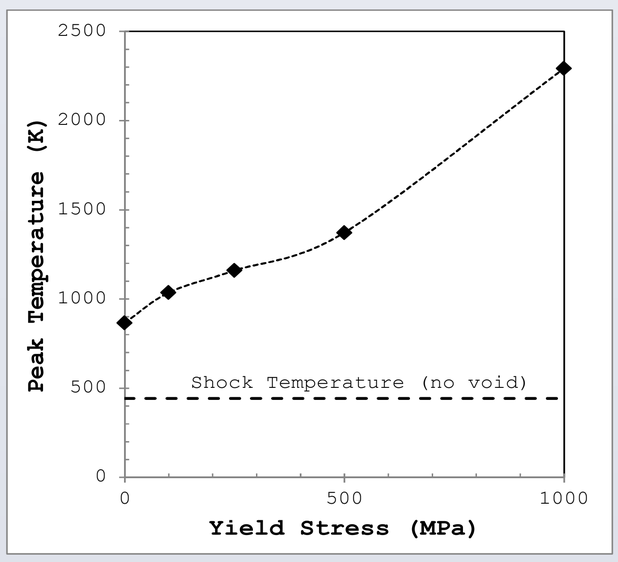
There are many model considerations that are unique to the grain-scale continuum approach. Most of these considerations revolve around the treatment of continuum model parameters, now applied to the fully dense matrix of material with dispersed discrete heterogeneous features. An examaple of this is how the equation of state (EOS) for a grain scale material must be the fully dense EOS, as opposed to the bulk EOS measured at lower densities. This poses unique validation and parameterization challenges, as most experimental data is gathered for bulk materials. We show how different theoretical tools for smaller length scales (MD, DFT-MD) can be used to calibrate the necessary models to achieve accurate simulation results. The average state around a collapsing pore is used as a target function in an evolutionary algorithm, to calibrate material strength parameters in a continuum shock mechanics calculation.

Motivation

As meso- or grain-scale models are used more and more for predicting behavior of heterogeneous materials [1], heightened scrutiny must be placed on the various constitutive and model inputs that govern the detailed response at grain scale features such as pores, particles, or inclusions. While extreme states lessen the influence of concepts such as material strength, predicting critical threshold regimes requires the analysis of such effects, and the production of accurate models in order to ensure confidence in the numerical results. The inclusion of a strength model in pore collapse simulations has been shown to have significant influence to the predicted temperatures. In temperature dependent reactive burn simulations, a difference of this magnitude can result in vastly different results.



CTH simulated pore collapse of a 100nm pore in HNS with different values of yield strength using an elastic perfectly-plastic (EPPVM) strength model [2].

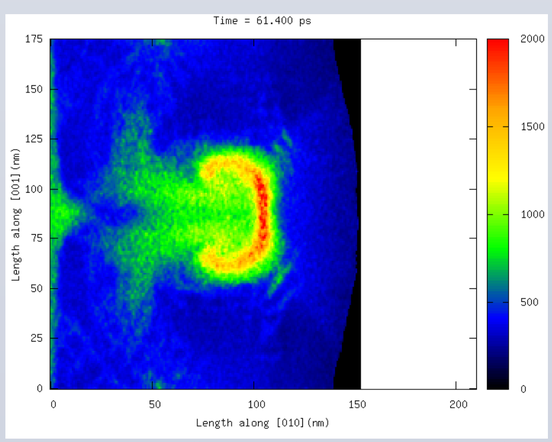


Plot of peak temperature during pore collapse simulations, after jet impact, as a function of the EPPVM yield stress [2].

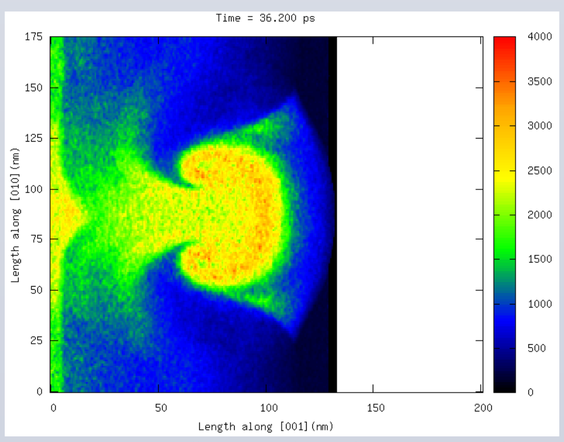
Much attention has been paid previously to the thermodynamic EOS for HNS [3], by using DFT-MD in conjunction with variable specific heat models to generate consistent tabular EOS for HNS, however, placeholder strength models were used. The lack of crystalline HNS experimental data precludes experimental calibration of strength models for fully dense HNS.

HNS Reax-FF MD Simulations

Molecular dynamics researchers have recently run MD pore collapse simulations using a reax-FF potential to investigate early time energy localization and reactant/product species concentrations of HNS [4]. Given the effort in calibrating the potentials for these simulations, an added benefit is the possibility of extracting information on material strength.



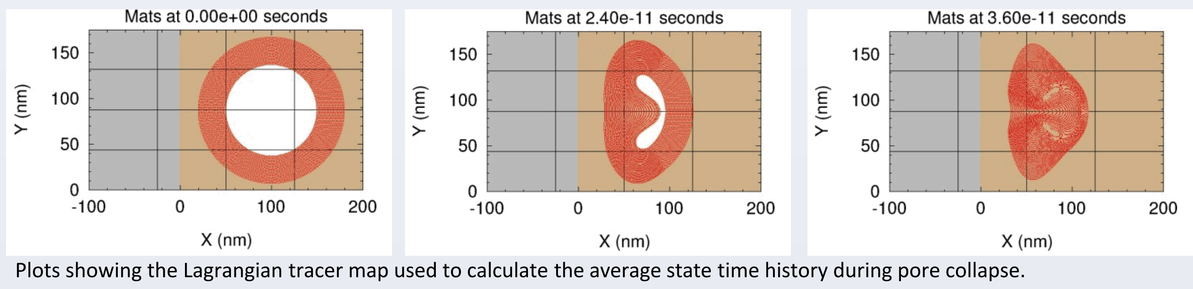
ReaxFF MD pore collapse simulation for a 100nm void in CTH, impacting an infinite impedence wall with particle velocity of 1.25 km/s.



ReaxFF MD pore collapse simulation for a 100nm void in CTH, impacting an infinite impedence wall with particle velocity of 2.25 km/s.

Method

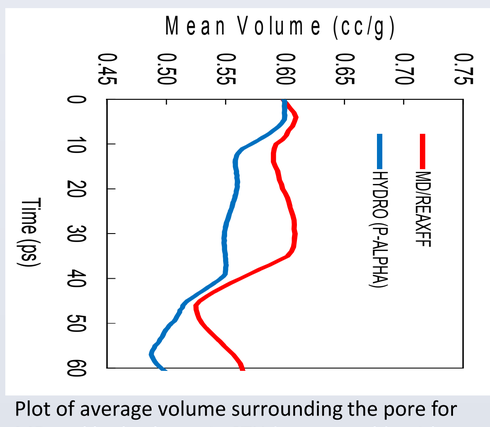
In order to calibrate a strength model, DAKOTA [5], a framework for design optimization, parameter estimation, uncertainty quantification and sensitivity analysis, was used to find the best fit to an objective function by modifying the strength model parameters. To obtain a function that best captured the effect of strength on pore collapse, a series of Lagrangian tracers were placed in concentric circles immediately surrounding the 2-dimensional pore. At each time step, the state values were recorded, and averaged, until the pore was completely collapsed. Using DAKOTA, these automated runs each resulted in a time history for the state variable that could be compared to a similar trace obtained through the MD simulations. Parameter guesses and iteration proceeded according to the evolutionary algorithm, resulting in a final “best-fit” model parameters vector. This procedure allows one to assess the feasibility of using single crystal MD simulations for strength model calibration, and the sensitivity of the results to the parameters.



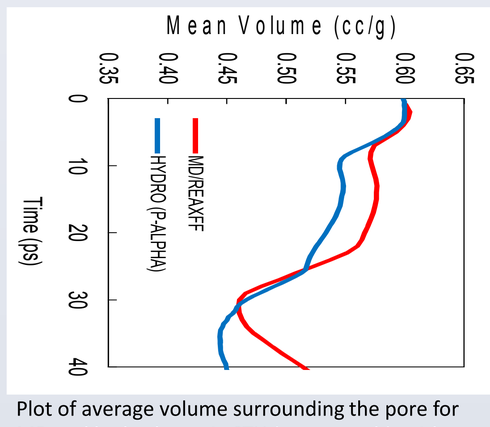
Plots showing the Lagrangian tracer map used to calculate the average state time history during pore collapse.

Results

It was desired initially to quantify the difference between a continuum result without strength, and the MD simulation, through the target function. The plots show that hydrodynamic calculations do result in different average states upon collapse.

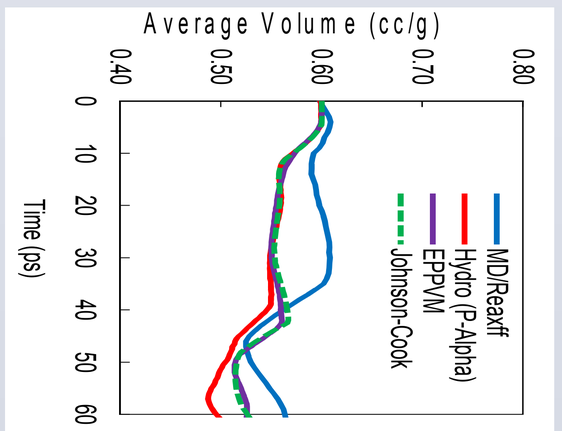


Plot of average volume surrounding the pore for MD and hydrodynamic CTH (no strength), with an impact velocity of 1.25 km/s.

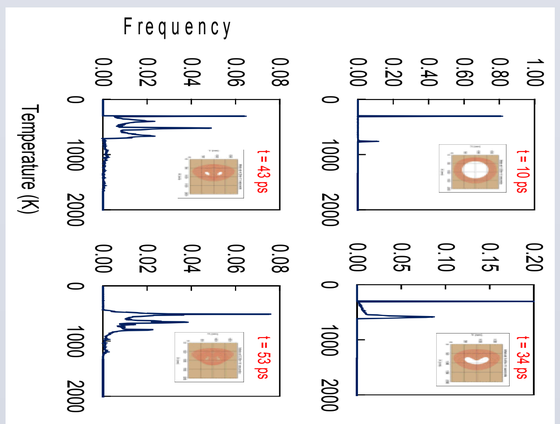


Plot of average volume surrounding the pore for MD and hydrodynamic CTH (no strength), with an impact velocity of 2.25 km/s.

When the target function is used to optimize the strength parameters, the best fits do not show excellent agreement with the MD result or published strength data [6], however some insight is gained into more efficient means of calibrating the models. Using the distribution of states can allow precision in choosing an averaging domain, and the use of an objective that targets the irreversible work could both result in a more direct comparison. The use of several explosive grains may also yield more physical results.



Baseline, worst and best case fits of the average response to the target function for 2.25 km/s impact.



Baseline, worst and best case fits of the average response to the target function for 1.25 km/s impact.

This first take approach has shown promise in theory, but more work is still needed to ensure that unique fits are obtained, and that the pore collapse simulation is adequate for strength model calibration. This will be accomplished through precise targeting of the material most affected by the strength through analysis of the state histograms, and through use of metrics more sensitive to strength effects, such as irreversible work.

References

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