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Multiscale Analysis of Cavity Collapse in High Explosives

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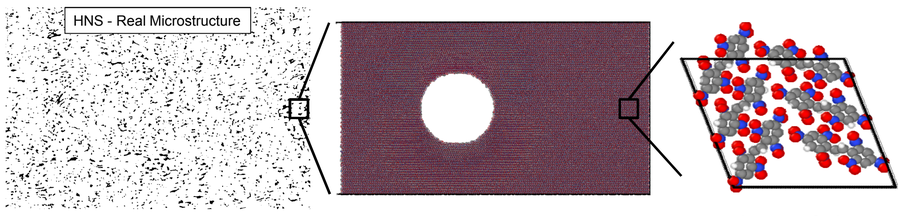
Problem

Predict margins on explosive components

- Modelling/simulation tools must capture accidental and intentional ignition scenarios.
- Bracket conditions for expected outcomes i.e. detonation, deflagration or just mechanical damage.

Understand how microstructure controls ignition

- Which hot-spot mechanisms are relevant i.e. jetting, viscoplastic heating and shear banding?
- How does this change with strength of the shock?



>10 µm, 1 µs

<1 µm, 0.1 µs

Physical Considerations
- Strain rates from creep to shock (~10^{-1} to 10^{8} s^{-1})
- Elastic and plastic deformation
- Thermal / Acoustic / Electromagnetic

Material Considerations
- PBX / pressed / granular / deposited
- Variations in sample preparation
- Vastly different length and time scales (nm - mm, fs - ms)

Approach

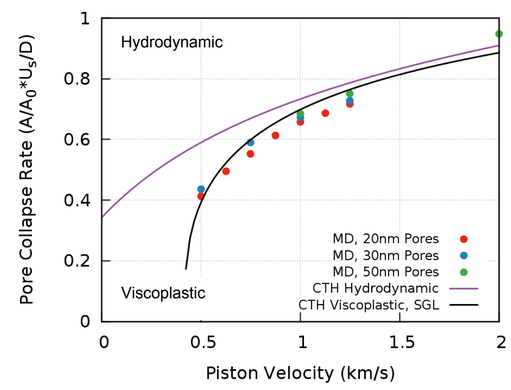
- CTH is an Eulerian continuum multi-dimensional multi-material modelling technique
- LAMMPS is a computational engine for classical molecular dynamics simulations.

Training data, detailed mechanisms

Microstructure effects, rapid prototyping

- Requires an equation of state, heat capacity parameterization and a strength model per material
- Reactive interatomic potentials (ReaxFF) capture chemistry naturally, fitted from *ab initio* database.
- Computationally inexpensive, can use real micrographs as simulation input
- Computationally expensive, is used to generate training data for CTH

- Strain rate dependent strength model needed to match MD results; Elastic-Perfectly Plastic von-Mises(EPPVM) strength model is insufficient.
- Optimized Steinberg-Guinan-Lund (SGL) strength model parameters against MD predictions(right)

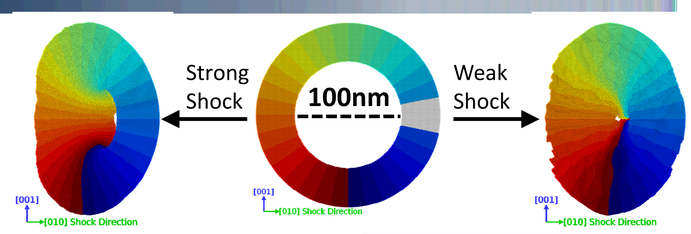


(Above) A scaled pore collapse rate from MD is shown as points which is used as the training objective of the SGL model (black) within CTH. The previous strength model (purple) is unable to capture the MD result.

Results

LAMMPS Molecular Dynamics

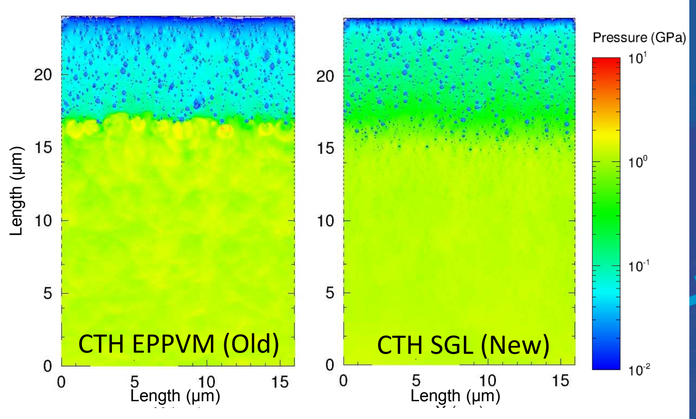
- Limiting cases of shock response captured within all-atom MD
- Strong shocks result in both shear banding and jetting from pore collapse
- Weak shocks only show shear banding

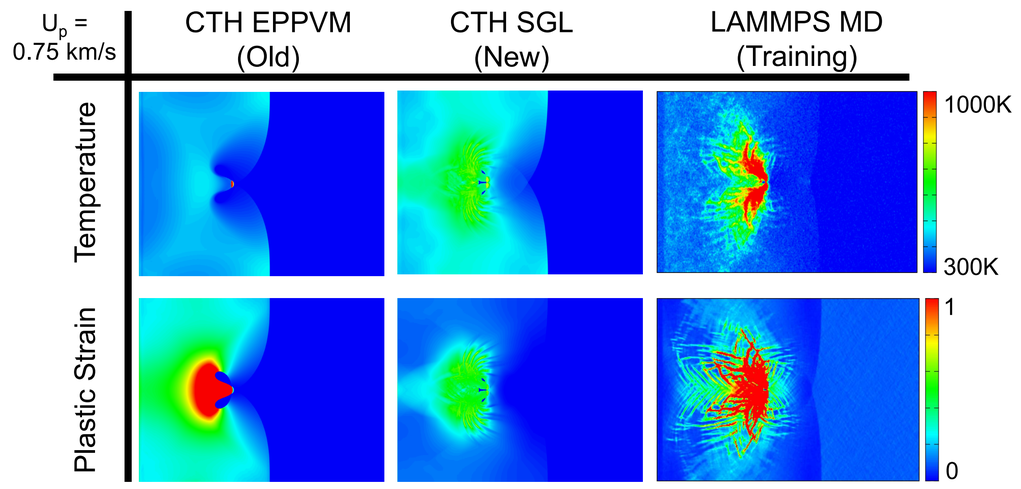


Hydrodynamic Response | Viscoplastic Response

CTH Hydrodynamics

- Old, EPPVM model only predicts jetting for all shock strengths
- New, SGL model shows a more uniform pressure distribution behind the shock
- Approximately 10^6 times cheaper than all-atom simulation





(Above) Qualitative comparison of the CTH model improvement relative to the MD result for the temperature and strain fields around a collapsing pore of diameter of 0.1µm. The EPPVM model has very little heat generated at regions of high strain, the SGL model corrects for this shortcoming.

Significance

Addressing a need for improved explosive components modelling
- MD simulations provide scientific basis for ignition predictions
- Demonstrated how shear banding causes localized heating, incorporated this effect into strength for continuum simulations

Enables identification of critical microstructure features for ignition
- Transfers knowledge from LAMMPS to CTH, greatly extending accessible length and timescales
- Improved predictions of initiation threshold for realistic microstructures, intractable within LAMMPS

HPC critical for connecting atomistic and CTH length/time scales
- KOKKOS implementation of LAMMPS efficiently use advanced computing architectures (GPUs, KNL), enabled atomistic simulations at unprecedented scales
- Accumulated $> 10^8\ cpu \cdot hrs$ on ACES and CTS-1 machines

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