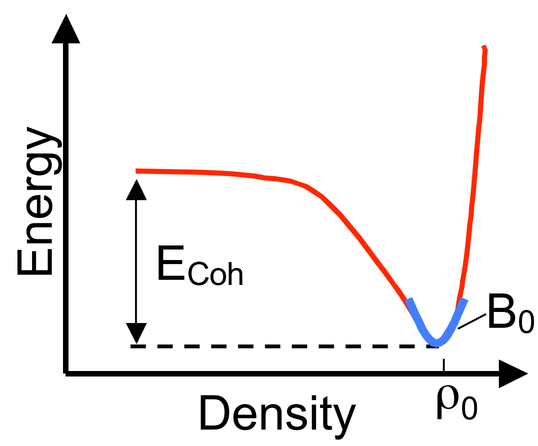
We write the global EOS in terms of three components

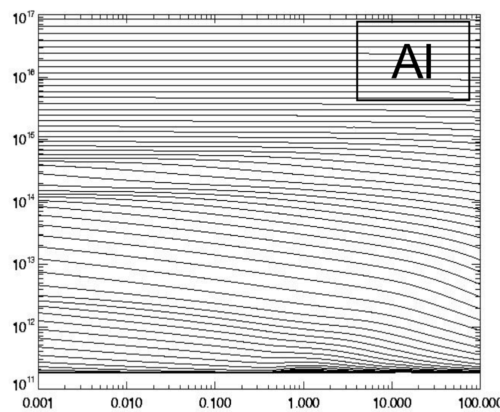
$$F[\rho,T] \quad = \quad E_{Cold}[\rho] \quad + \quad F_{Elec}[\rho,T] \quad + \quad F_{Ion}[\rho,T]$$

Cold Curve



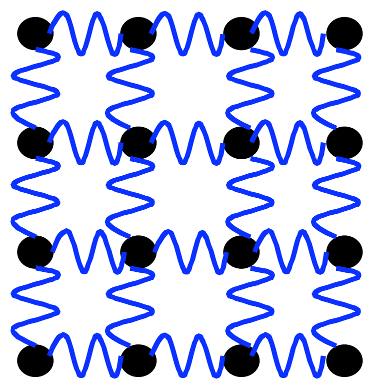
Cold curve may include additional parameters to modify $\rho < \rho_0$ and $\rho > \rho_0$ behavior

Electron-Thermal



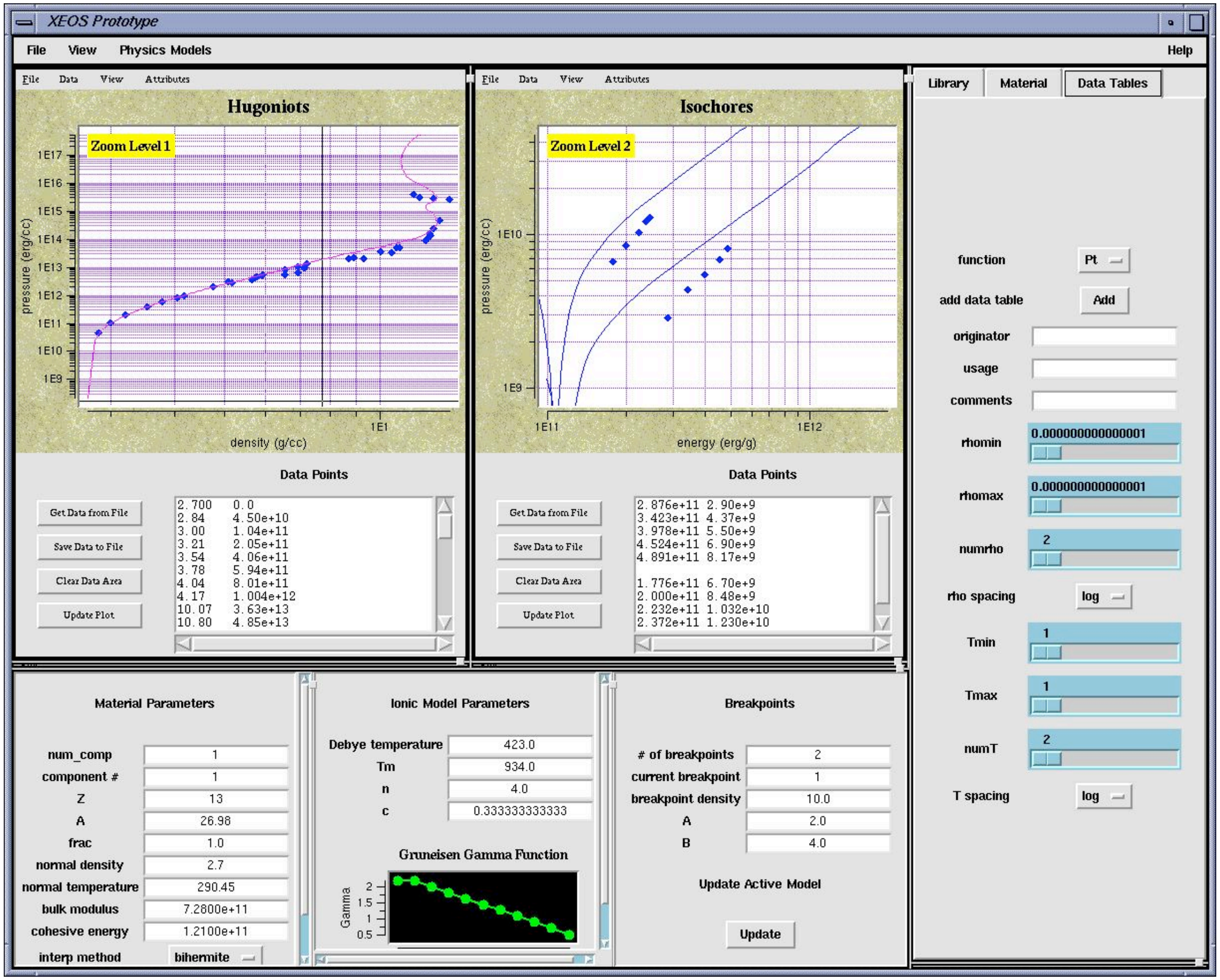
Ionization features seen in Purgatorio-based electron-thermal energy and entropy.

Ion-Thermal



Ion thermal contribution from Debye model and density-dependent Grueneisen $\gamma[\rho]$

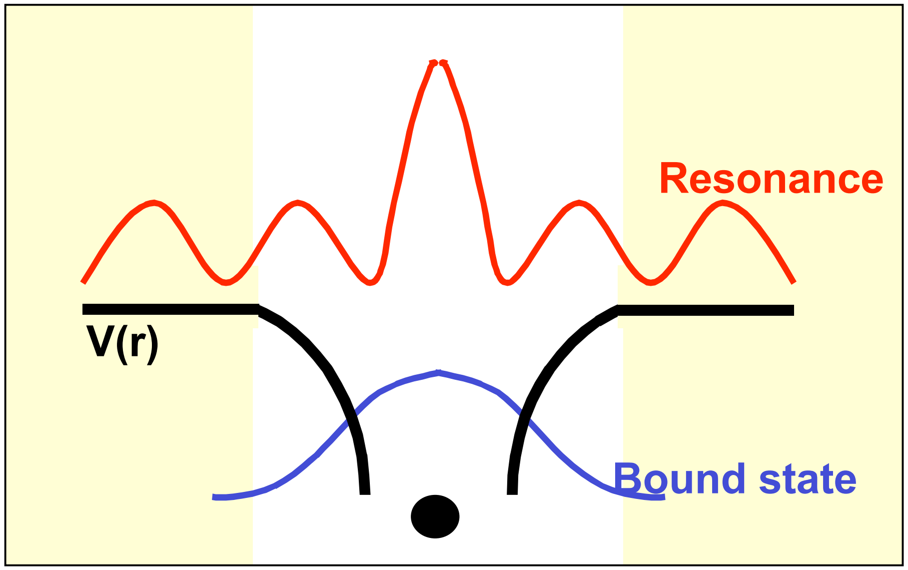
XEOS facilitates the interactive construction of new EOS tables



XEOS Features

- Multiple thermodynamic tracks
- Automatic plot update with parameter changes
- Experimental data overlay
- Extensible – new models and thermodynamic tracks can be added
- Uses Purgatorio electron EOS data

Purgatorio model: single atom in a homogeneous electron gas

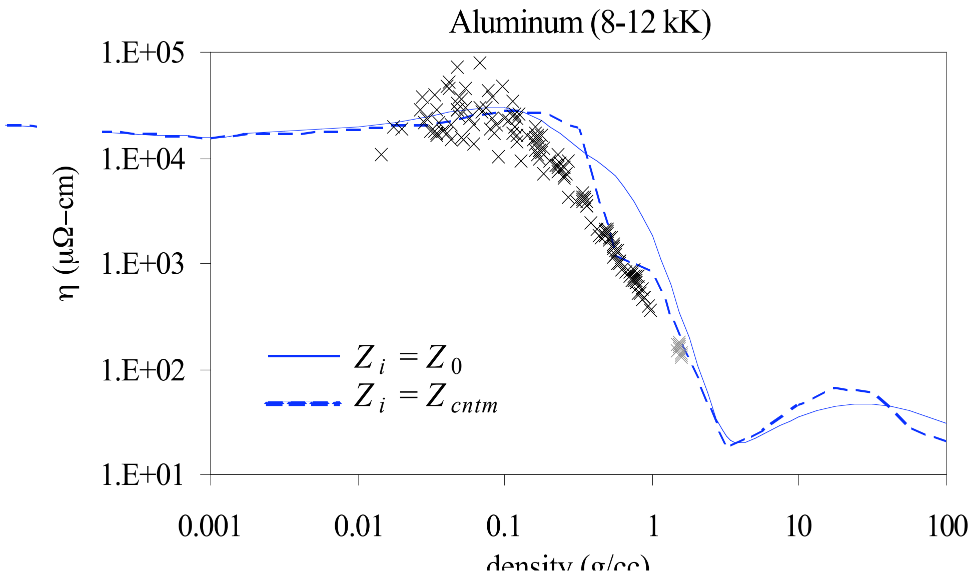


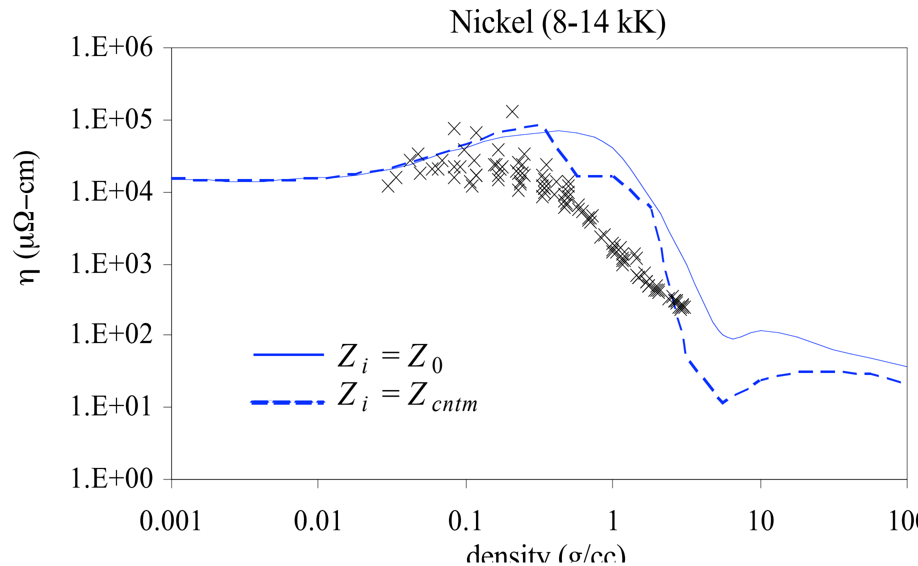
Our Purgatorio model is a modern reimplementation of David Liberman's Inferno Code :

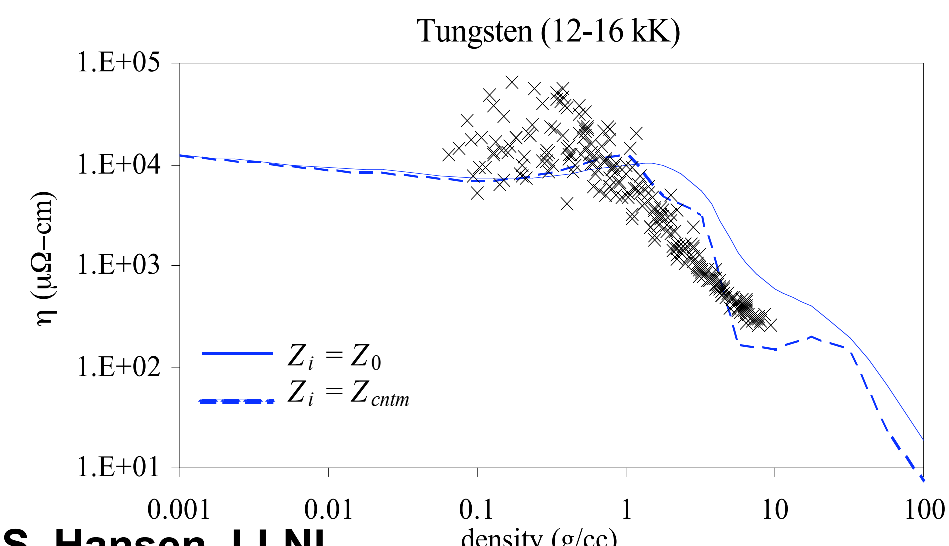
- Fully relativistic *ab initio* muffin-tin model of a single atom in jellium
- Charge neutrality enforced within atomic sphere
- Production code that works across the periodic table for a wide range of temperatures and densities
- Phase-amplitude method gives more accurate solutions for high energy, angular momentum states
- Automatic integration refinement resolves sharp resonances in density of states

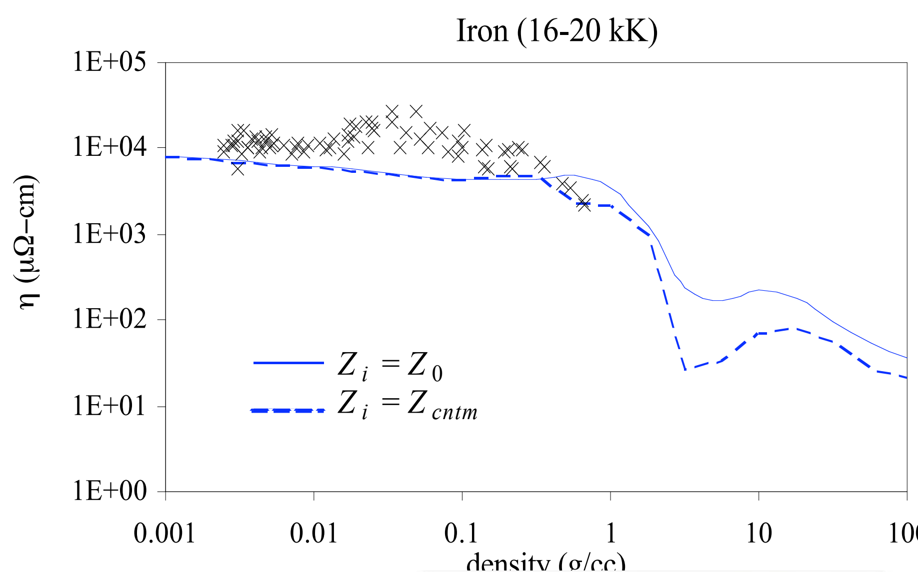
Purgatorio is an important enabling tool for future research since we can build on it to incorporate more physics. We have already extended it to calculated electron conductivities.

Comparisons with η measurements from capillary experiments (courtesy Alan DeSilva, U. Maryland)





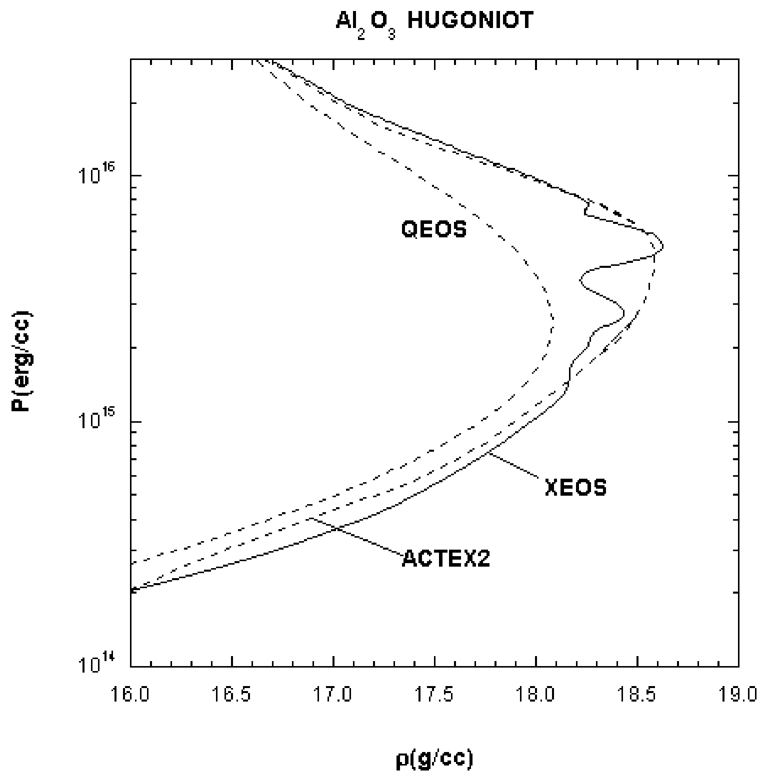


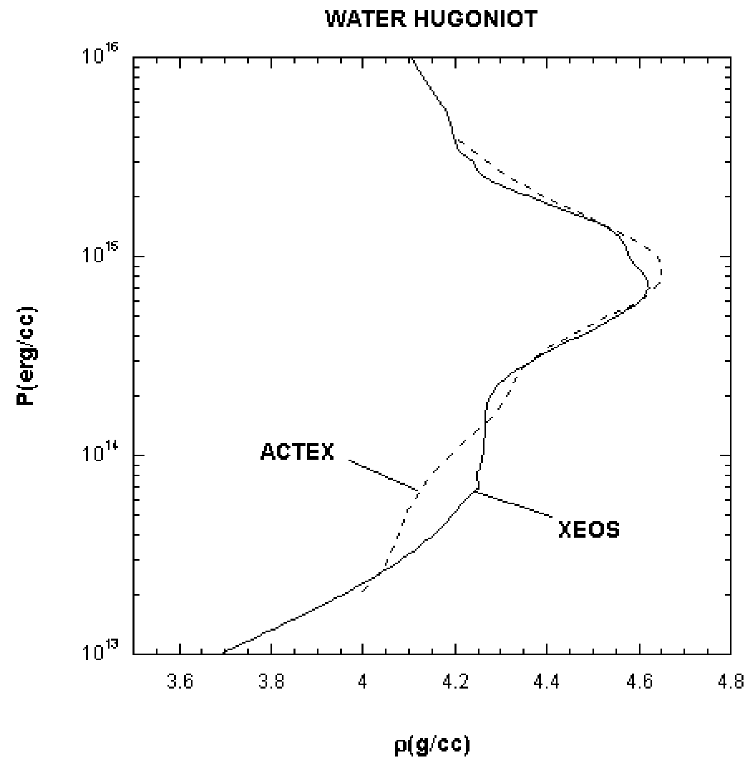


S. Hansen, LLNL

Mixtures

Constant-pressure mixing

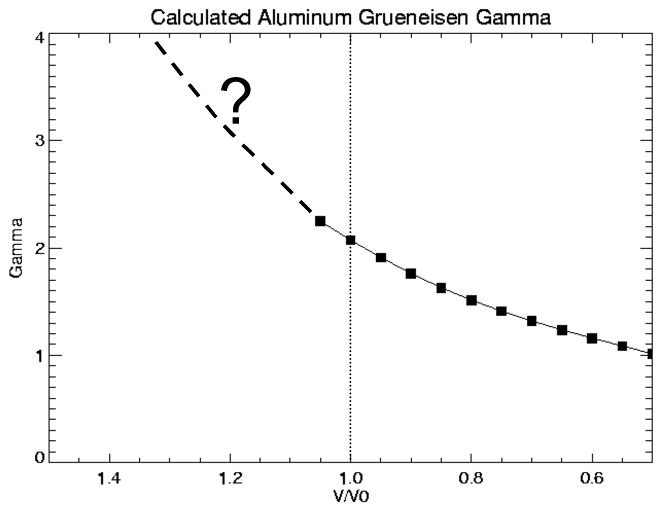




Purgatorio gives a better description of maximum compression than TF.

Purgatorio shows ionization shell features that may be suppressed in real mixtures

Porous material data shows a sensitivity to the Grueneisen Gamma parameter variation at low densities



First principles electronic structure calculations show that γ increases as density decreases.

Our current EOS models set $\gamma=\gamma(\rho_0)$ for $\rho<\rho_0$.

Is this increase in γ important for understanding porous shock data?