SAND2009-7517C

Mixed equation of state: dynamical materials experiments on Z and multi-scale simulations

T.R. Mattsson, S. Root, T.A. Haill, R.W. Lemke
Sandia National Laboratories

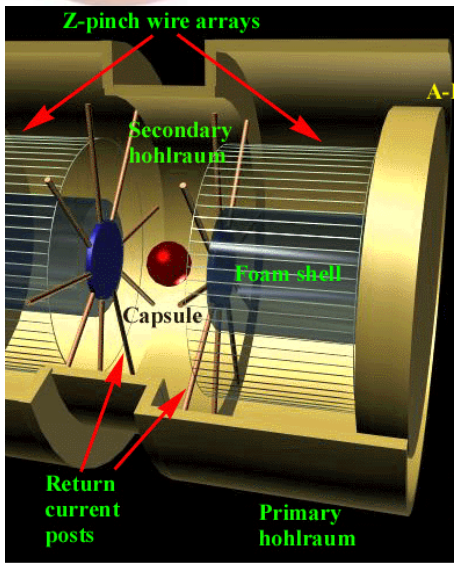
N.L. Bruner
Voss Scientific

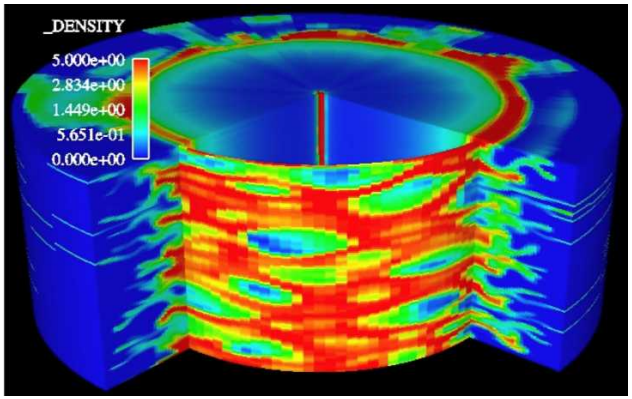
APS DPP meeting talk CO5.00006
Atlanta, GA
November 2, 2009

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Sandia National Laboratories

Modeling the behavior of materials under high energy-density conditions is a foundation for progress



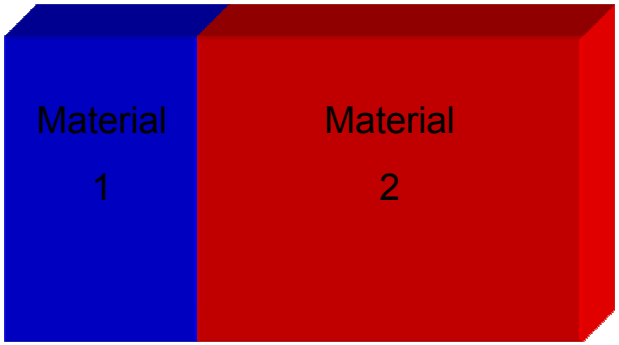


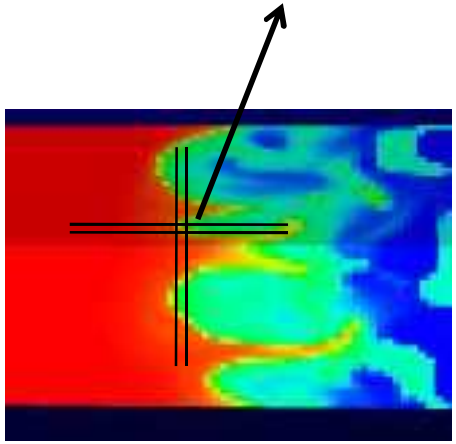
Simulation of imploding Z pinch: involved flows lead to mixing

- Many materials in HEDP experiments
- Experiments require simulations for design, optimization, and analysis
  - Warm-dense matter: eV temperature, solid density, 100 GPa
- Equation of state (EOS) of mixed materials
  - Apply rules to blend pure EOSs
  - We use a doped CH_2 foam to investigate mixing rules
  - Multi-scale simulations: DFT/QMD, classical MD and rad-hydrodynamic
- *Validate multi-scale simulations by sets of Mbar shock experiments*

EOS Mixing Rules (aka Multi-Material Treatment) in ALEGRA – Sandia multi-physics code

Cell with two materials with volume fractions: f_k



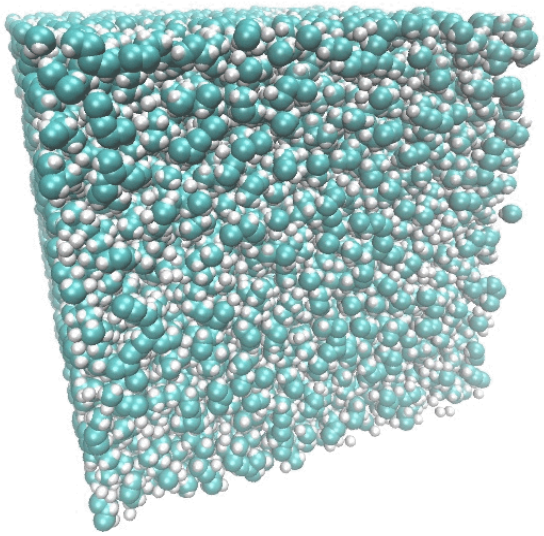


- How do volume fractions change as a cell compresses or expands?
- Densities, specific internal energy, temperature and pressure depend on it
- Isentropic compression method: update volume fractions by difference in bulk modulus

$$\frac{df_k}{dt} = f_k\left(\frac{\overline{B} - B_k}{B_k}\right)\nabla \bullet \vec{u} - \frac{f_k}{\overline{P}}\frac{dP_k}{dt}$$

- Re-normalize volume fractions under mass- and energy conservation
- Update EOS
- *Rules must be validated by experiments*

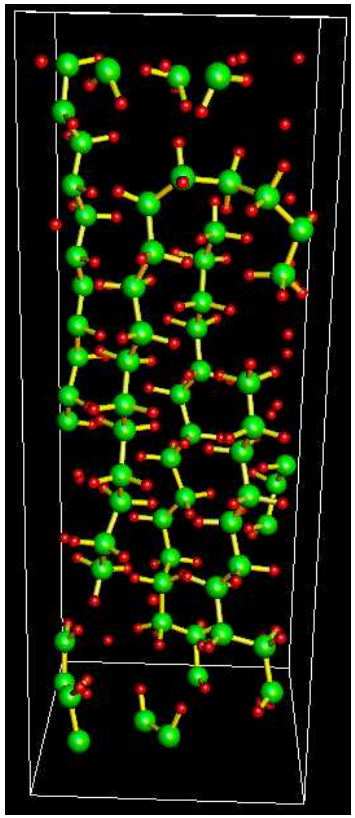
We employ a multi-scale approach to modeling foam, doped foam, and the effects of mixing



Simulation cell for classical MD

- Foam is polymers and void
- *Modeling the dense polymer plastic is a key step to modeling the foam*
- Macromolecules are large systems with long timescales – classical MD simulations
- Using LAMMPS: **lammps.sandia.gov**
  - Classical MD code developed at Sandia
  - Many interaction potentials (force fields)
- Study shock response of two polymers
  - *Polyethylene: linear semi-crystalline*
  - *Poly-methyl-pentene (PMP) branched hydrocarbon and the base of TPX foam*

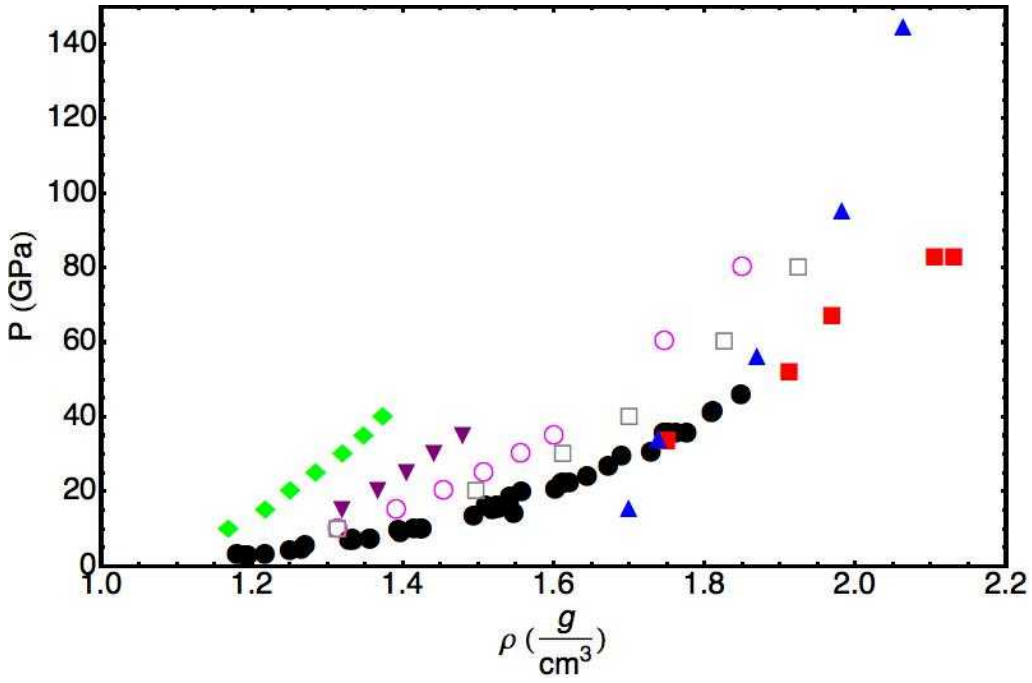
Density functional theory (DFT) based MD is a well-established approach, but is far from a black box



Snapshot of 0.955 g/cm^3 crystalline poly-ethylene

- VASP 5.1 code (Georg Kresse, Vienna, Austria)
  - Plane-wave basis-set
  - Finite-temperature DFT (Mermin)
- Accuracy of DFT calculations depends on the exchange-correlation (xc) functional
  - Sandia developed AM05 functional (Armiento and Mattsson, Phys Rev B 2005)
  - DFT research at Sandia: **dft.sandia.gov**
- *Demanding large scale DFT-MD simulations: 200 atoms polyethylene and 440 atoms PMP cells*
  - Polyethylene: Desjarlais/Cochrane
  - PMP/TPX: Mattsson
  - Utilizing Red Storm at Sandia

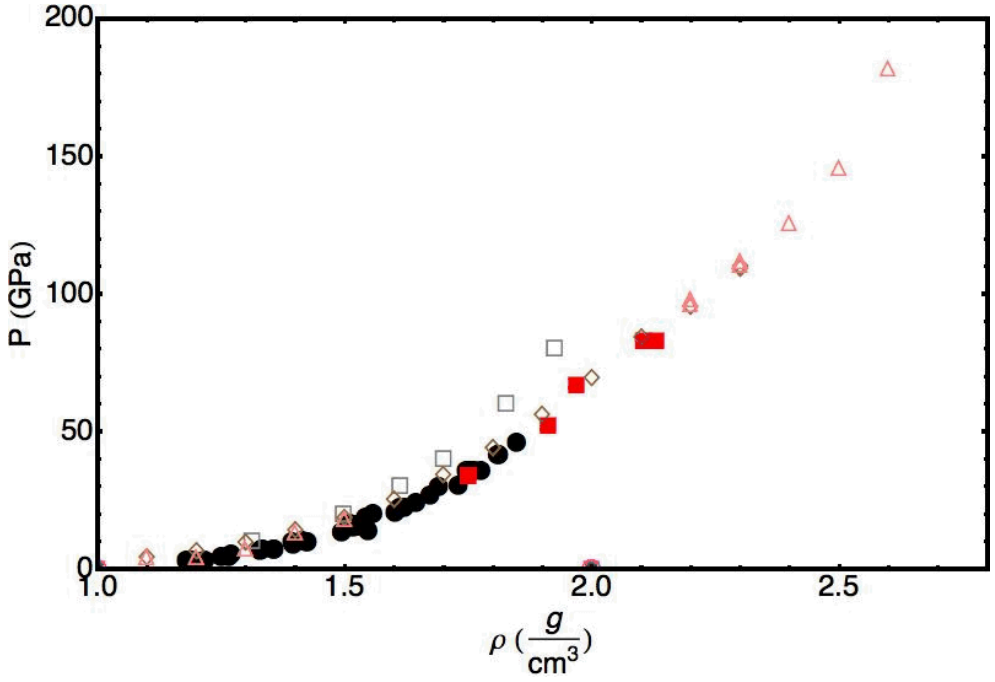
None of the classical force-fields are of high fidelity for strong compression – ReaxFF works for weak shocks



- Tight-binding (J.D Kress et al SCCM 1999)
- AIREBO
- OPLS
- Borodin-Smith (exp6)
- ReaxxFF
- Experiments (Nellis/ LASL handbook)

- LASL shock handbook plus high-pressure work by W.J. Nellis and co-workers (J. Chem. Phys. 1984)
- *Tight-binding* – state of the art 10 years ago
- *OPLS, Borodin-Smith-exp6* are fixed-bond force-fields commonly used for polymers
- *AIREBO*, reactive force with Lennard-Jones core repulsion
- *REAXFF*, recent reactive force field, van Duin et al Caltech. It is complex and decidedly slower than the other classical potentials

DFT/QMD delivers a high-fidelity description of shocked polyethylene



ReaxxFF

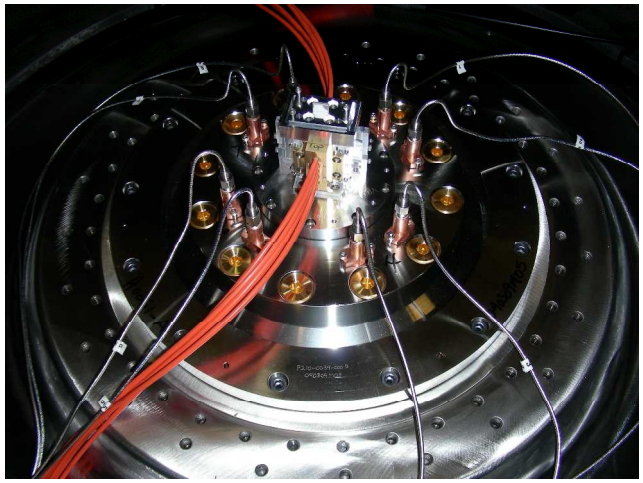
DFT-AM05

Experiments (Nellis/ LASL handbook)

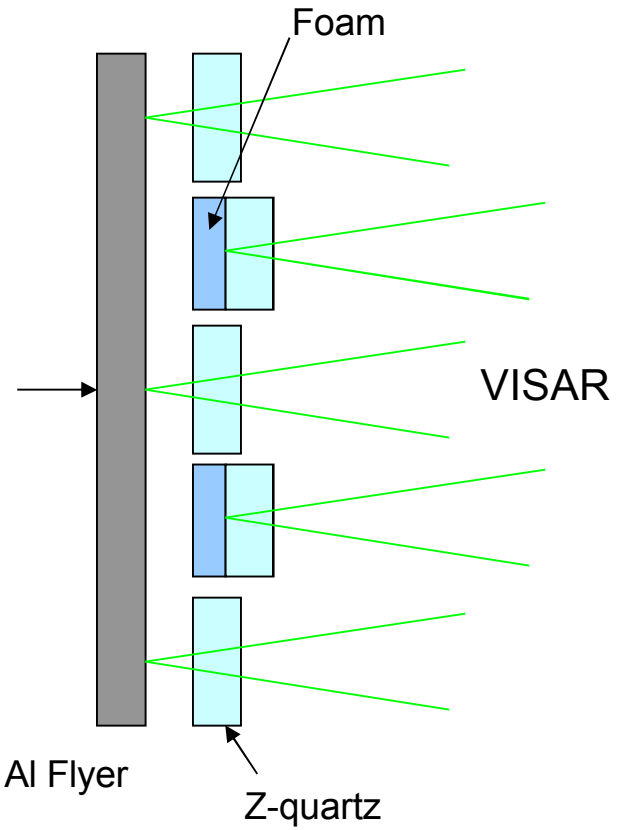
- *DFT-QMD/AM05 in quantitative agreement with shock-data for all compressions.*
- ReaxFF shows qualitative behavior for weak shocks
- Predictions for multi-Mbar shocks in polyethylene

Magnetically accelerated flyer impact experiments

- Four experiments in April 09:
  - 2 – pure, 2 – doped.
- One experiment in August 09:
  - Dense PMP/TPX plastics
- Pure/doped foam in September 09.
- Flyer Velocities:
  - 20.5 km/s to 25.8 km/s



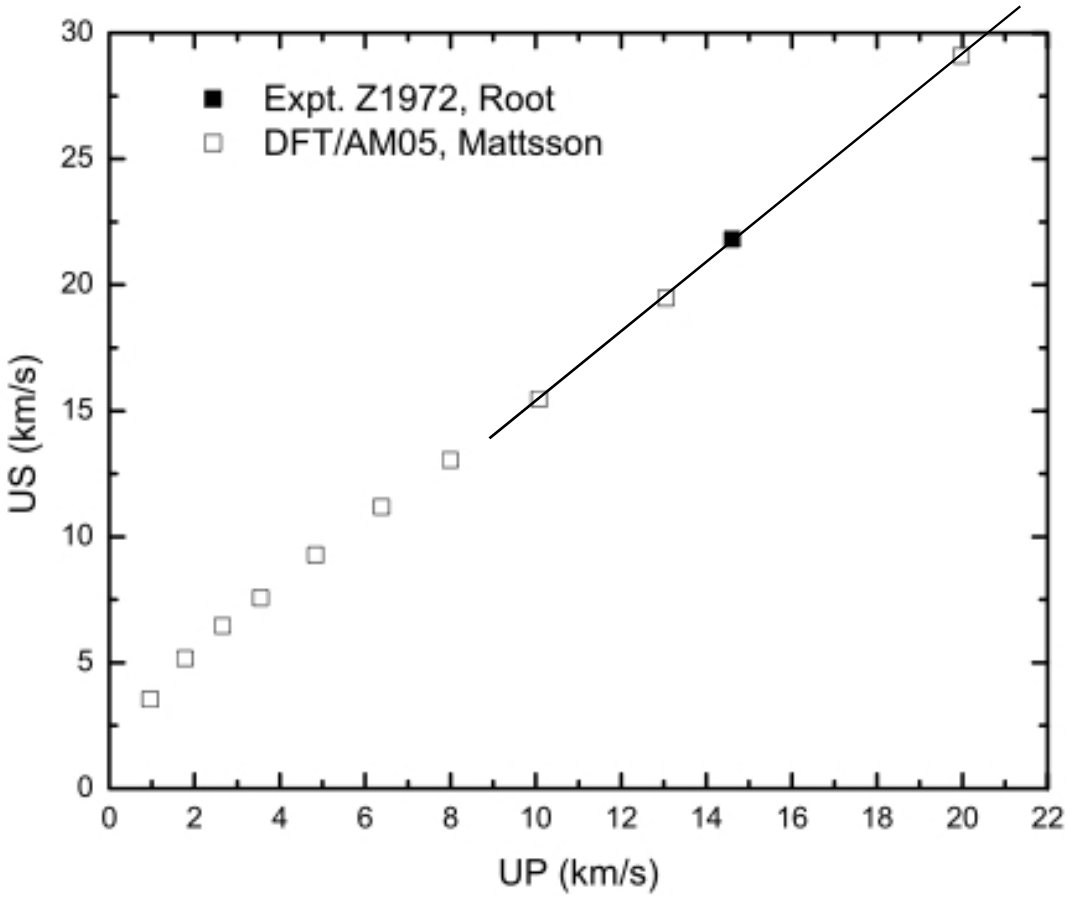
Seth Root experimental PI



VISAR Measurements as main tool:

- Shock velocity from arrival at Foam/Quartz Interface
- Flyer velocity and impedance matching with aluminum standard

Recent Mbar experiments on Z confirms the DFT/AM05 predictions for shocked poly(4-methyl 1-pentene) (PMP)

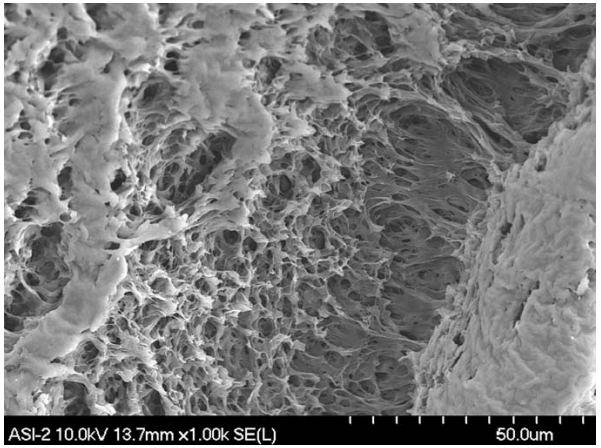


- DFT-QMD/AM05 simulations for PMP
- Flyer plate experiments on Z (Seth Root)
- Excellent agreement between experiments and theory
- *DFT-QMD/AM05 yields results of high fidelity for shocked polymers in the Mbar regime*

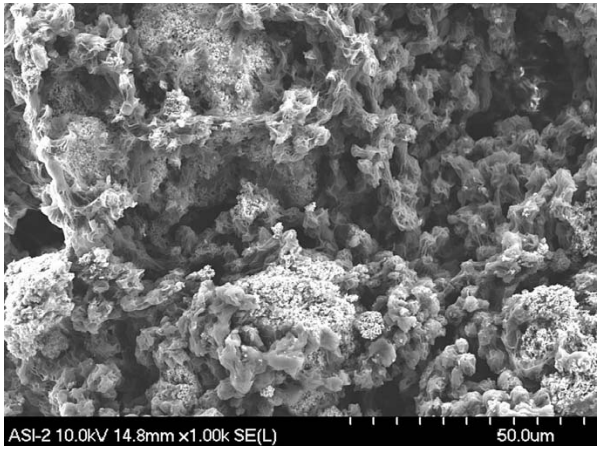
Foam targets made by General Atomics

- Poly-methyl-pentene (PMP/TPX) foam: chemical composition CH_2
- Platinum dopant (150 – 450 nm):
- 50% Pt by weight
- Undoped density = 0.309 g/cm³
- Pt-Doped density = 0.293 g/cm³

- Targeting *50% mass fraction* for largest deviations from simple mix rules
- *99.3% foam and 0.7% platinum by volume*

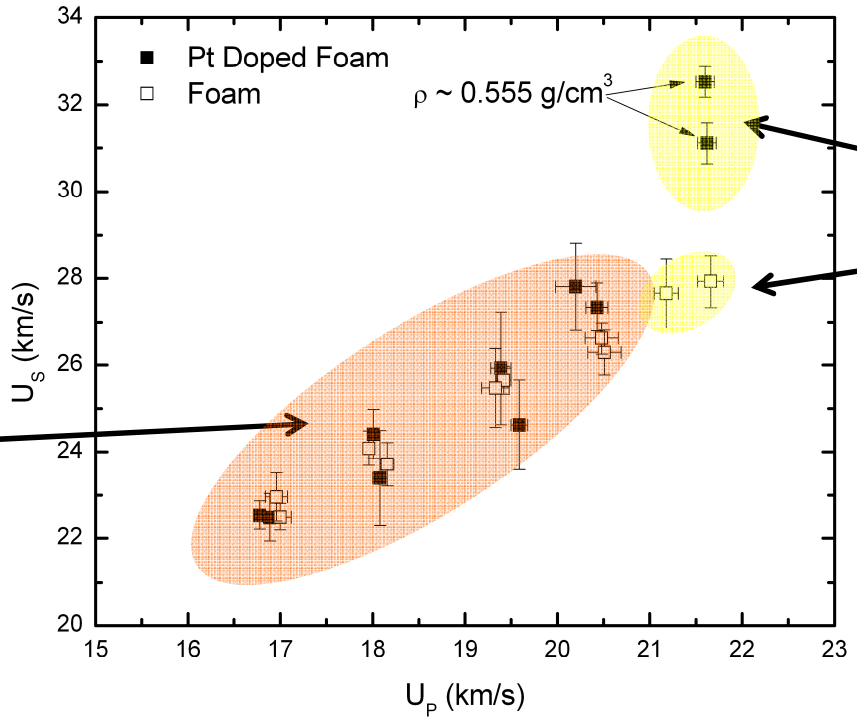


Pure Foam



Pt doped foam

Experimental results: the doped and pure foams show similar response – and the foam response is reproducible

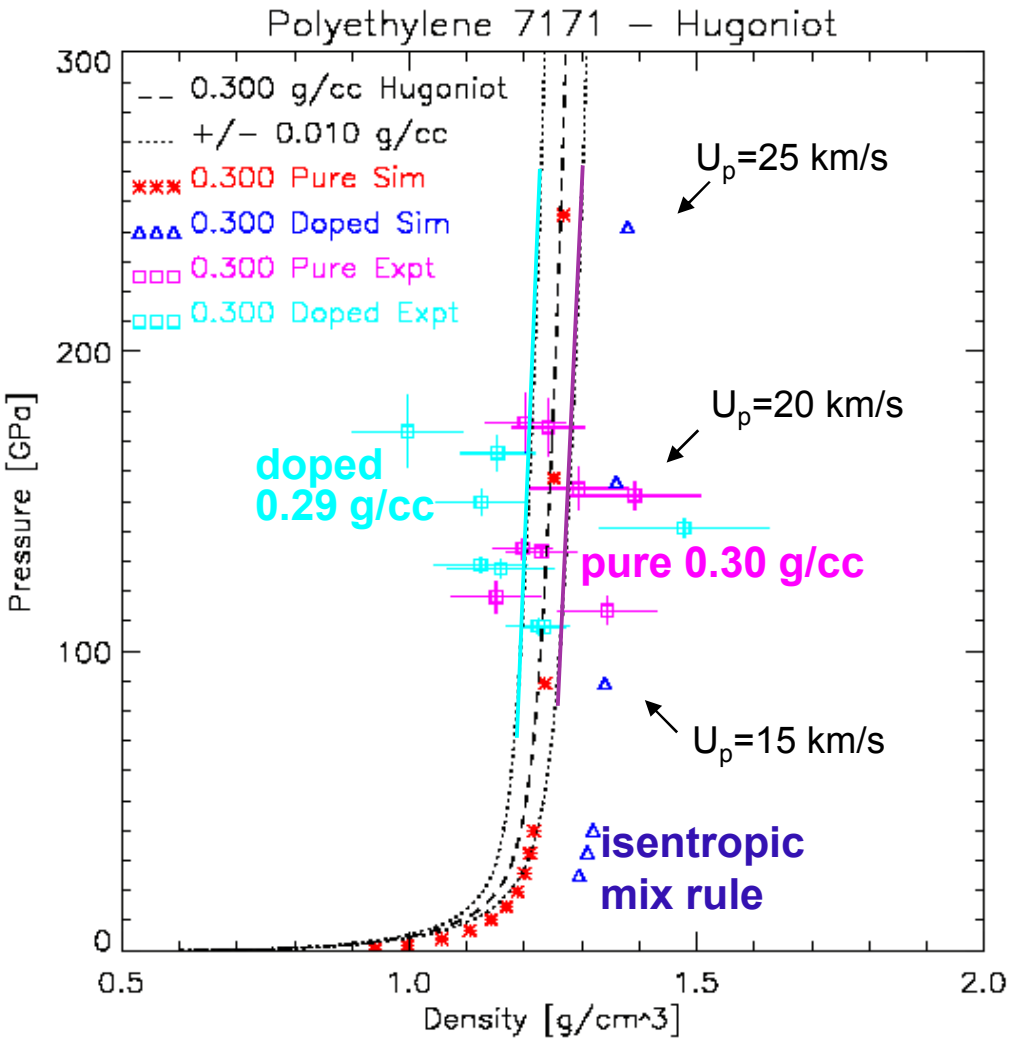


Two experiments in September

Experimental series in April 2009.
Pure: 0.31 g/cm^3
Doped 0.29 g/cm^3
(*the difference matters*)

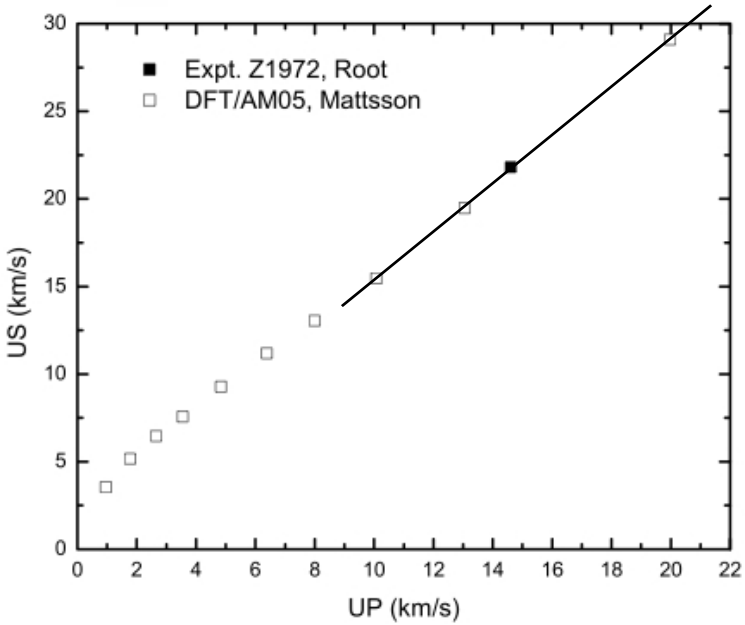
Within experimental uncertainty, pure and doped foam show similar shock response – not what we expected.

Comparing experiments on pure and doped foam with ALEGRA simulations applying the isentropic mix rule

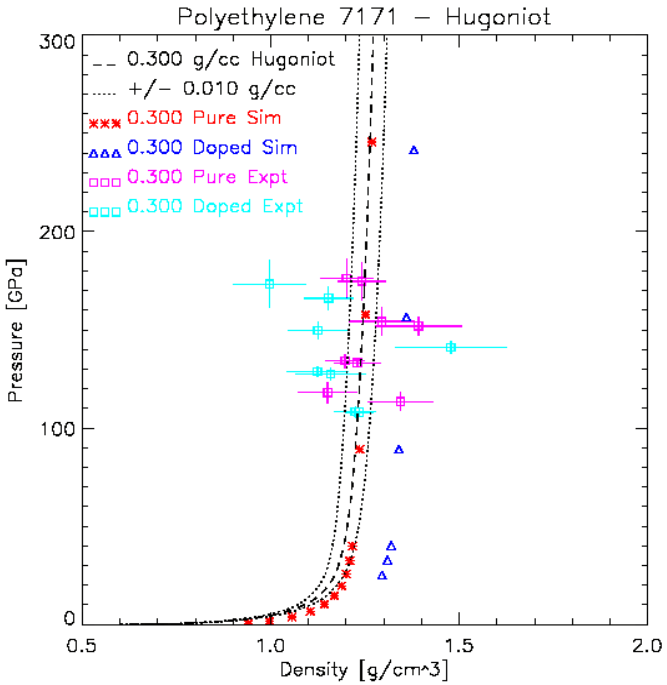


- Lines are simulations for *pure foam* at 0.29, 0.30, 0.31 g/cm^3
- Simulation: isentropic compression mix-rule predicts shock to lower pressure
- *Although the experimental data has significant scatter, the isentropic mix rule has a different trend than the data*
- This needs more work: additional experiments and application of different mixing rules

Summary: shock response of dense PMP/TPX can be predicted – doped foam a promising platform to study mix



DFT-QMD/AM05 results for high-pressure PMP/TPX Hugoniot validated by experiments on Z.



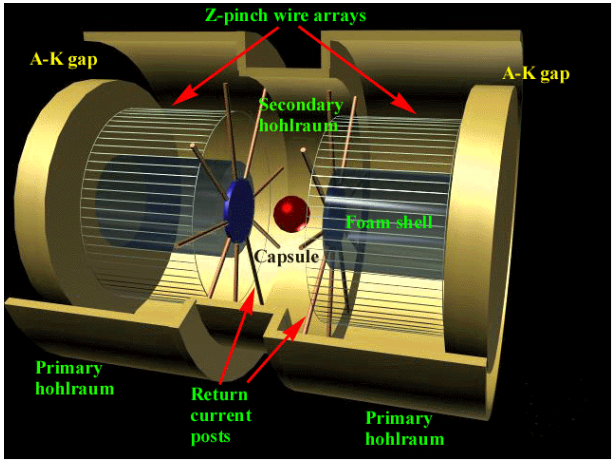
Promising results for CH_2 foam as a system to validate models for mixed equation of state

Gary Grest, Matt Lane, Aidan Thompson, Kyle Cochrane, Michael Desjarlais, Seth Root, Tom Haill, Nikki Bruner, Ray Lemke, Dawn Flicker, Tom Mehlhorn.

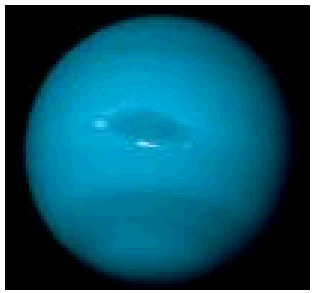
Extra slides for questions following the presentation

Thank you, any questions?

Properties of shocked hydrocarbon foams is of importance to modeling inertial confinement fusion



Double-ended Z pinch with a cm sized foam-shell capsule



Dynamical materials experiments reach conditions of giant planets like Jupiter and Neptune

- A commonly used foam is based on poly(4-methyl 1-pentene) (PMP/TPX)
- Modeling the dense plastic as a step to modeling the foam
- Macromolecules are large systems with long timescales, bonded force-fields are commonly used for MD simulations
  - OPLS (W. L. Jorgensen et al 1996)
  - Borodin-Smith exp6 (O. Borodin et al 2006)
  - AIREBO (S.J. Stuart et al 2000)
  - ReaxxFF (K. Chenoweth et al 2008)
- *Benchmarking/validation is everything*
- *First-principles simulations to investigate the fidelity of these force-fields*
- *Magnetically launched flyer plate experiments to validate mixing rules and DFT/QMD results*

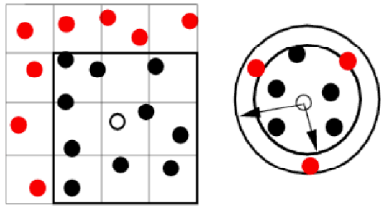
Molecular Dynamics with the Sandia code LAMMPS

What LAMMPS is…

- MD engine for atoms, molecules, or particles at any length/time scale using Newton's equations. Steve Plimpton main developer
- Integrated MPI for parallel or serial for stand-alone *designed for portability and highly efficient parallelization*
- FFT for long-range Coulomb-interactions
- *Many pre-coded potentials:*
  ReaxFF, AIREBO, EAM/MEAM, LJ, Yukawa, Tersoff, etc.
- Open source (GPL)
  http://lammps.sandia.gov

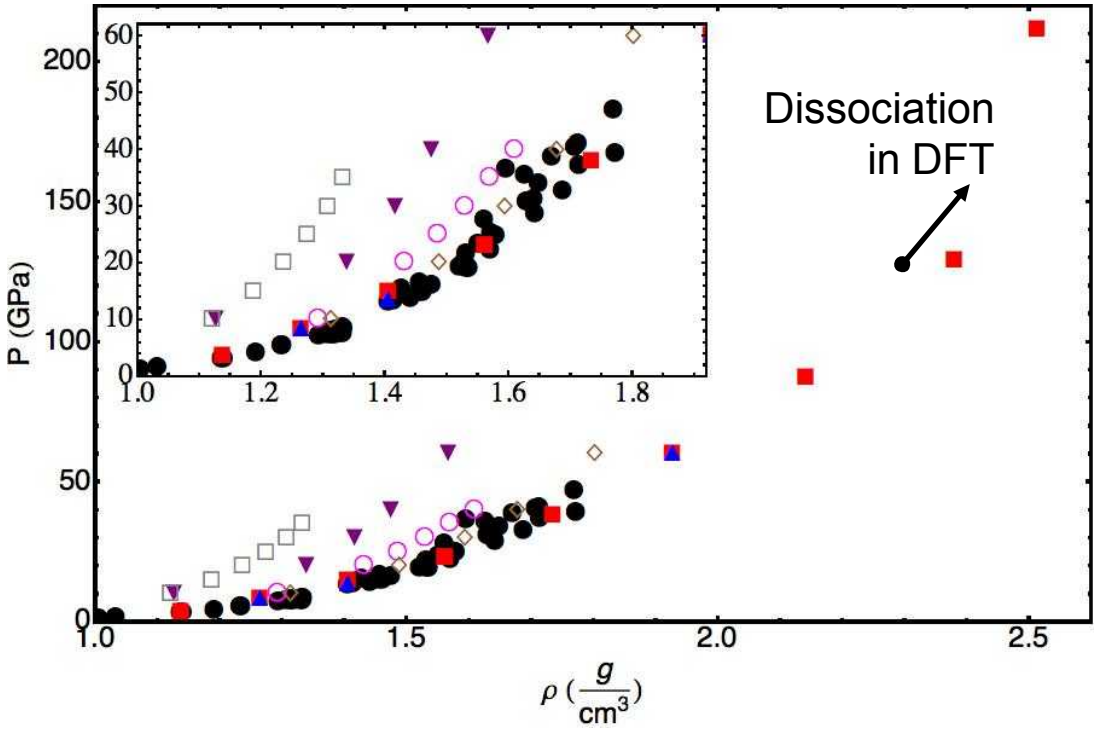
What LAMMPS is NOT…

- Limited pre-processing support for building systems configurations
- Limited on-the-fly diagnostics
- Limited post-processing analysis and visualization
- However, add-on tools and modules are available to accomplish these on website



Computationally efficient neighbor analysis algorithm

Similar differences in behavior for shocked poly(4-methyl 1-pentene)



- AIREBO and OPLS both give *significantly too stiff shock response at all pressures*
- Borodin-Smith and ReaxFF work well for weak shocks in PMP
- *Only the DFT-AM05 simulation of high fidelity for all shocks*
- *Significant deviations already far from the regime where dissociation occurs*
- Classical MD: Gary Grest, Matt Lane, and Aidan Thompson
- DFT-QMD: Polyethylene: Cochrane & Desjarlais, TPX/PMP: Mattsson
- T.R. Mattsson et al, submitted (2009).

Shocked foam hydrodynamics simulations using the Sandia code ALEGRA

Driver / method

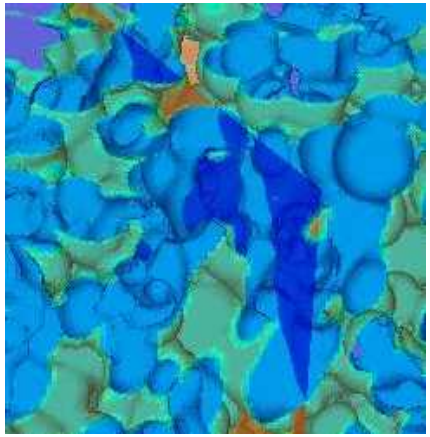
- Constant velocity piston driver
  - Classical shock problem used to generate the Rankine-Hugoniot relationship within the code
- Constant velocity piston driven foam with explicit flyer
  - Reveal issues with driving non-uniform foam with uniform flyer
- Hydrodynamics simulation that includes graded density/temperature flyer at time of impact
  - Initial flyer conditions from MHD simulation of flyer only
- Full MHD drive simulation of flyer / foam / window
  - Future
- Lagrangian simulations

Target material models

- Homogenous low-density plastic
  - Initialize uniform material at average foam density
- Porosity homogenous target
  - Invoke the P-alpha model
  - Specify solid plastic density as reference
  - "$\alpha = \rho_{solid} / \rho$" is the distention parameter reduces to 1.0 as void compressed from foam
- Mesoscale direct simulation of foam
  - Explicitly model plastic matrix with voids
  - Development state
- Mix models
  - Volume fractions
  - Isentropic mix

Porosity is modelled in ALEGRA using the P-α model

- The distention parameter α is defined and advanced in time
  - $\alpha = \rho_{solid} / \rho_{foam} \geq 1$
  - Evolution equation for α
- Pressure and energy/temperature tables are evaluated at the compressed solid density when $\alpha > 1$
  - $P(\rho_{foam}, T_{foam}) = 1/\alpha\ P_{table}(\alpha^*\rho_{foam}, T_{foam}) = 1/\alpha\ P_{table}(\rho_{solid}, T_{foam})$
  - $E(\rho_{foam}, T_{foam}) = E_{table}(\alpha^*\rho_{foam}, T_{foam}) = E_{table}(\rho_{solid}, T_{foam})$
  - Otherwise tables are evaluated normally when $\rho > \rho_{solid}$ (i.e., $\alpha = 1$)
- References:
  - W. Herrmann, J. Appl. Phys., 40 (6) 2490, May 1969.
  - M.M. Carroll and A.C. Holt, J. Appl. Phys, 43 (4) 1626, April 1972.
  - G.I. Kerley, SAND92-0553, SNL, April 1992.

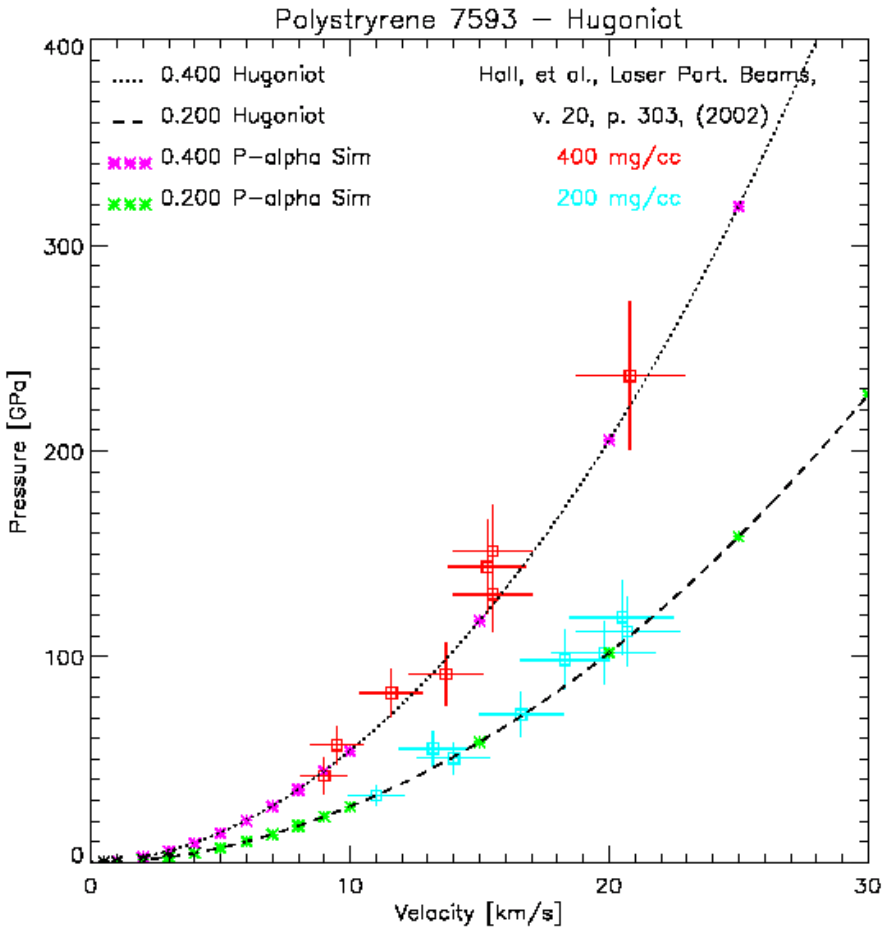


- Pressure reduced by distention parameter since a porous material can't sustain the pressure of the bulk material
- Energy from bulk material (neglect surface effects) questionable assumption in high surface/volume materials like foam
- *Must validate the model*

Validation of P-α Model for Polystyrene

- Partial Hugoniot data in literature for TMPTA foam
- Polystyrene is a close approximation
  - Hall, et al., used 7592
  - We use Aneos 7593
    - » More complete
    - » More consistent
- Laser driven shock experiments on LULI, France
- ρ = 20, 50, 100, 200, 400, and 1100 mg/cm^3
- We model ρ = 200 and 400 mg/cm^3

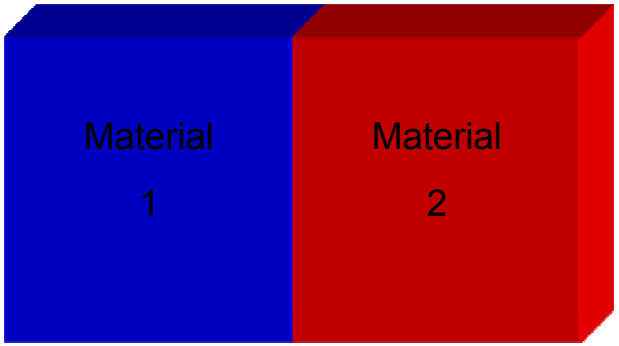
- *Data and simulations agree without tuning, initial density is not a free parameter*



EOS Mixing Rules (aka Multi-Material Treatment) in ALEGRA – Sandia multi-physics code

- Whenever a cell compresses or expands, how do the volume fractions change?
- This affects densities and specific internal energy
- Hence also affects temperature and pressure

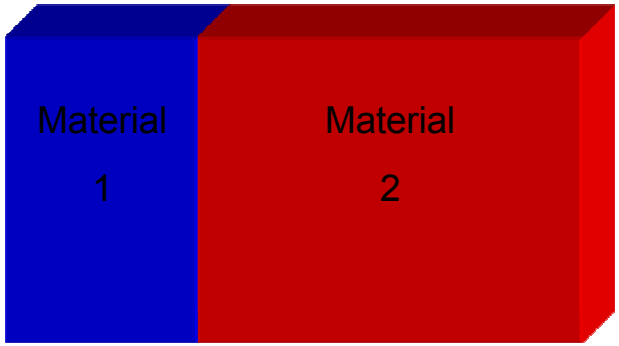
- Default (legacy) method:
  - Volume fractions, f_1 and f_2 , held constant
  - Density & energy adjusted for each material separately
    - » $\rho_{new} = \rho_{old} * (V_{old} / V_{new})$
    - » $e_{new} = e_{old} * (\rho_{old} V_{old} / \rho_{new} V_{new})$
  - Temperature & pressure updated by EOS evaluation



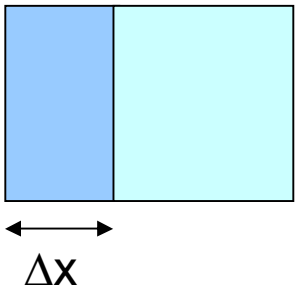
- Isentropic Compression Method (new):
  - Update volume fraction for each material *k* using bulk modulus B_k

$$\frac{df_k}{dt} = f_k\left(\frac{\overline{B} - B_k}{B_k}\right)\nabla \bullet \vec{u} - \frac{f_k}{\overline{P}}\frac{dP_k}{dt}$$

- Normalize volume fractions to 1.0
- Enforce mass & energy conservation
- Update EOS



Experimental analysis: shock transit time and impedance match with Al standard



- $T_{Transit} = T_{Shock\ Arrival} - T_{Impact}$
- $U_S^{Foam} = \Delta x / T_{Transit}$
- With Al Hugoniot properties, U_S^{Foam}, and ρ_0, we can determine P, U_P, and ρ

Rankine – Hugoniot Equations:

$P = \rho_0 U_S U_P$

$\rho_0/\rho = (U_S - U_P)/U_S$

$E - E_0 = 0.5(P+P_0)(V_0-V)$