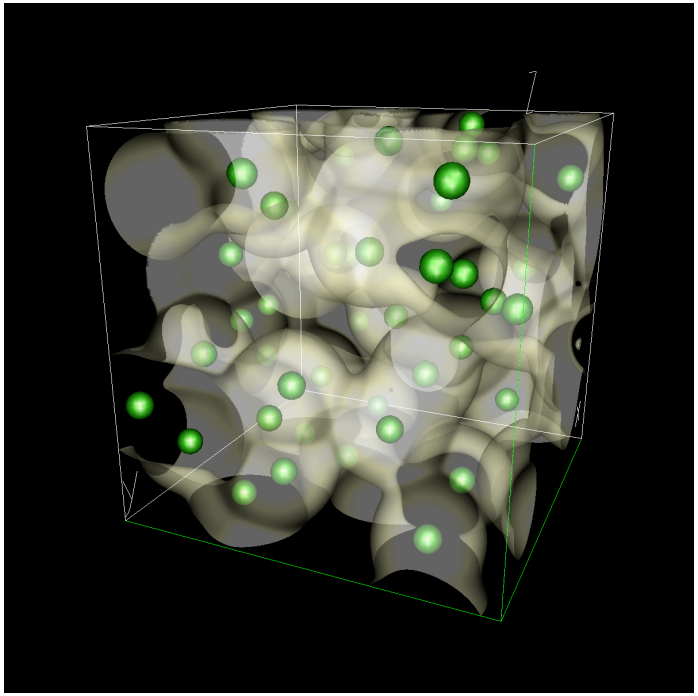
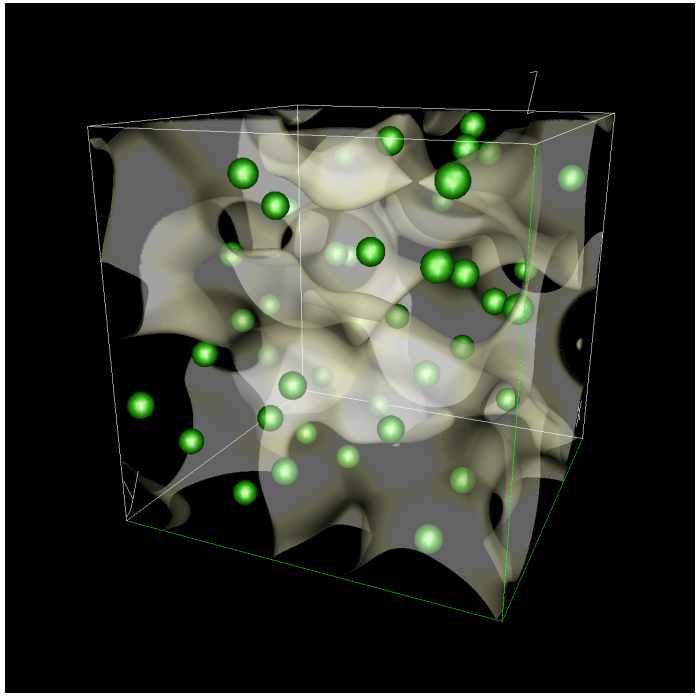
QMD Simulations of Warm Dense Matter in support of High Energy Density Physics Experiments on the Z Machine



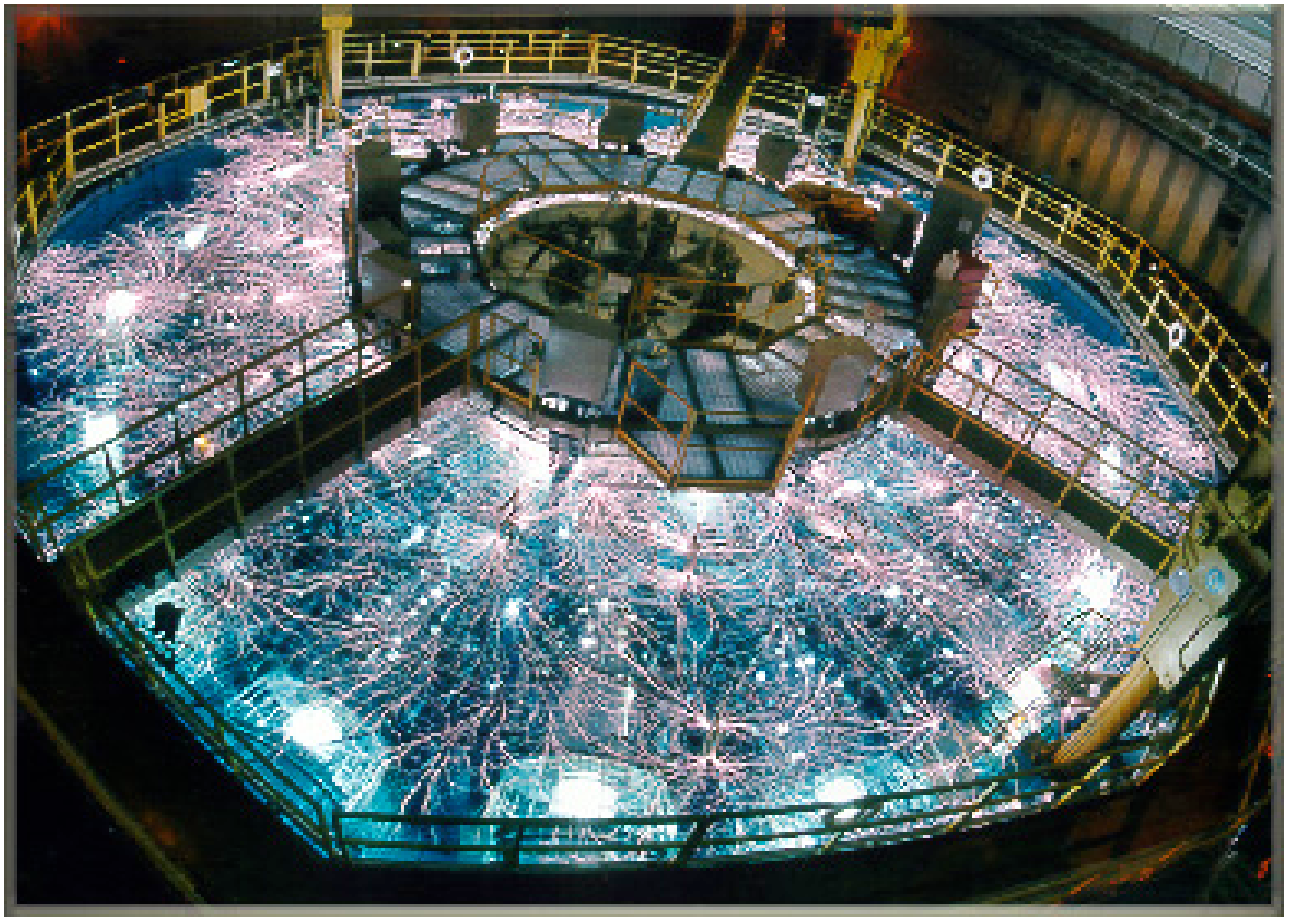


Mike Desjarlais
HEDP Theory &
ICF Target Design
Sandia National Laboratories

Workshop on
Accelerator-Driven
Warm Dense Matter
February 22-24, 2006

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's Z Machine is used for several HEDP experimental campaigns



Z pinches for Inertial Confinement Fusion

Magnetically launched flyer plates for EOS studies

Isentropic compression for EOS studies

The Z machine delivers more than 20 million Amperes of current
ZR will generate more than 25

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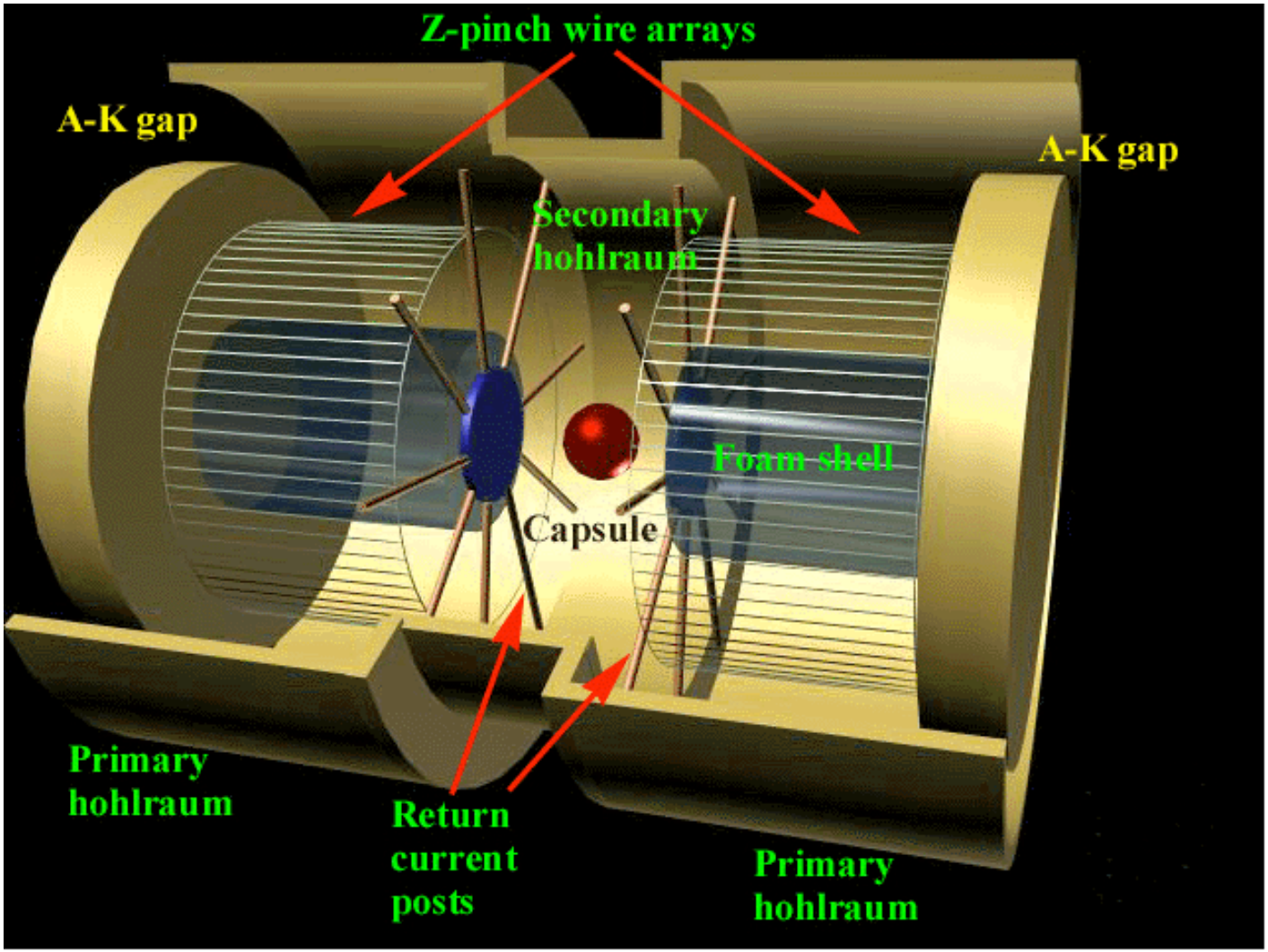
We routinely perform large scale computer simulations to model the complex geometries and physics in our HEDP experiments



This is a double-ended Z pinch with an ICF target in the center

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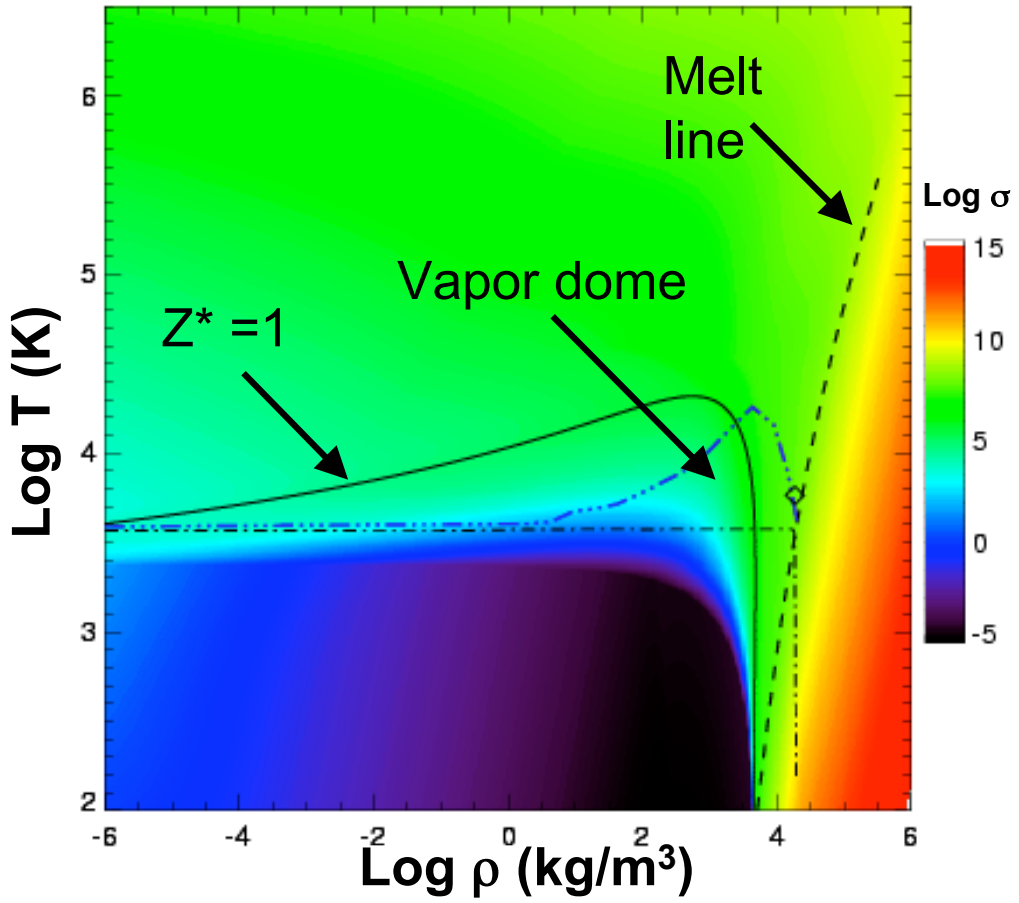
HEDP computer simulations rely on "physics packages": Conductivities, Equations of State, and Opacities

Tungsten Conductivity



This highly structured portion of phase space is Warm Dense Matter

Definitions of Warm Dense Matter are varied, but generally center around **strongly coupled ions and moderately degenerate electrons** --- many different interactions are comparable.

A **quantum mechanical** treatment is generally necessary.

Most wide-range equations of state interpolate through this difficult area.

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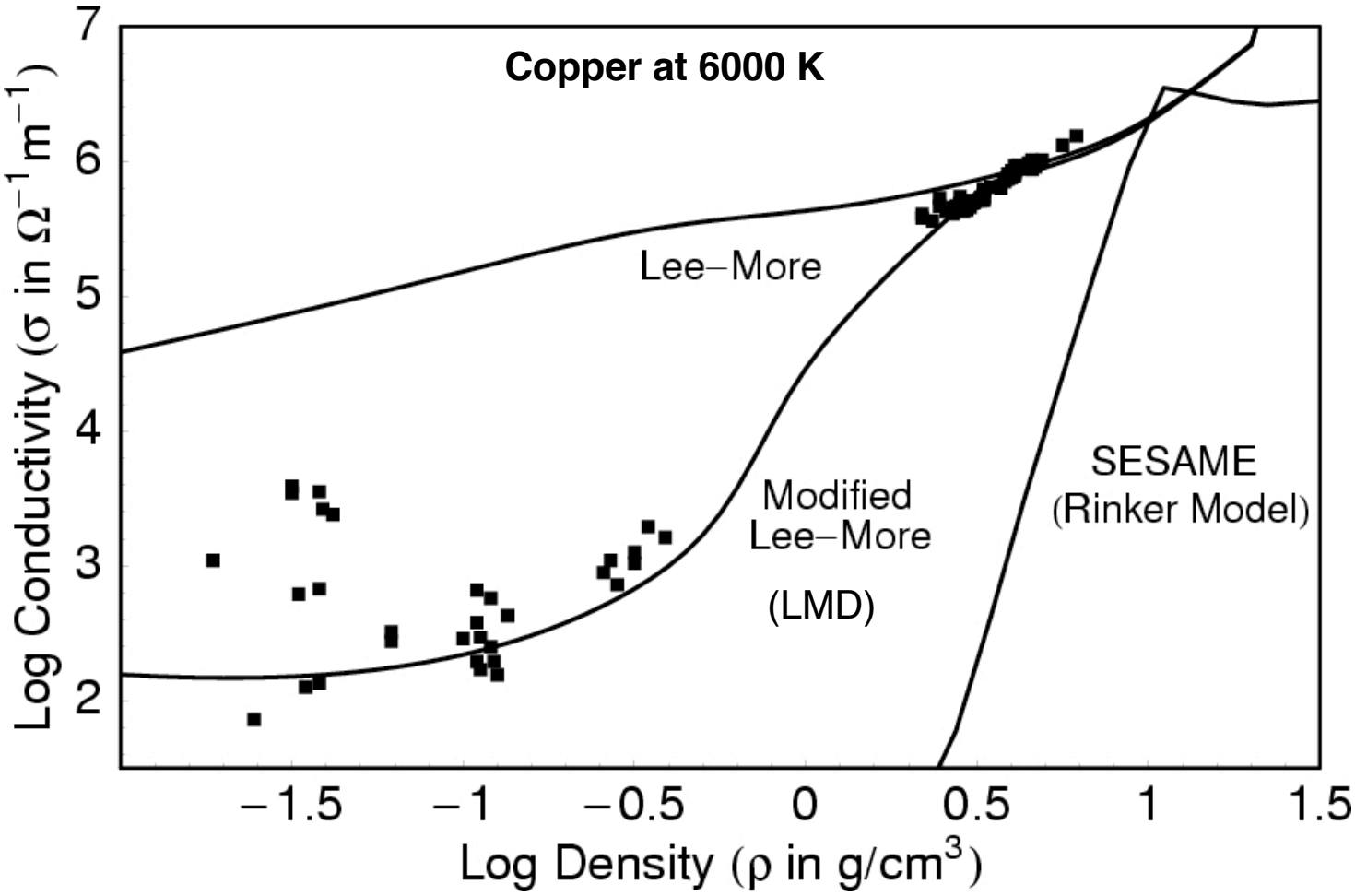
Modifications of the Lee-More algorithm were made to obtain an improved wide-range model*

* M. P. Desjarlais, Contrib. Plasma Phys. **41** (2001) 2-3, 267-270



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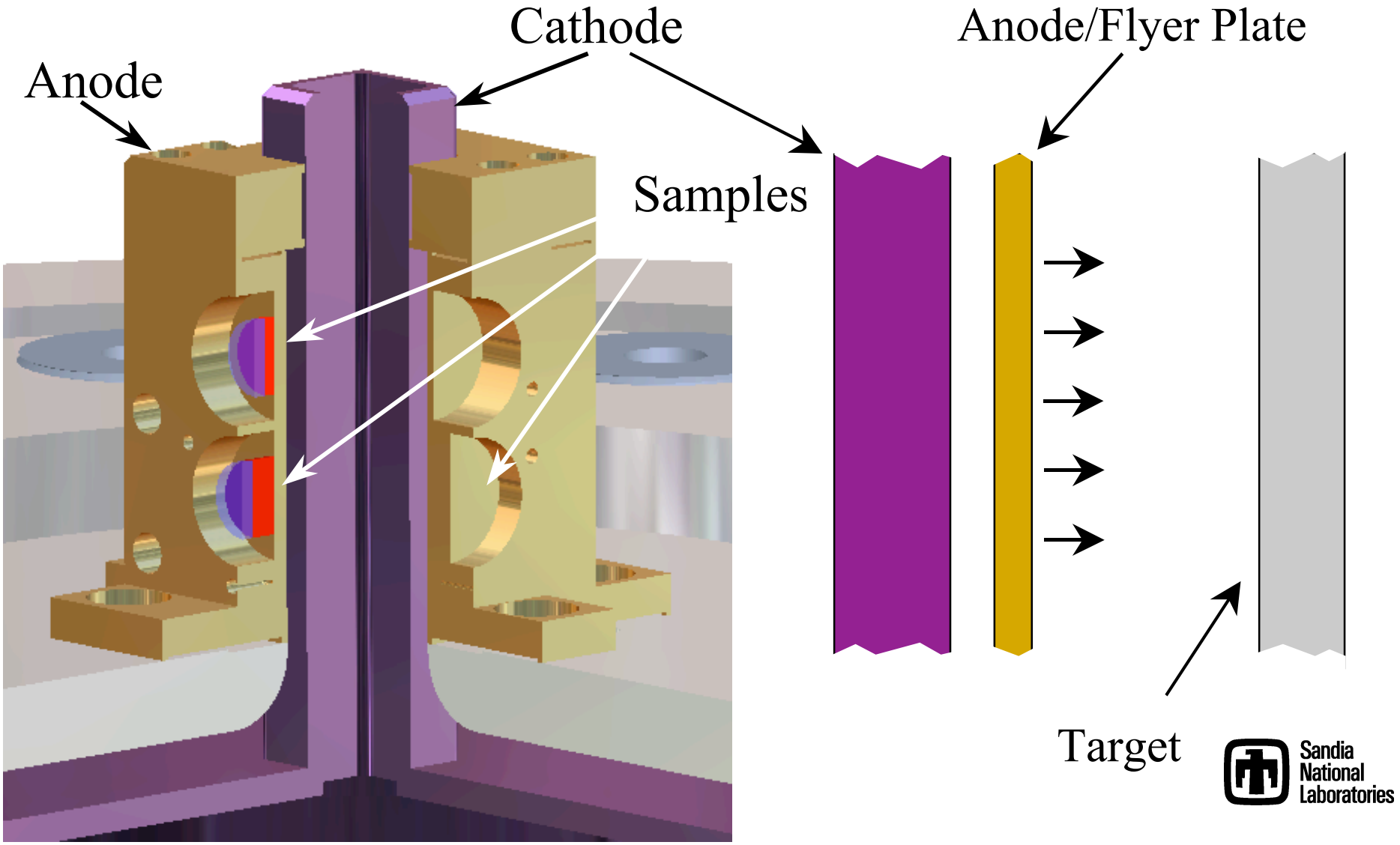
A demanding application: Ultra-high velocity magnetically launched flyer plates (30 km/sec, Multi-Mbar pressures)



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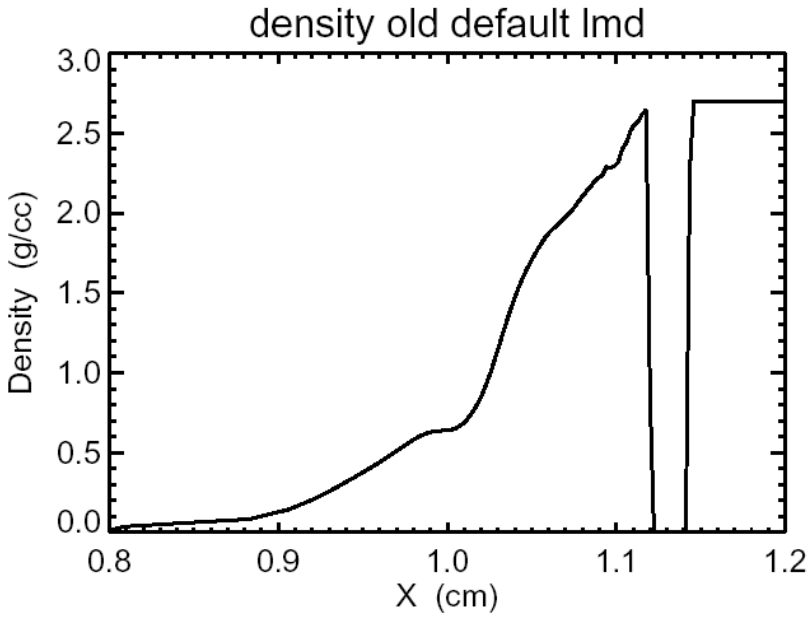
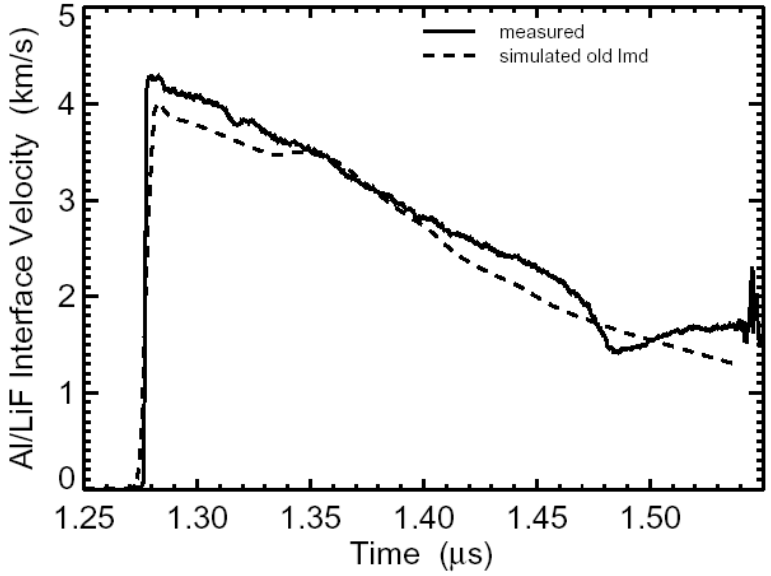
We simulated these magnetically launched flyer plates using the modified Lee-More (LMD) conductivities

Detailed comparison between simulations and experiments for magnetically launched flyer plates suggested that our *improved* conductivities were still not sufficiently accurate for the warm dense liquid aluminum.

Simulations by Ray Lemke with Sandia's 3D Rad-MHD ALEGRA code





For many of our applications we require conductivities accurate to well within a factor of two.

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We are using Density Functional Theory (DFT) to perform Quantum Molecular Dynamics (QMD) simulations of Warm Dense Matter

•The simulations are performed with VASP (Vienna Ab initio Simulation Program), a plane wave density functional code

•Exchange and Correlation functionals are Generalized Gradient Approximation (GGA/PBE)

•We typically use up to 256 atoms, but it varies depending on density and the number of electrons we need to carry (the valence); We use Projector Augmented Wave (PAW) all-electron, frozen core potentials for the atoms

•We generally perform our simulations in the Canonical Ensemble (N,V,T) using either velocity scaling or a Nosé-Hoover thermostat to regulate the temperature; Fermi statistics for the electrons

•Typical runs cover one to twenty picoseconds

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The Kubo-Greenwood formula is used to calculate the frequency dependent electrical conductivity

$$\sigma_{\mathbf{k}}(\omega) = \frac{2\pi e^2 \hbar^2}{3m^2 \omega \Omega} \sum_{\alpha=1}^{3} \sum_{j=1}^{N} \sum_{i=1}^{N} (F(\varepsilon_{i,\mathbf{k}}) - F(\varepsilon_{j,\mathbf{k}})) \left| \left\langle \Psi_{j,\mathbf{k}} \left| \nabla_\alpha \right| \Psi_{i,\mathbf{k}} \right\rangle \right|^2 \delta(\varepsilon_{j,\mathbf{k}} - \varepsilon_{i,\mathbf{k}} - \hbar\omega),$$

where *e* and *m* are the electron charge and mass. The *i* and *j* summations are over the *N* discrete bands of the triply periodic calculation for the cubic supercell with volume Ω. The coordinate index is α and in general we average over α to improve the statistics. $F(\varepsilon_{i,\mathbf{k}})$ is the Fermi weight corresponding to the energy for the *I*-th band at ***k*** with wavefunction $\Psi_{i,\mathbf{k}}$.

We integrate over the Brillouin zone using the method of special **k**-points

$$\sigma(\omega) = \sum_{\mathbf{k}} \sigma_{\mathbf{k}}(\omega) W(\mathbf{k}) \quad ,$$

and average over 10 to 20 configurations selected from the MD run.

This is really nothing more than the quantum analog of the classical current-current correlation function representation of the conductivity

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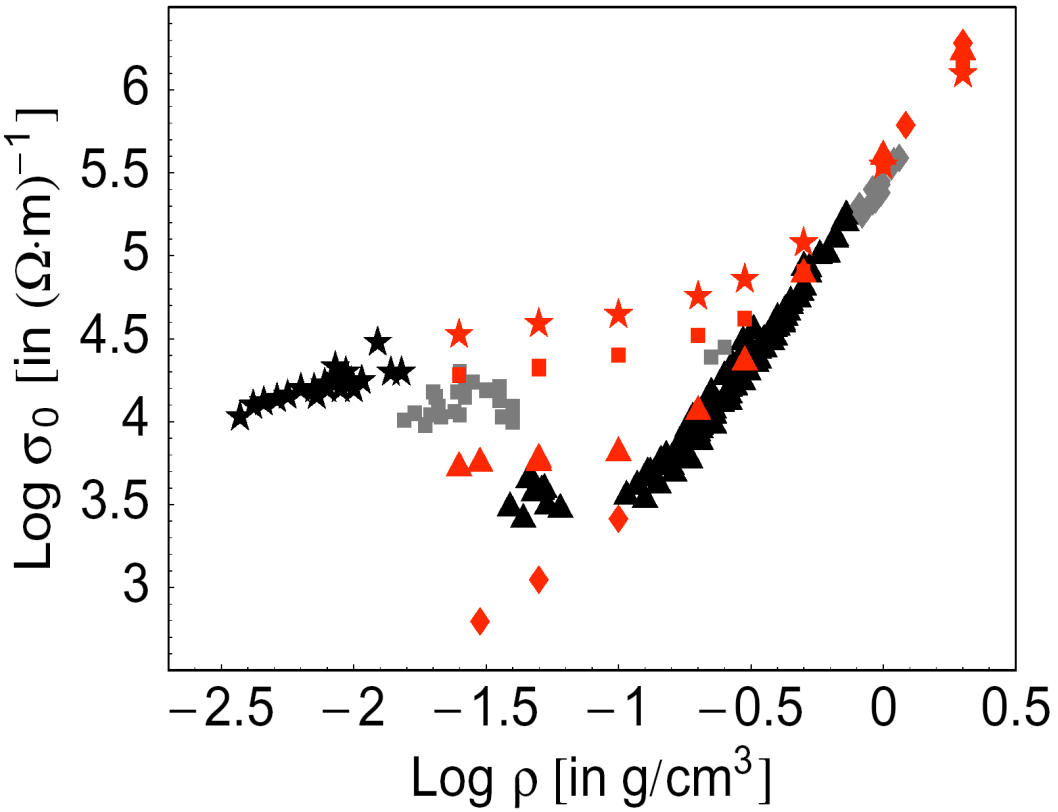
The QMD-KG results are in good agreement with DeSilva's data over a two decade range of density



DeSilva and Katsouros data in black or grey, MD-KG results in red

★ 30000 K, ■ 20000 K, ▲ 10000 K, ◆ 6000 K

[Desjarlais, Kress, and Collins, PRE **66,** 025401(R) (2002)]

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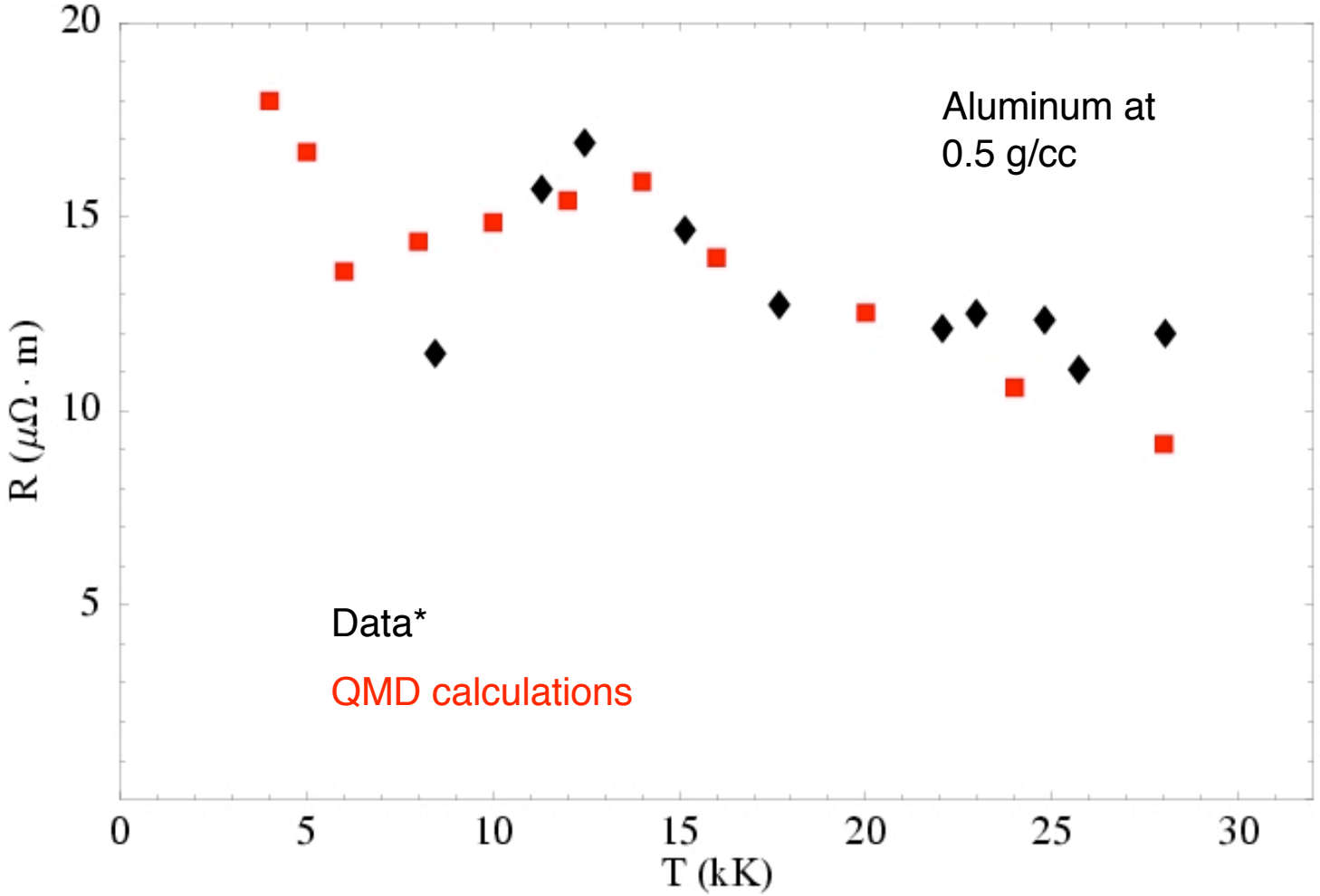
We find good agreement with isochore resistivity data from tamped exploding foil experiments*



*Data from Korobenko, Rakhel, Savvatimski, and Fortov, PRB **71** 014208 (2005)

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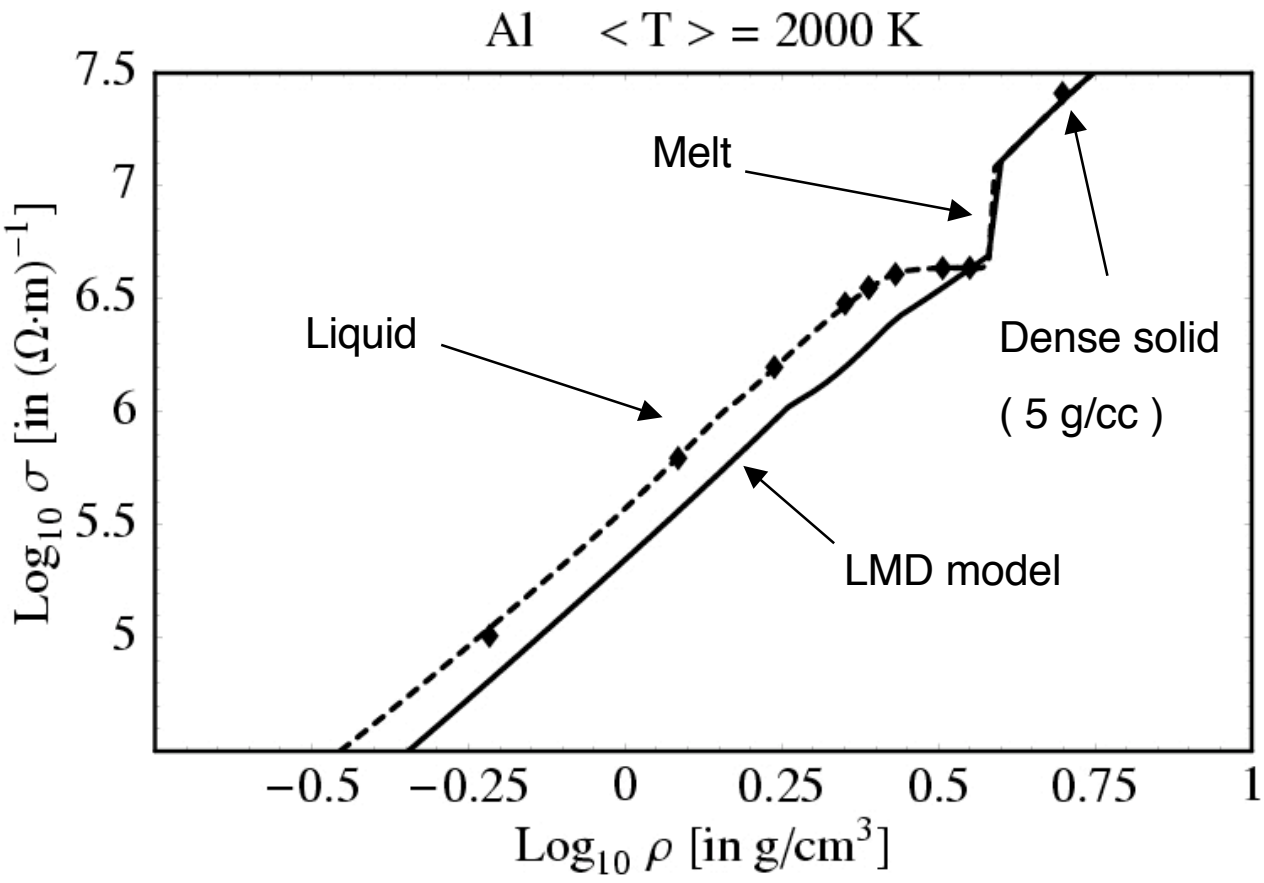
The calculated liquid aluminum conductivities are higher than the *improved* Lee-More (LMD) model predictions



The dashed line shows the 2000 K isotherm from our QMD-tuned wide-range aluminum model

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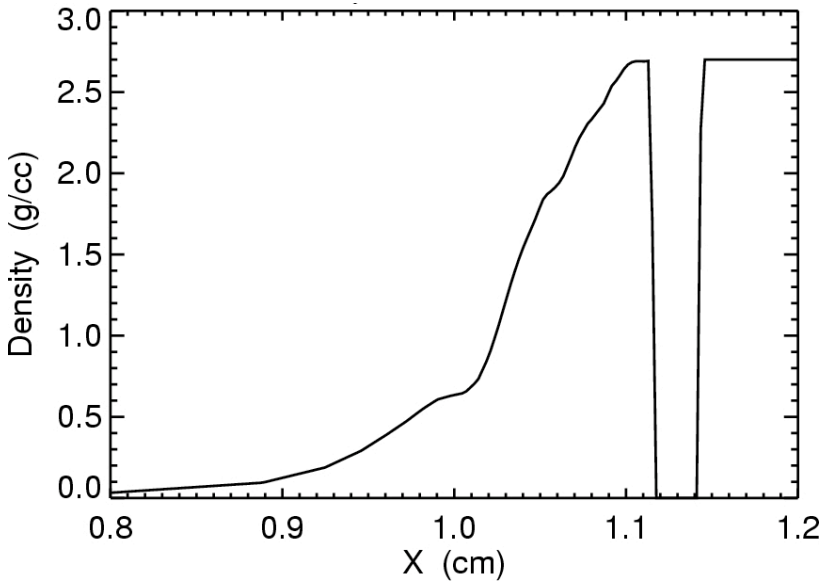
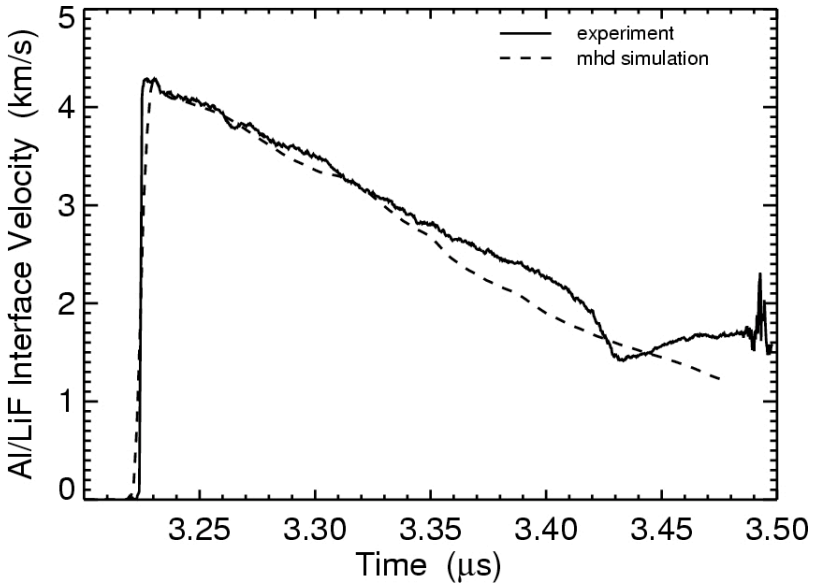
Flyer plate simulations with the QMD based conductivities give very good agreement with experiment

Simulations by Ray Lemke with Sandia's 3D Rad-MHD ALEGRA code





Conductivities based on the QMD calculations have given us a new predictive capability.

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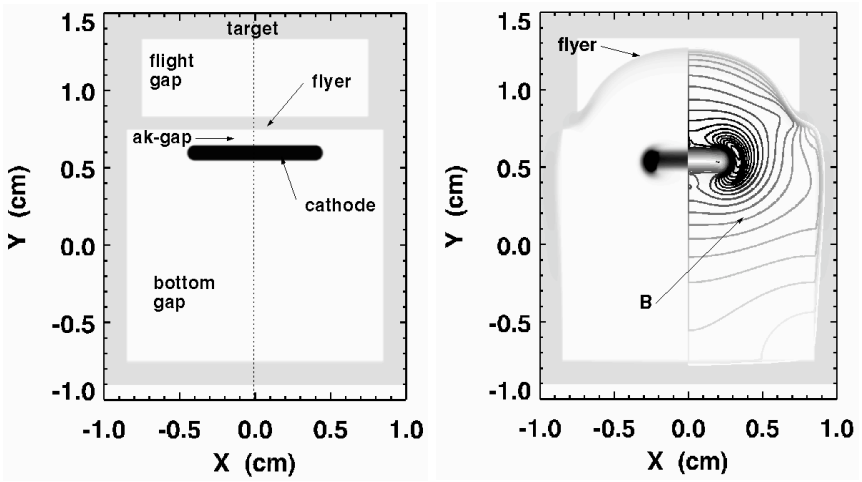
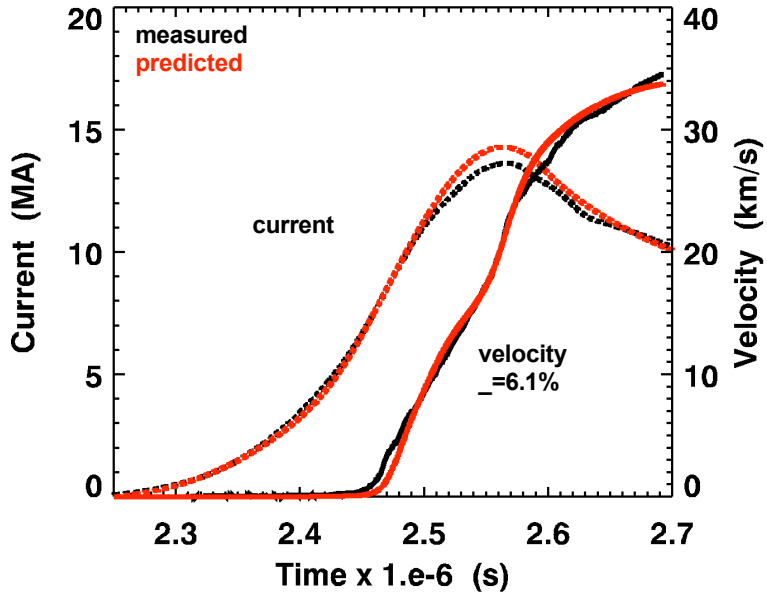
We have used our simulation capability with the new aluminum model to optimize flyer performance on Z



Measured / predicted current & flyer velocity (850 _m Al)



The simulations were performed by Ray Lemke using Sandia's ALEGRA code in 2-D

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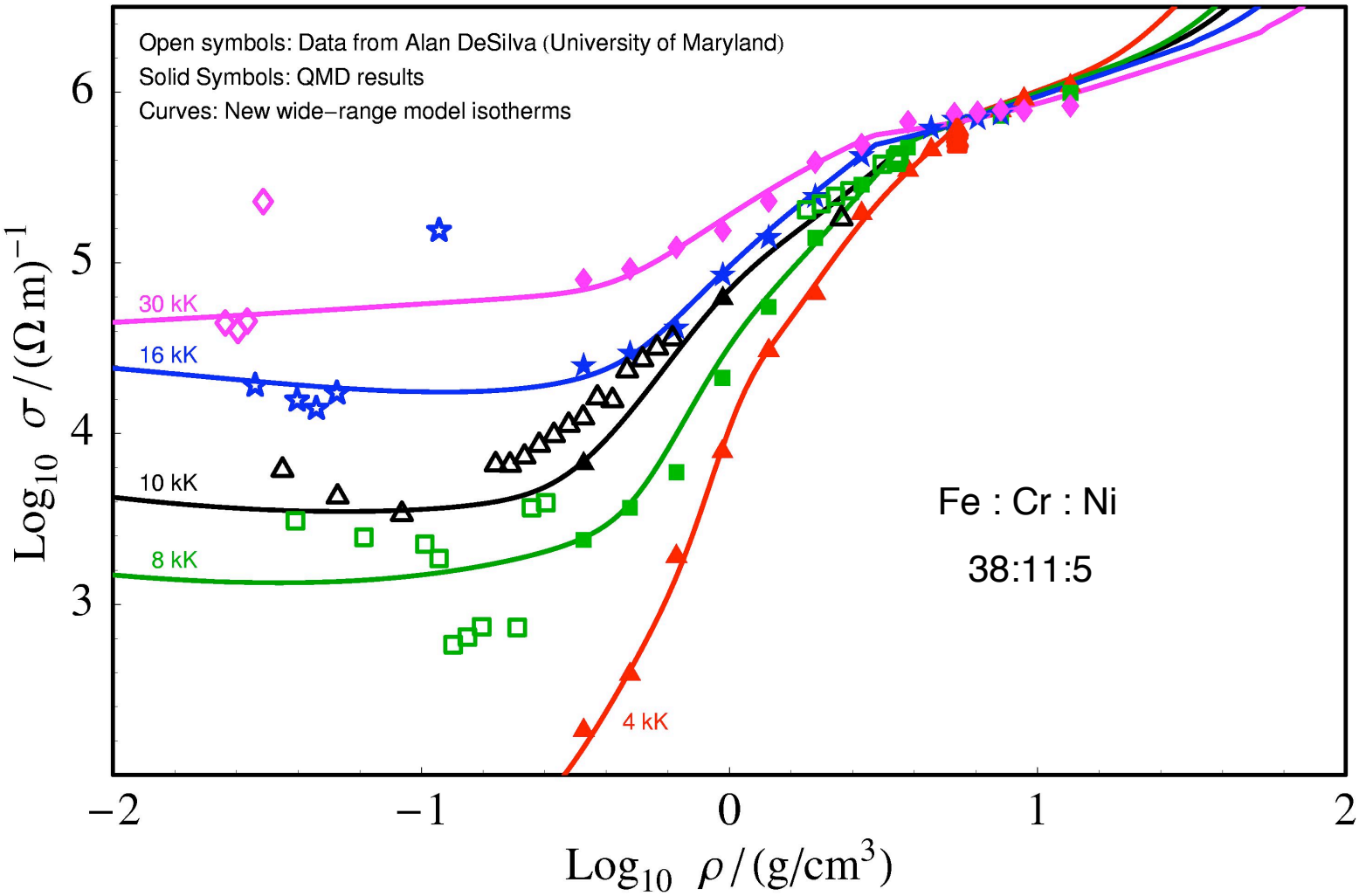
We have applied the QMD/KG approach to develop a high fidelity conductivity model for stainless steel



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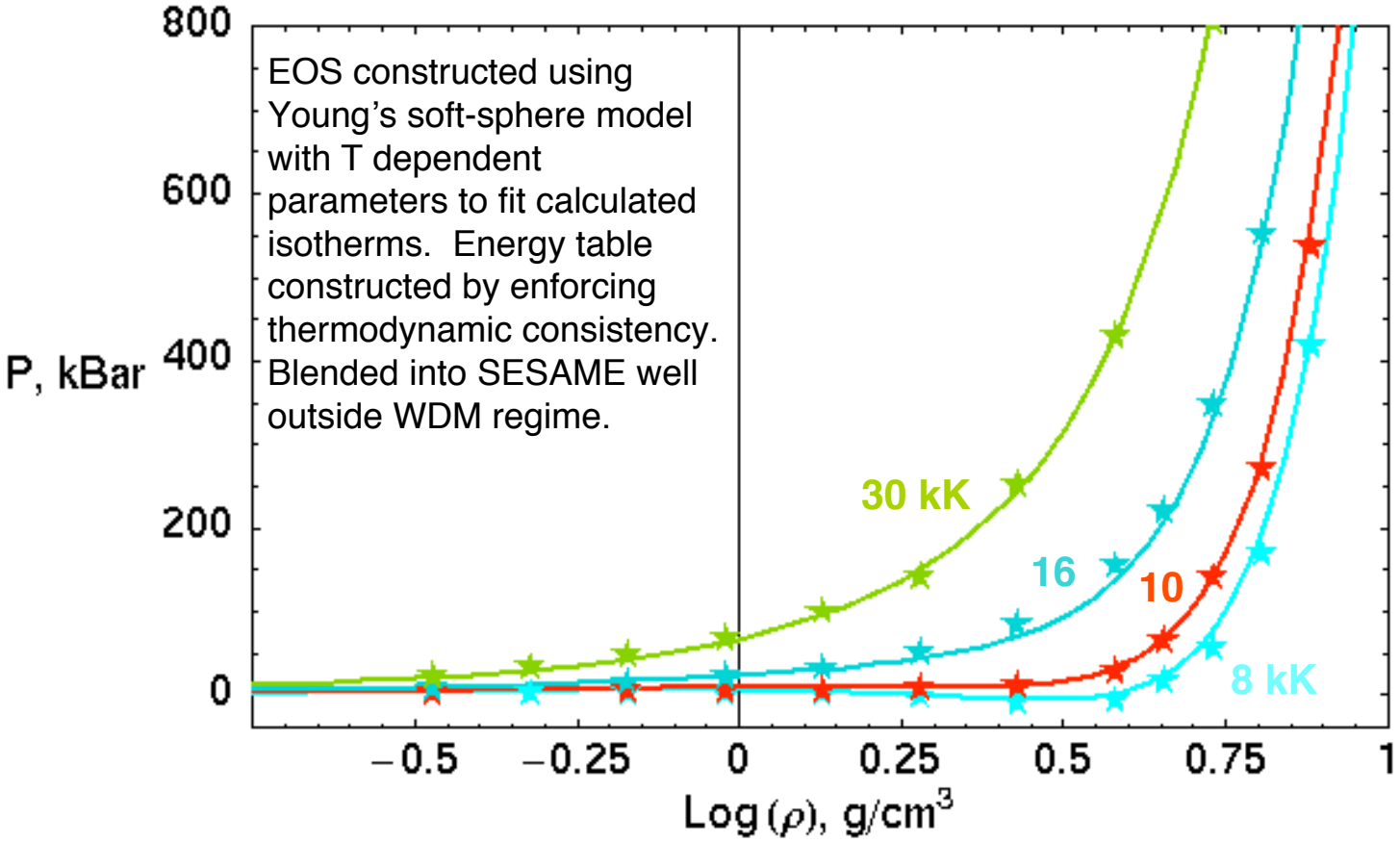
We have used QMD to generate an Equation of State for Stainless Steel, consistent with the conductivity model



We find the stainless steel liquid-vapor critical point to be at 10,000 K and 2.0 g/cc

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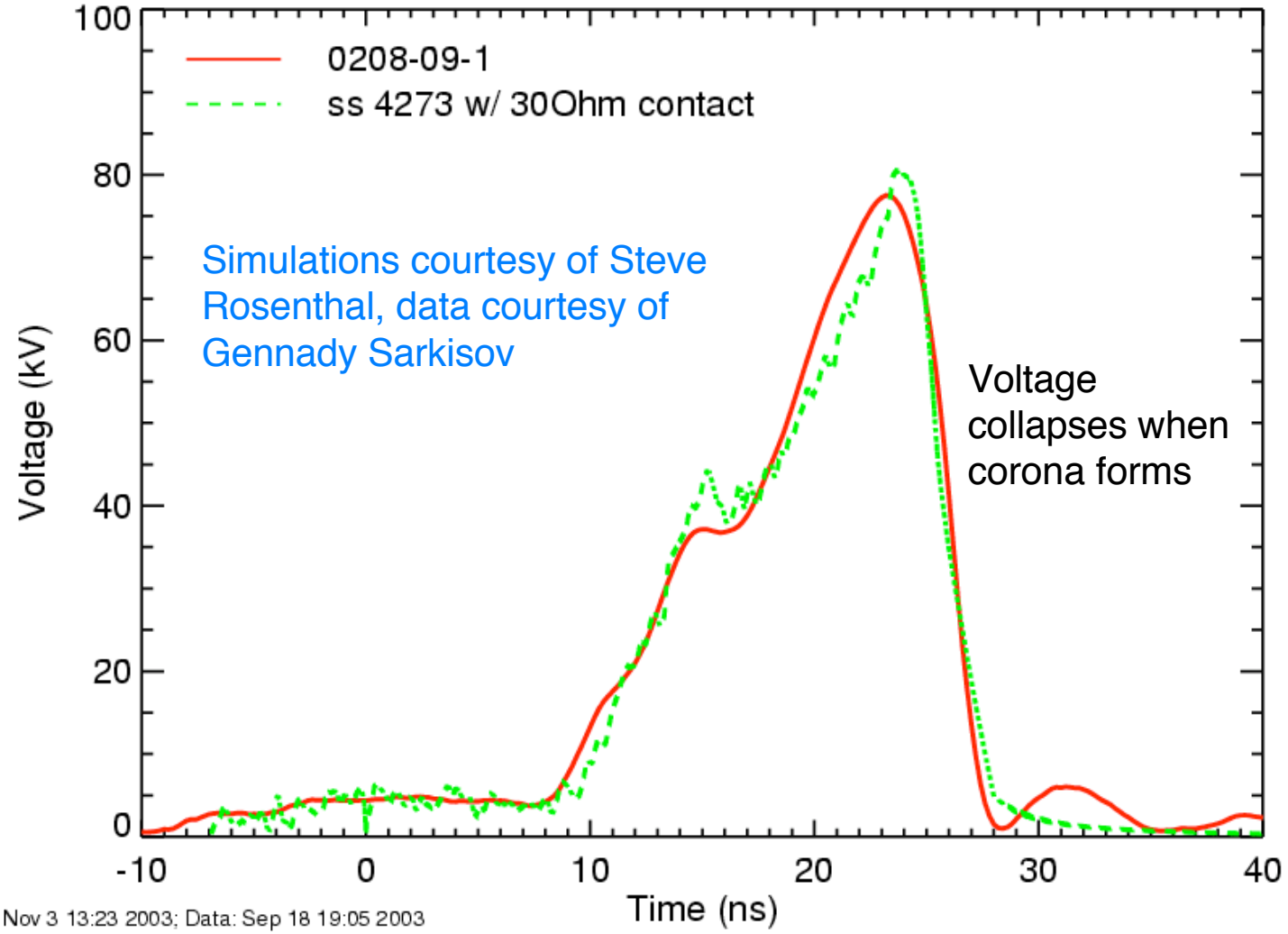
Simulations of exploding stainless steel wires with the new models are in very good agreement with experiment



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Conductivity in water -- electronic conduction and proton conduction increase the complexity

Electronic contribution

- Kubo-Greenwood theory
- 20-30 snapshots from a long QMD simulation
- Uniform and reproducible

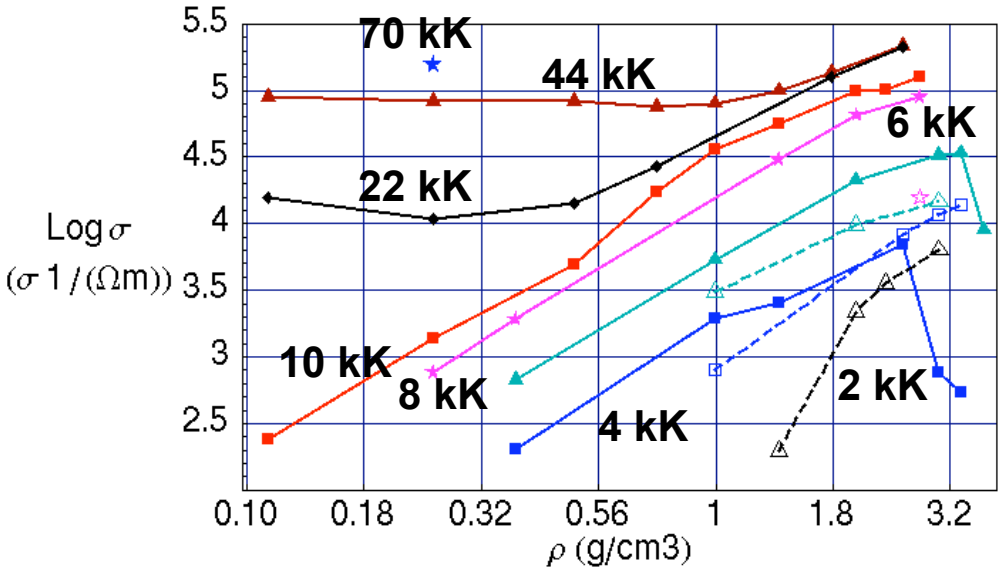
Proton contribution

- Classical Kubo expression

$$\sigma = \frac{ne^2}{m}\int_0^\infty \frac{\langle v(\tau)v(0)\rangle}{\langle v(0)v(0)\rangle}d\tau$$

- 10-20 ps QMD simulations.
- Long enough simulations to obtain converged correlation functions

Electrical conductivity of HEDP water



- Full lines: electronic conductivity
  - Suppressed in the superionic phase
  - Dominates above 6000 K
- Dashed lines: proton conduction
  - Dominates below 4000 K
- Quantitative conductivity over a large region of phase-space

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Calculations and analysis by Thomas Mattsson

We are using QMD/DFT calculations to produce accurate compression and release isentropes

$$dS = \frac{\partial S}{\partial T} dT + \frac{\partial S}{\partial V} dV$$

$$\frac{\partial S}{\partial T} = \frac{1}{T} \frac{\partial E}{\partial T}$$

$$\frac{\partial S}{\partial V} = \frac{\partial P}{\partial T}$$

$$\frac{1}{T} dT = -\frac{\partial P / \partial T}{\partial E / \partial T} dV = -\left.\frac{\partial P}{\partial E}\right|_V dV$$

Piecewise integration gives

$$\frac{T_{i+1}}{T_i} = \exp\left[-\int_{V_i}^{V_{i+1}} \left.\frac{\partial P}{\partial E}\right|_V dV \right]$$

We can make direct comparisons between the QMD isentropes and data from Isentropic Compression Experiments (ICE) on Sandia's Z machine

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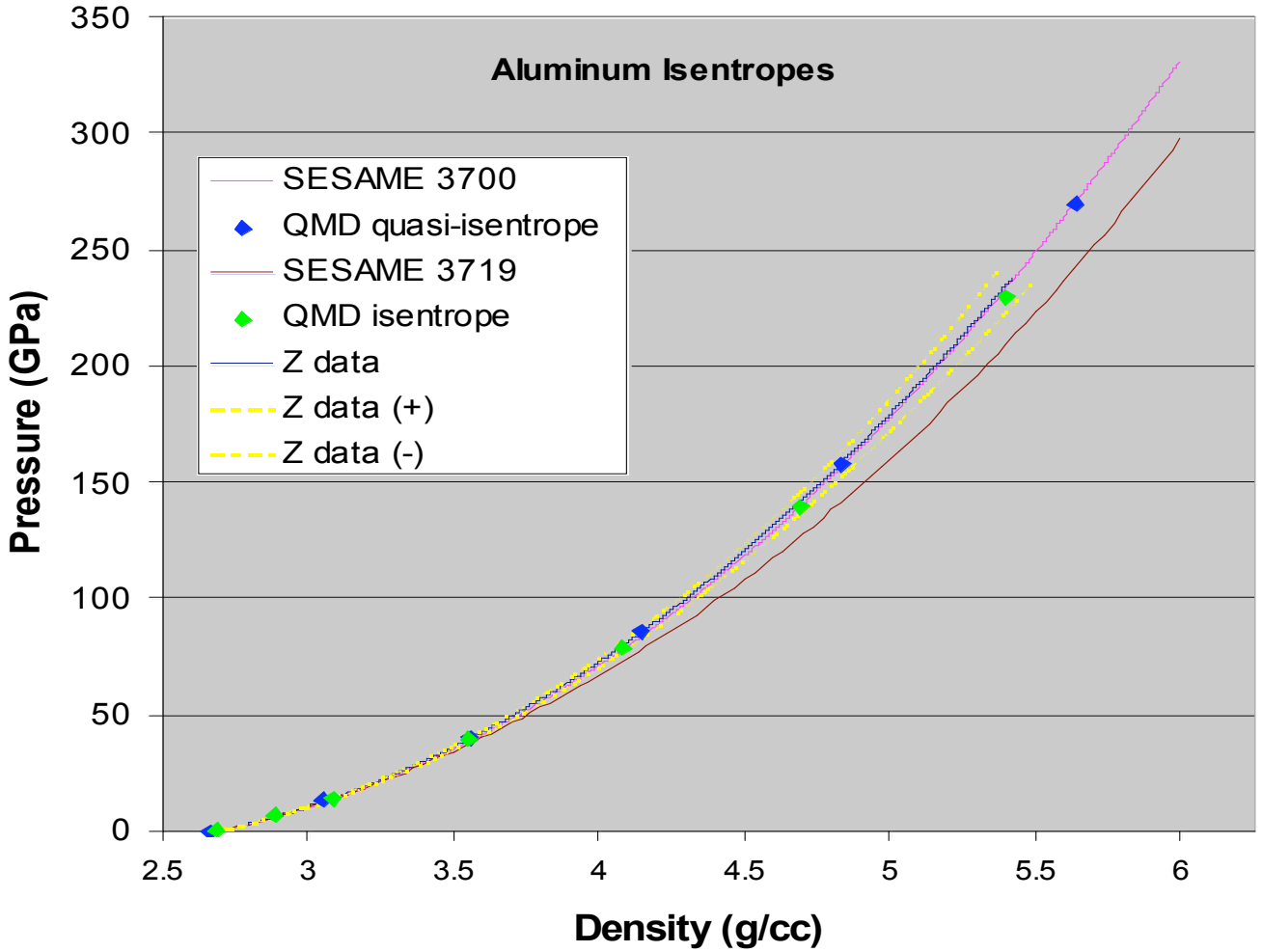
Our calculated principal isentrope for aluminum is in excellent agreement with data from Sandia's Isentropic Compression Experiments (ICE) on Z



Data from **ICE** experiments on Z courtesy of Jean-Paul Davis

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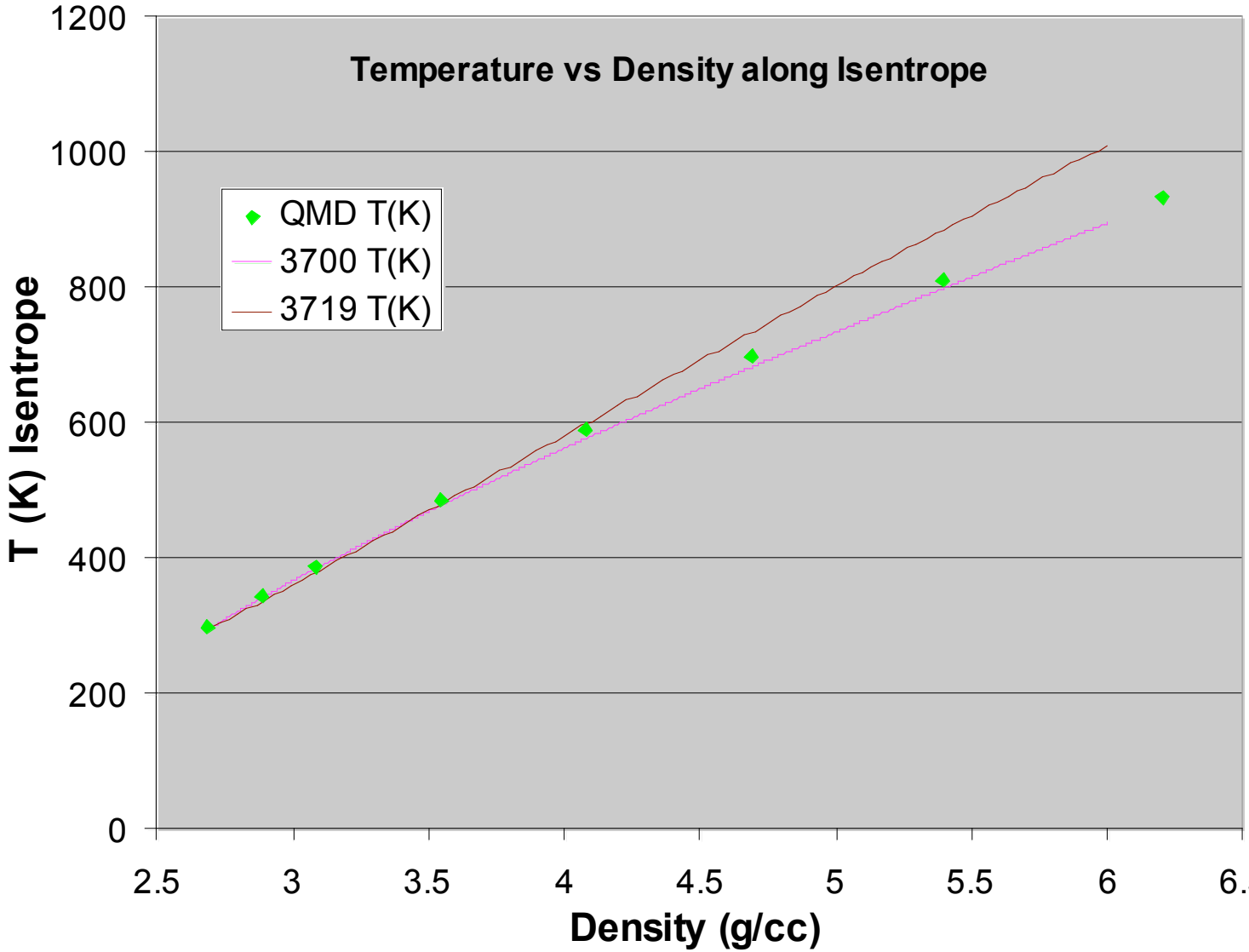
The temperature versus density along the isentrope is also in excellent agreement with SESAME 3700 (Kerley)



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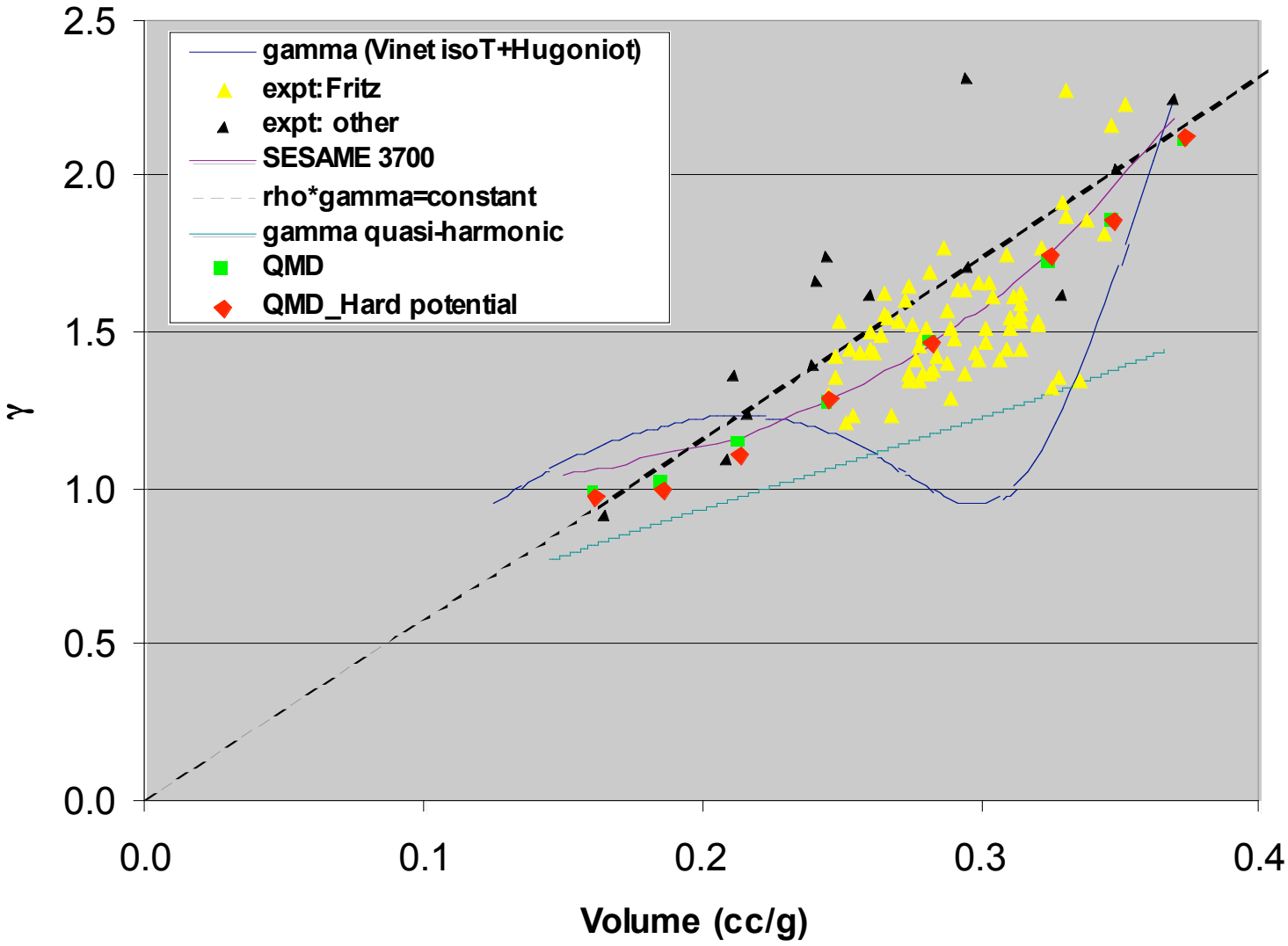
Our calculated Gruneisen γ for solid aluminum is in very good agreement with data



$$\gamma \equiv V \frac{\partial P}{\partial E}$$

Data and model compilation courtesy of Dennis Hayes

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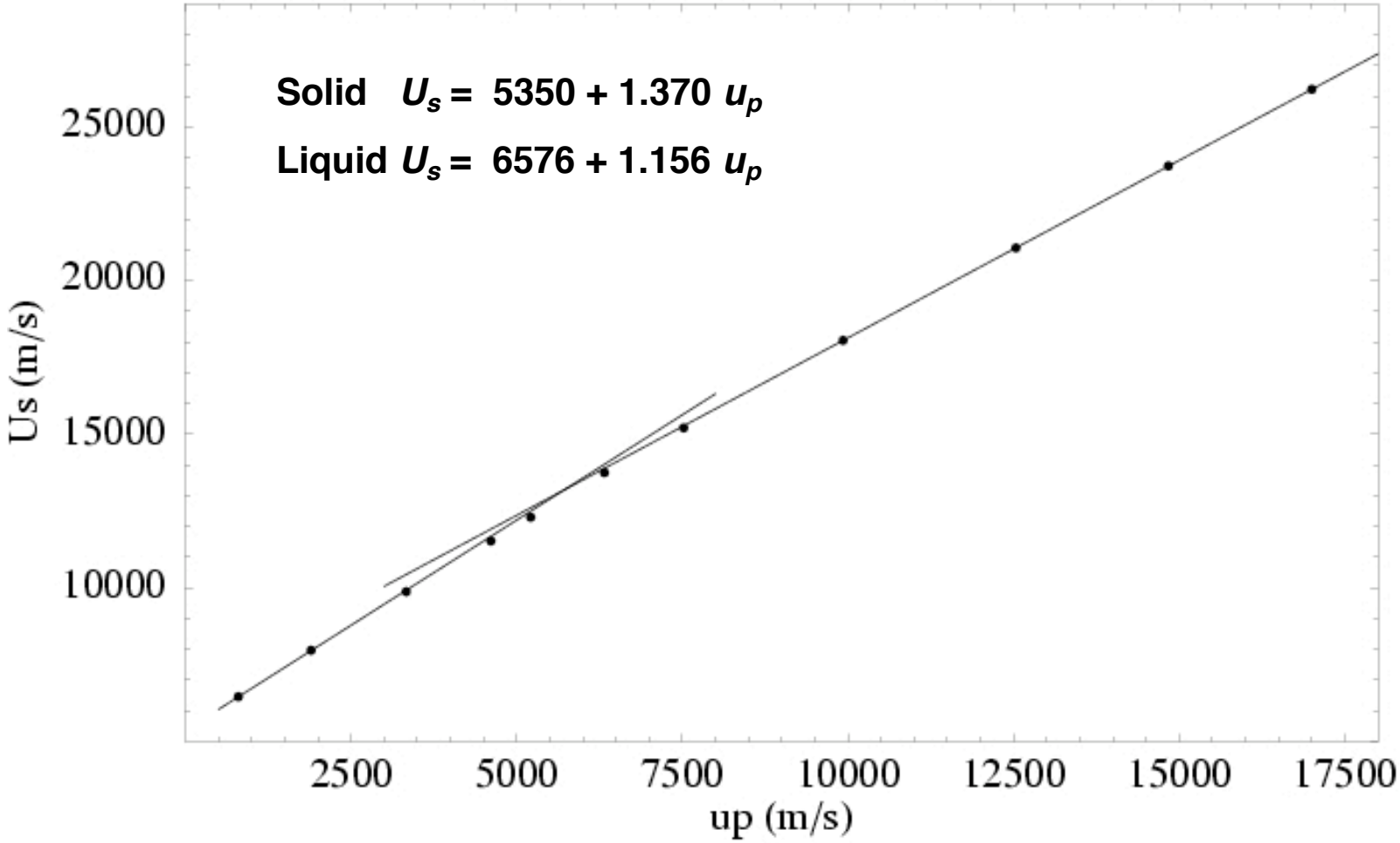
We have calculated the aluminum Hugoniot from solid density up to 12 Mbar



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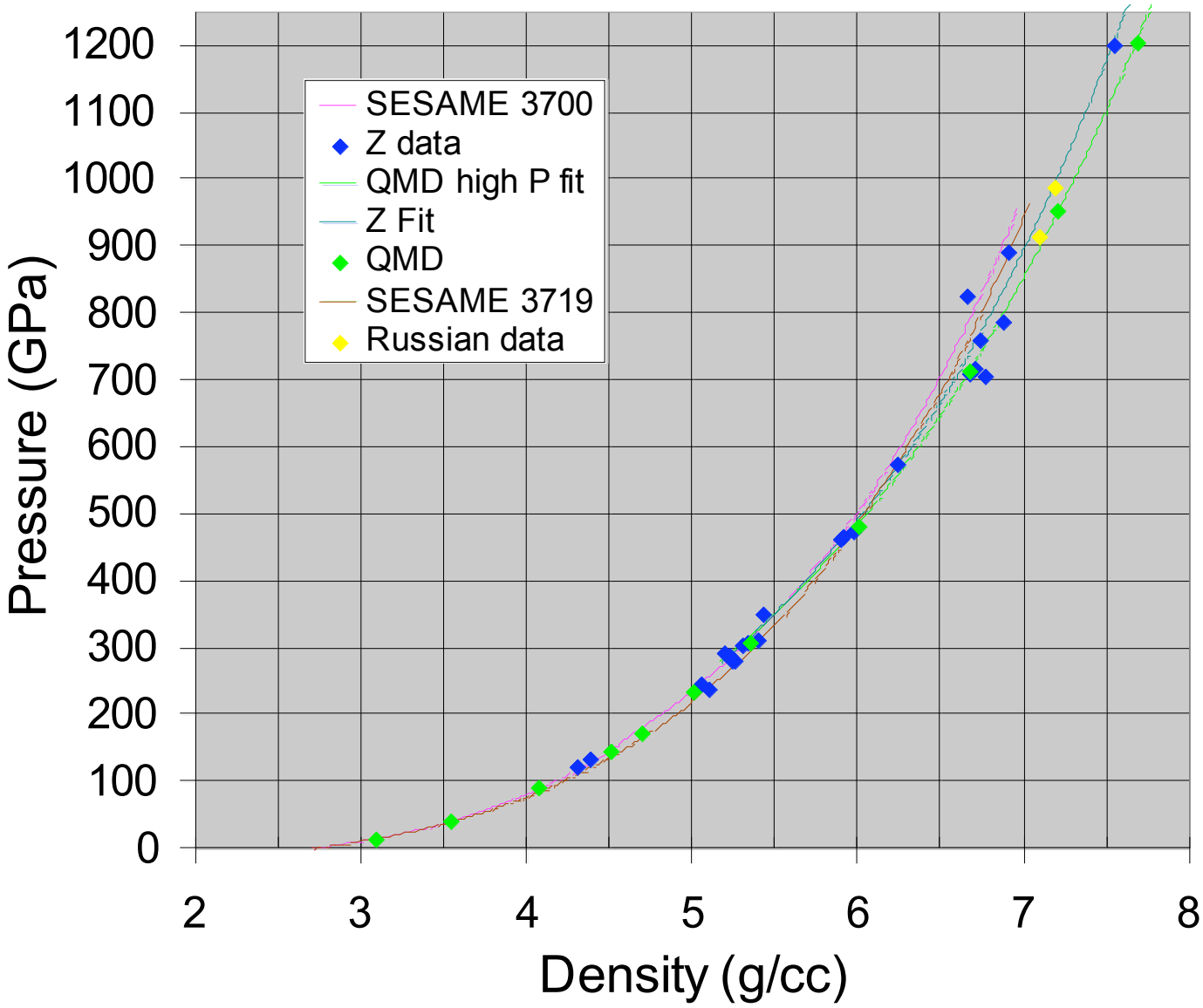
Our aluminum Hugoniot is in very good agreement with data



3700 appears to give a good isentrope, but the Hugoniot is too stiff

Al Hugoniot data courtesy of Marcus Knudson

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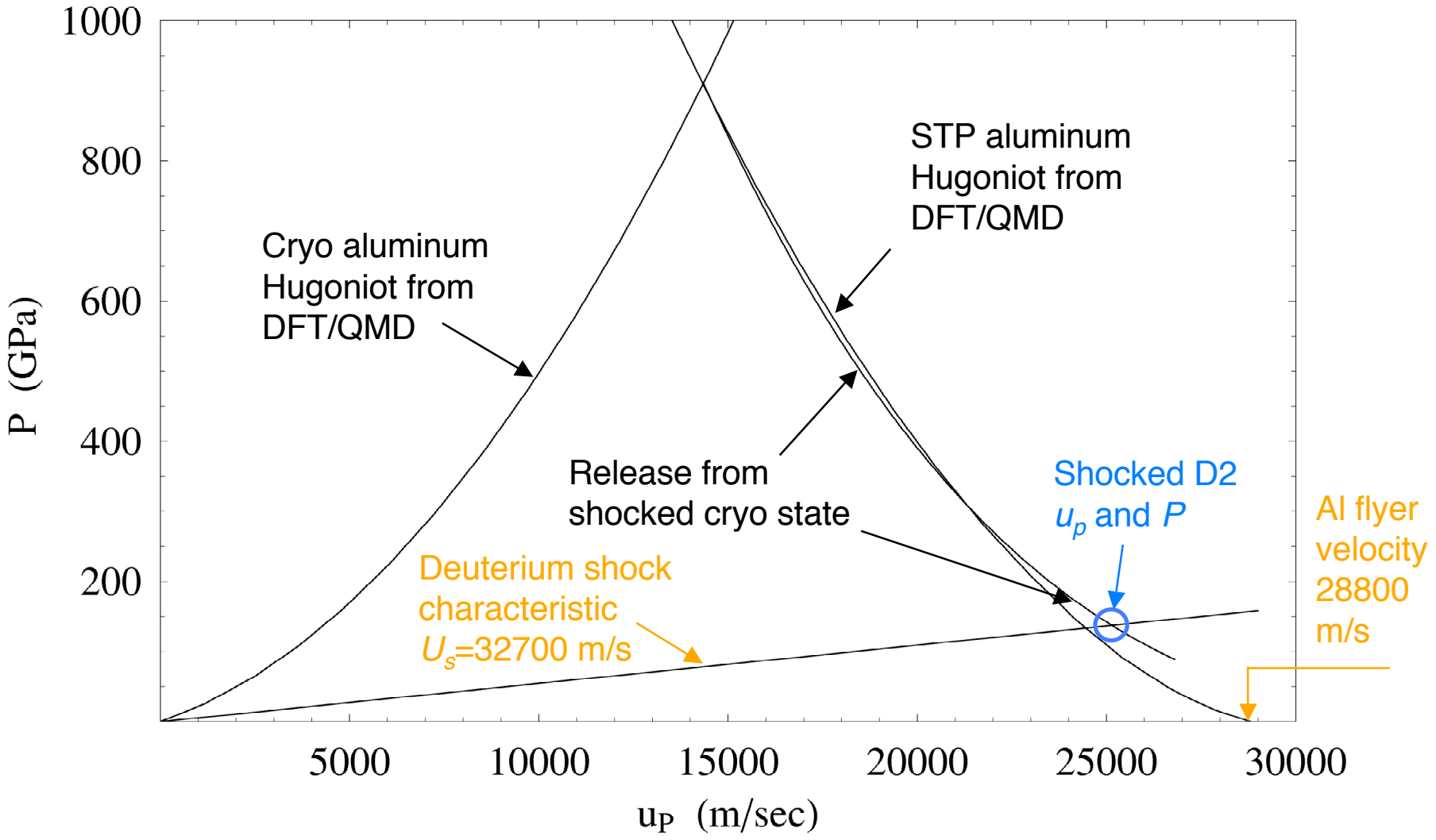
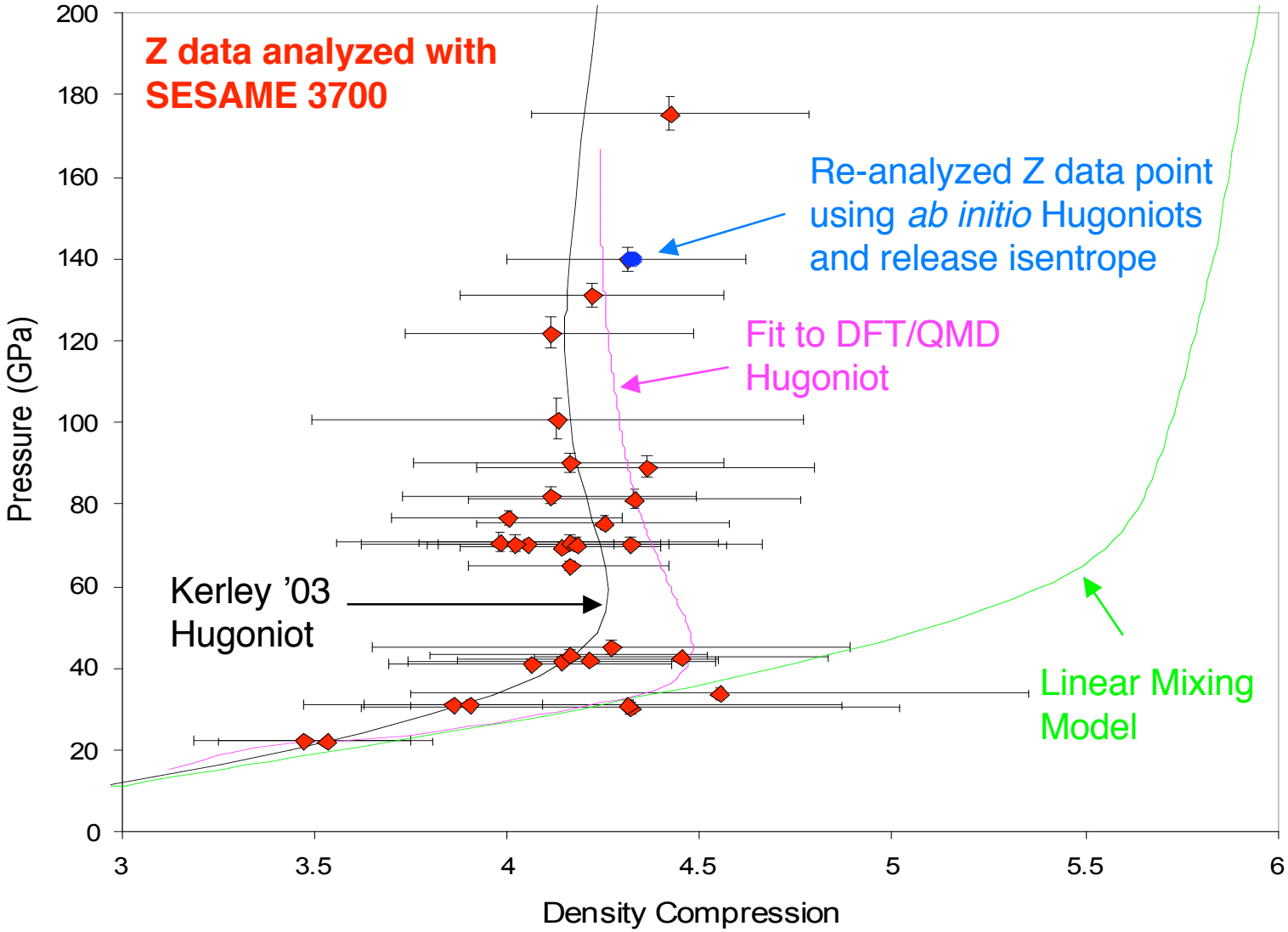
We have all the pieces to do *ab initio* impedance matching calculations



Our re-calculated impedance match point is very close to that obtained with SESAME 3700



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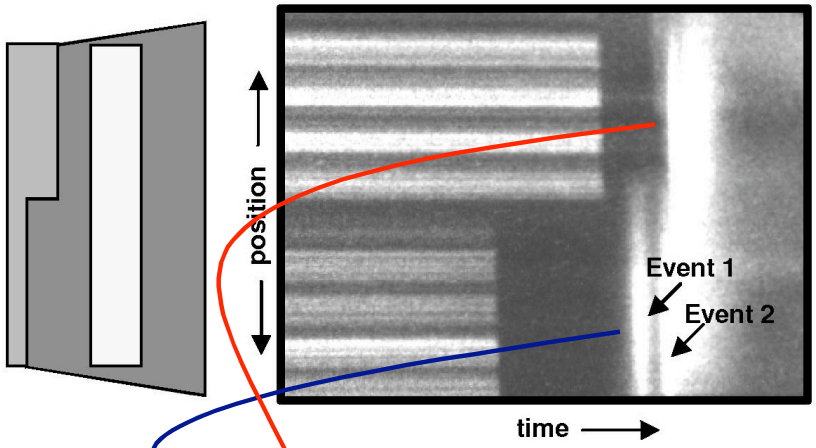
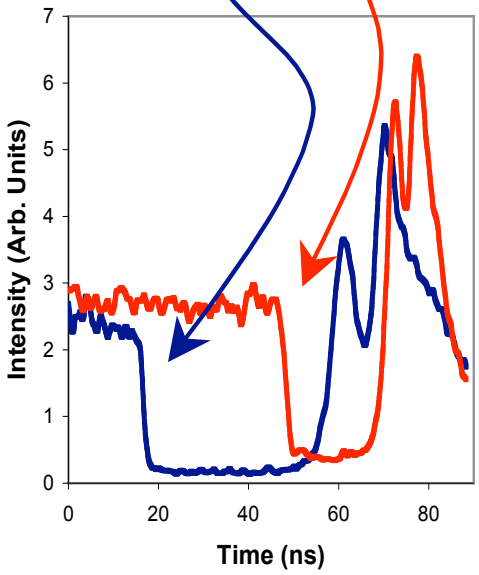
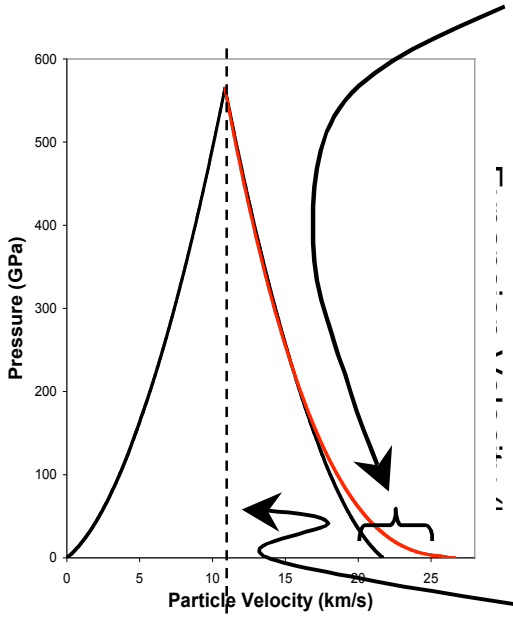
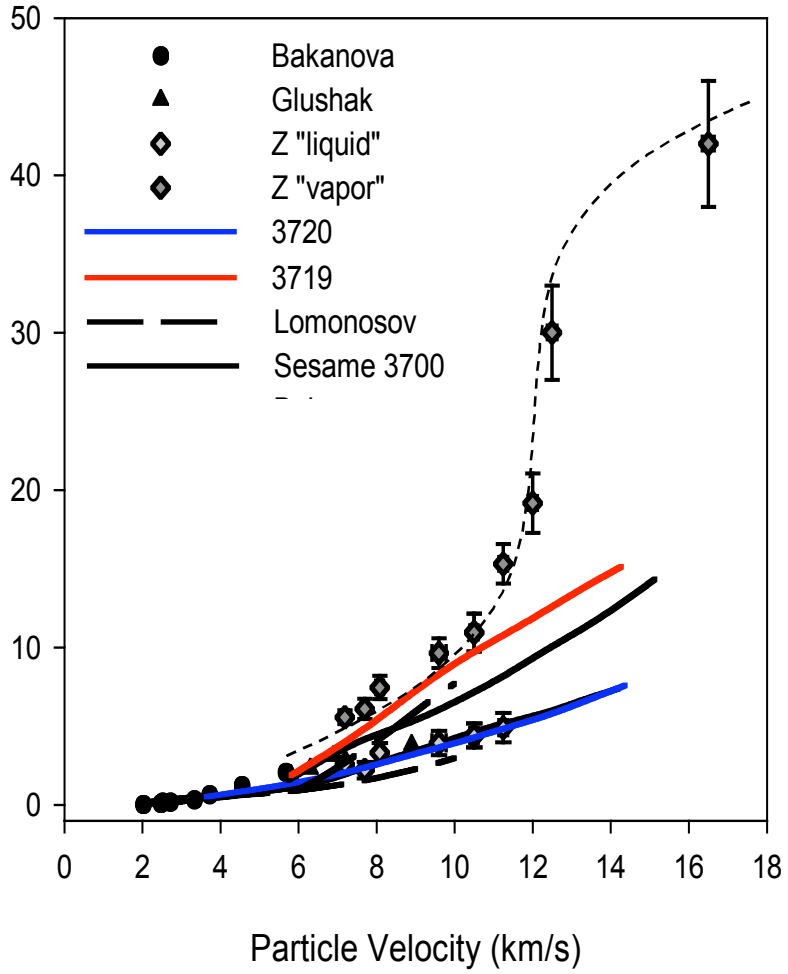
Full release measurements are being performed on Z









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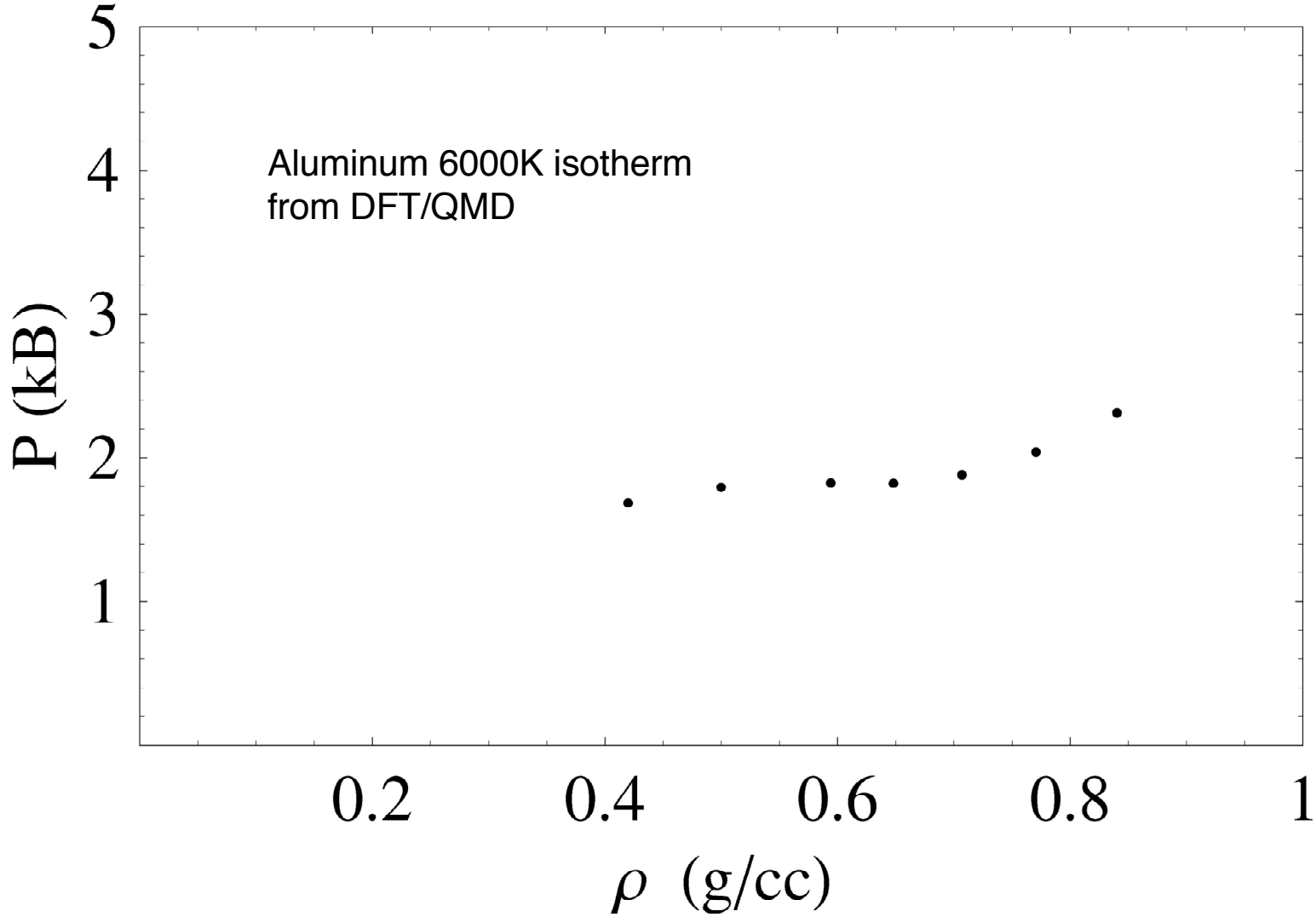
Our calculated liquid-vapor critical point for aluminum appears to be very close to 6000 K, and at 0.6 g/cc



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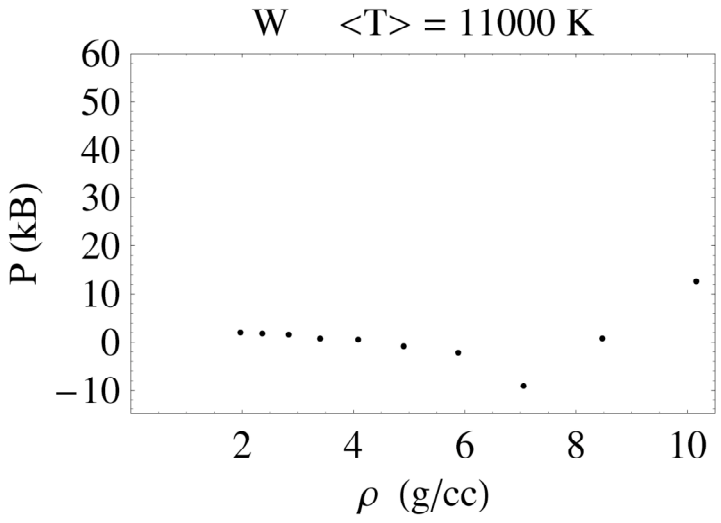
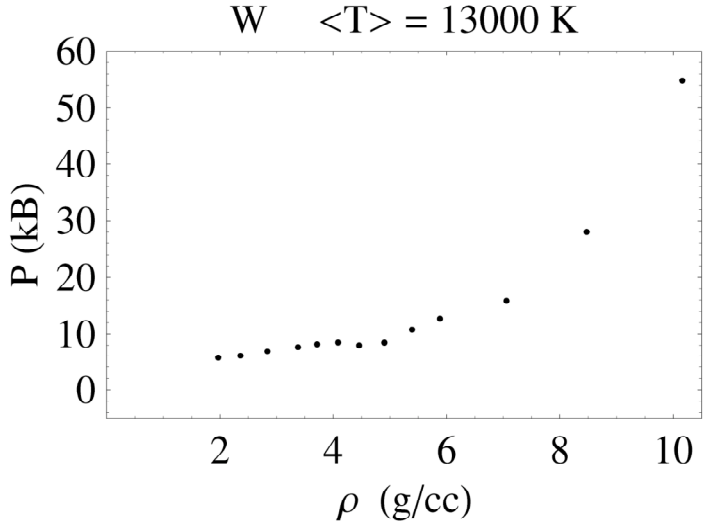
Isotherms for W have been calculated for EOS development in collaboration with Richard More

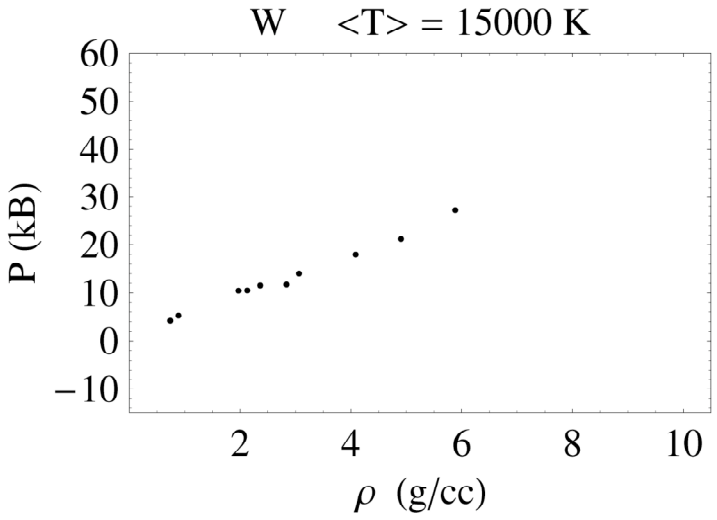


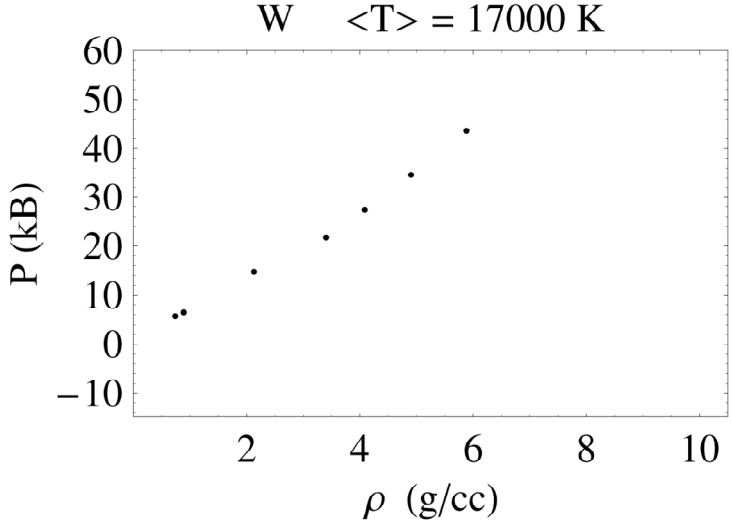


Liquid-vapor critical point

~13000 K

~ 4.5 g/cc





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Recent and active research areas

- QMD based conductivity models for Al, W, Be, and SS
- Reflectivity of shocked xenon
- Principal Hugoniot and reshock properties of deuterium
- Principal and release isentropes of Al
- Principal Hugoniot of Al and W
- Liquid-vapor critical points (Al, W, SS)
- Electrical and thermodynamic properties of water at high energy densities
- Equations of state for SS, Al, and W
- Research on advanced electronic structure methods for HEDP (finite temperature Exact Exchange, finite temperature GW)

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