Summary report
Working Group 3: Computer Codes

A snapshot of the state of the art

Alex Friedman, working group chair

Workshop on Accelerator-Driven Warm Dense Matter Physics

February 22-24, 2006

Four Points Sheraton Hotel, Pleasanton, CA

Participants

- Mike Desjarlais
- Alex Friedman
- Dave Grote
- Enrique Henestroza
- Marty Marinak
- Gregg Penn
- Dave Rose
- William Sharp
- Ed Startsev
- Philip Sterne
- Peter Stoltz
- Naeem Tahir
- Jean-Luc Vay
- Jonathan Wurtele

Outline

- Perspective (by the group)
- Cartoon of accelerator-driven WDM experiment and simulation
- “Taxonomy” of codes; list of codes by “genus”
- “Axes” and other thoughts
- Notes on some of the codes
- Philip Sterne’s presentation to the working group

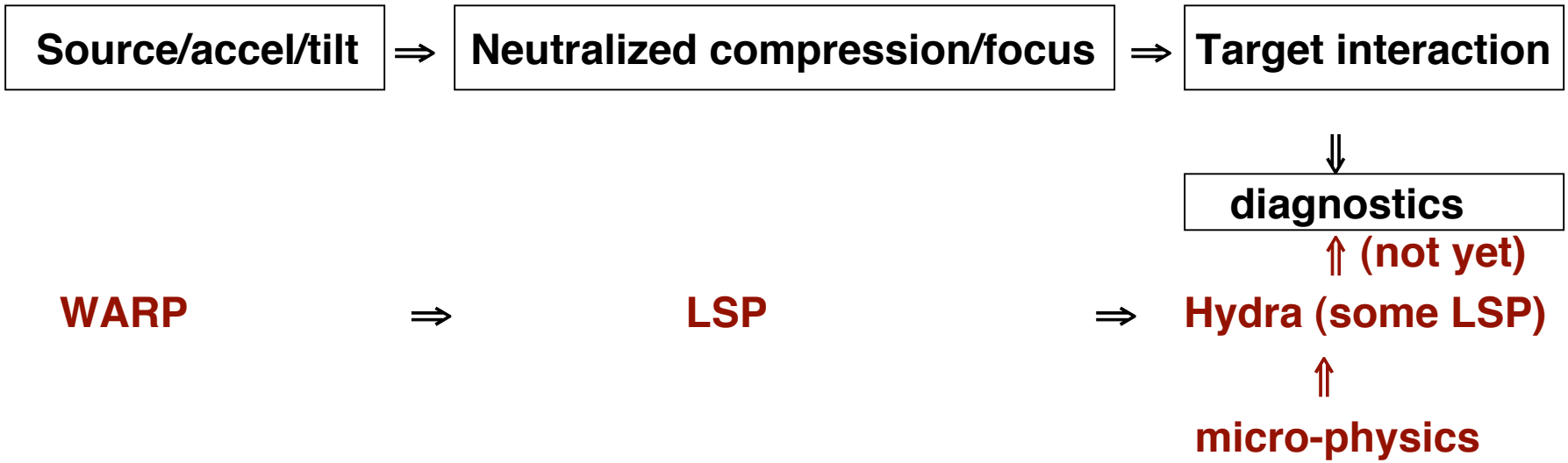
Perspective (by the group)

- **Existing tools provide a good jumping-off point for modeling accelerator-driven WDM physics**
- **We stand on the shoulders of giants (and giant programs …)**

but

- **We did not have sufficient time to systematically assess the limitations of the various tools**
- **We concurred that the needs of the WDM physics community (in general) are not fully met by existing codes, *e.g.*:**
  - **EOS's not yet satisfactory for multi-phase systems, foams**
  - **Differing e and i temperatures not handled well**
  - **QM models unable to provide benchmark all regions of interest**

Cartoon of an accelerator-driven WDM experiment as simulated by the HIFS-VNL



- The beam physics tools are quite advanced, but require further development for "plasma" problems
- Hydra and other "target" codes are advanced, but EOS's, etc., are not yet fully mature for WDM regime
- "Synthetic" diagnostics are essential; iterate as "real" diagnostics are developed

Taxonomy of codes

- Macroscopic (target and beam physics)
  - Kinetic
  - Hybrid
  - Fluid
- Mesoscale
  - Classical MD codes
- Microscale
  - First-principles low-to-medium T
  - First-principles medium-to-high T
  - Semi-classical MD
  - Semi-empirical (data-driven)
- Physics "packages" (for EOS, etc.)

Macroscopic codes for target and beam physics

- **Kinetic**
  - **WARP (Grote/Vay/Friedman):** 3D/rz/xy ES PIC; HIFS-VNL; general lattice; cut cells, AMR; SCL emission; e-cloud models; large Δt e-mover
- **Hybrid**
  - **LSP (Welch/Rose):** 3D/rz implicit/explicit PIC/fluid hybrid code; multiphysics; used by HIFS-VNL; also for fast ignition, other appls.
- **Fluid**
  - **HYDRA (Marinak)**
  - **[new AMR code] (Colella)**
  - **ALEGRA**
  - **LASNEX (Bailey)**
  - **CALE-ICF (Tipton)**
  - **MACH (Frese)**
  - **[none] (More)**

Mesoscale codes

- Classical molecular dynamics codes
  - For study of constitutive properties (tensile strength, grain boundaries, …)
  - Very large scale runs (many millions of atoms)
  - sophisticated potentials (Pair-wise and many-body)
  - LLNL (A. Kubota, F. Streitz), LANL (SPASM team), …

Microscale / basic physics input codes (1)

- First-principles low-to-medium T (< ~10 eV)
  - VASP+ (Sandia)

    KGOPTICS uses eigenvalues and -functions from VASP to calculate the Kubo-Greenwood response
  - ABINIT (freeware)
  - Wien

- First-principles medium-to-high T (> ~ few eV)
  - Path-integral MC method (for H, He; codes not generally avail.)
  - ACTEX ("Activity Expansion", by Forrest Rogers, LLNL); OK beyond He, but still limited to low Z by complexity
  - Inferno, Purgatorio ("cooler than Inferno"), SCAALP
    - provide approx results for all rho, T
    - based on single atom in "jellium;" no collective atom-atom effects

Microscale / basic physics input codes (2)

- Semi-classical MD + quantum corrections for stopping power
  - TCPproj: two-component plasma model with projectiles (Murillo & Jones)
  - Erlangen group (Zwicknagel)

- Semi-empirical for stopping power, secondary particles, …
  (based on experimental dats and scaling laws)
  - SRIM / TRIM (free, but source unavailable)
  - CRANGE (Tech-X; open source)

Physics “packages”

- EOS models (“sewing exercise” or “amoeba”?)
  - QEOS / MPQEOS
  - XEOS
  - (SESAME is a *format*)
- Conductivity models
- Opacity models
- Materials strength models
- Ion stopping models
- Atomic process models (ionization, c-x, stripping, …)
- Thermal relaxation models (e-i coupling, …)

- Consistency among the physics packages is an issue
  - “Who owns the charge state?”

"Axes" which characterize a code

- Physics models
- Numerical technologies
- Regime(s) of applicability
- Purpose
- Benchmarking
- Availability
- Limitations
- Plans/Goals
- Needs from "suppliers"
- "Speed" (relative to other codes in same domain)
- "Correctness" (likewise)

Other thoughts (1)

- "Macro" vs. "Micro"
  - Surface tension, boiling seem well described when they are viewed as microscopic physics used as subgrid models in a macro code
  - If a "macro" description of such processes is wanted, *e.g.*,
    - Detailed description of a small heated spot (where surface tension matters)
    - Boiling, but capturing where the splashes go

    … more physics (tensor description, kinetic processes, nonequilibrium models) may be needed

- Interactive exploration vs. automatic optimization
  - "Dakota" package automates simulation runs
  - EOS development

Other thoughts (2)

- Need to develop synthetic diagnostics
  - Backlit images
  - Spectra
  - VISAR
  - …
- How to diagnose?
  - Post-process data dumps using interactive or scripted tool, *e.g.*, Yorick
  - Produce plots as run progresses (pre-programmed; or via "user-steerable" code, *e.g.*, Python steers WARP)
- Much more work is needed here

Brief descriptions of some of the codes

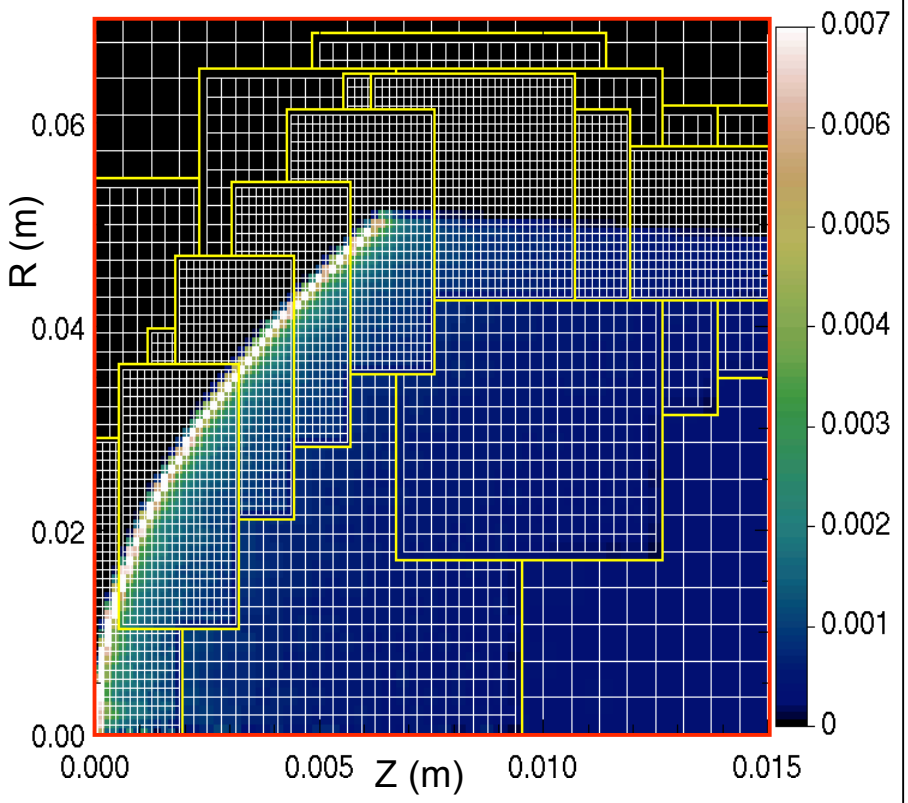
WARP (HIFS-VNL; description by D. Grote & J-L. Vay)

- **Physics models**
  - **beams in accelerator lattice + interaction with gas / low density plasma**
  - **3-D, R-Z (axi-symmetric), X-Y (slice); electrostatic / magnetostatic;**
  - **multi-species, models for generation and dynamics of electron clouds and gas, particle emission from solid and plasma sources**
  - **models for beamline elements at various levels of details with MAD-like syntax, warped coordinates for bends**
- **Numerical techniques**
  - **explicit Particle-In-Cell**
  - **cut-cell for internal conductors**
  - **Adaptive Mesh Refinement (AMR)**
  - **Boris particle pusher + drift for e^-'s in B field (bridges i/e time scales)**
  - **Monte-Carlo Collisions (ionization)**
  - **Parallel**
  - **"Steerable" (Python, GUI)**

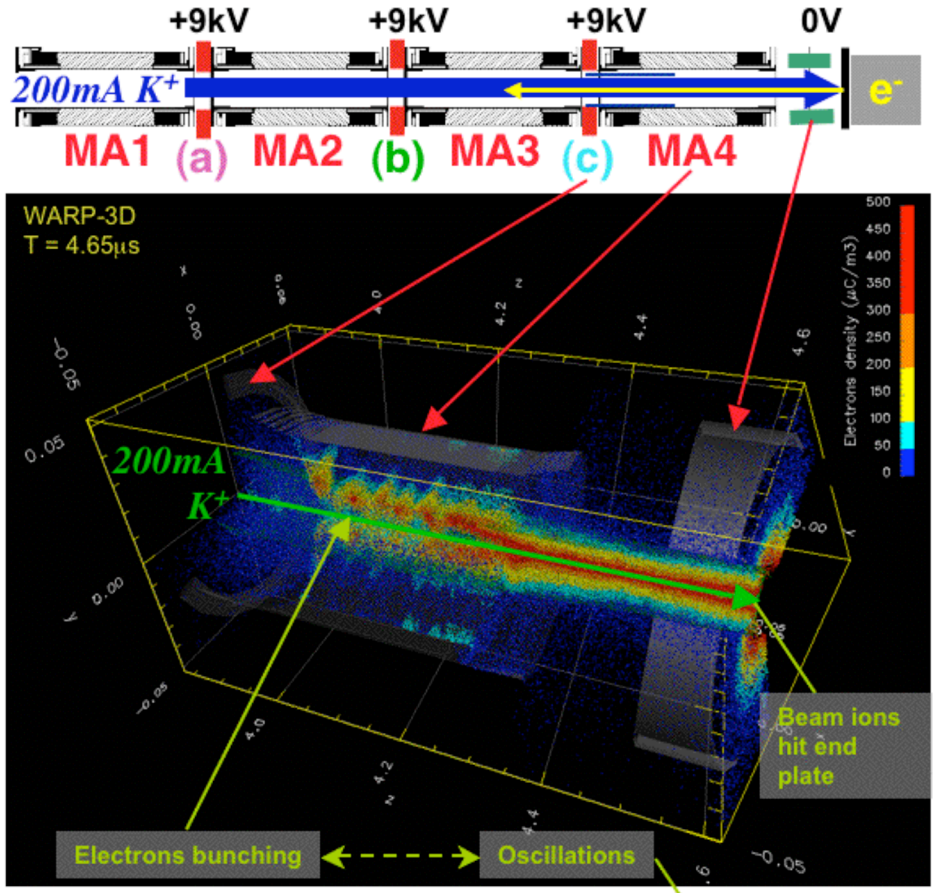
WARP (cont.)

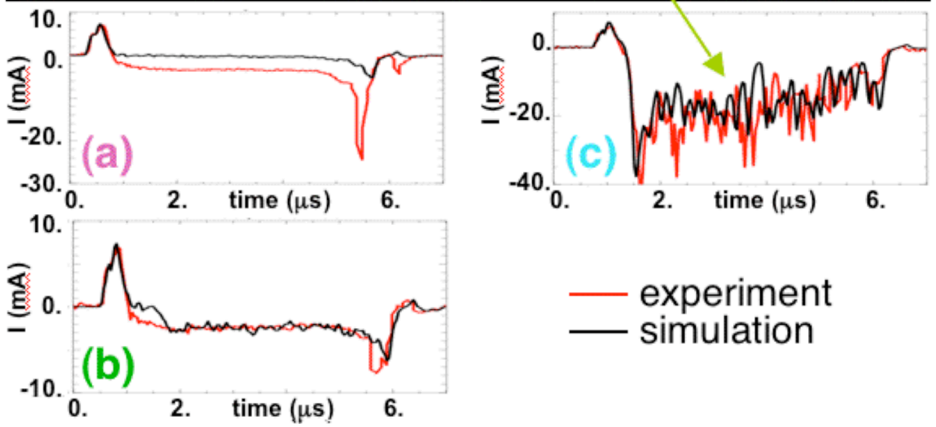
- **Regime of applicability**
  - **charged particle sources, accelerators, traps, low-ρ plasmas**
  - **"Space-charge-dominated" beams (non-neutral or neutralized by "electron cloud")**
  - **electrostatic and magnetostatic**
- **Benchmarks**
  - **High-Current Experiment (HCX)**
  - **Neutralized Transport Experiment (NTX),**
  - **Source test stand (STS500) / merging beamlet experiment**
  - **Dual Axis Radiographic Hydrodynamic Test (DARHT)**
  - **University of Maryland Electron Ring (UMER)**
  - **RIA front-end VENUS**
  - **PPPL Paul trap**
  - **LBNL/UC Berkeley multipole trap.**
- **Availability**
  - **Upon request**

WARP (cont.)



Time-dependent space-charge-limited emission using AMR-PIC





Electron-cloud buildup in HCX: simulation & experiment [J.-L. Vay, *et al.*]

LSP (description provided by Dave Rose)

- **Physics models:**
  - –Time-domain, electromagnetic, plasma dynamics code for 1,2,3-D modeling generation / evolution / stability of fully and/or partially ionized plasmas.
  - –Treats arbitrary electron and ion distributions kinetically and contains models for fluid descriptions by species.
  - –Fully parallel code (MPI) with dynamic load balancing
  - –Electron scattering and energy loss in materials via Moliere/Muller methods or via the Sandia ITS algorithms (implemented internally) including photon generation (not transport)
  - –QEOS (see Dale Welch's presentation)
- **Benchmarks**
  - –Broad range of fundamental and applied plasma physics benchmarks are an integral part of research conducted with LSP
  - –LSP test suite is available for testing of established modes of code operation (diodes, beams, collision models, etc.)

LSP (cont.)

- **Numerical Methods:**
  - **Fields:**

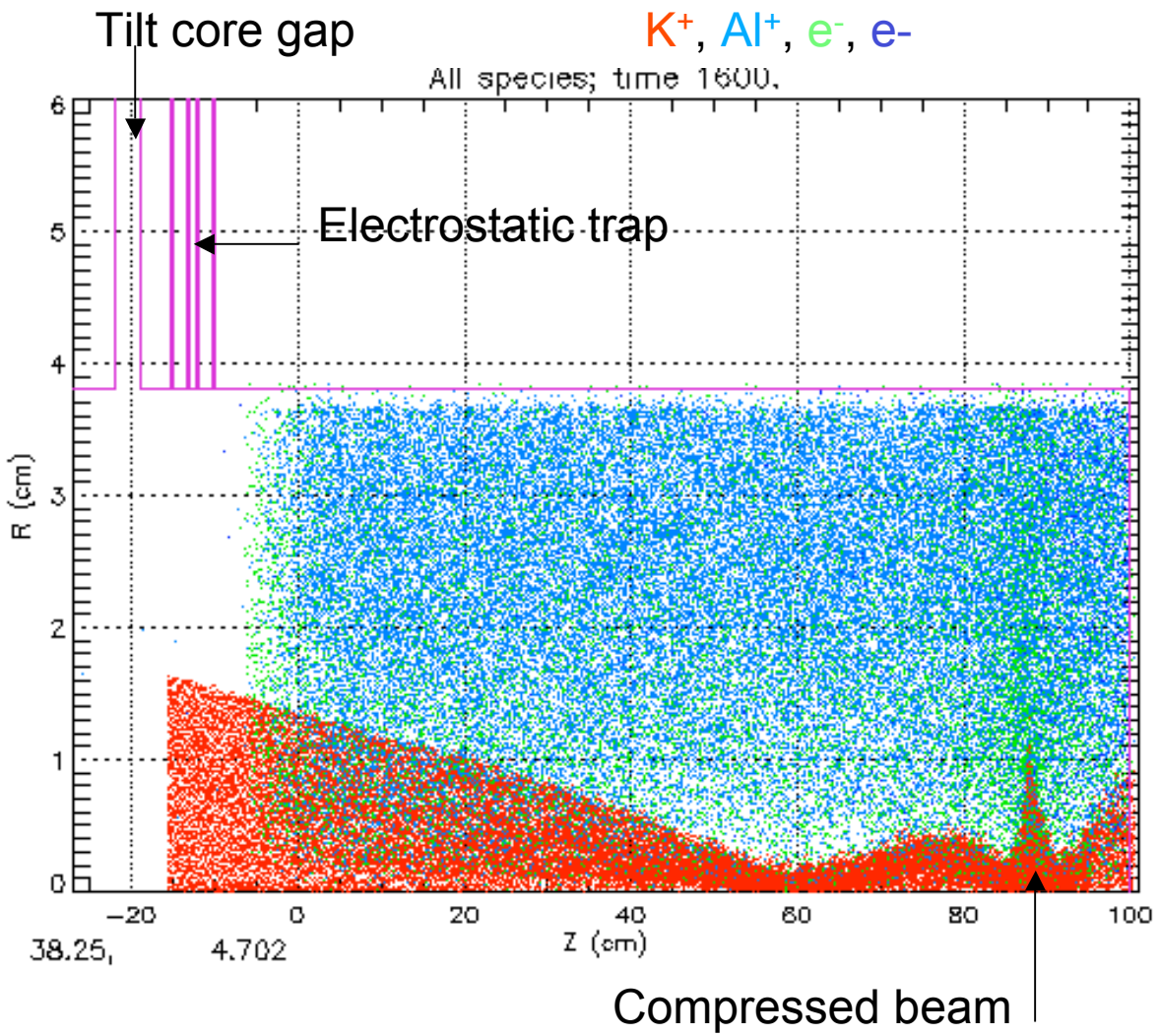
    Electrostatic solvers (SOR, ADI) and EM solvers (explicit and implicit)

    Quasi-neutral (EMHD) model, inertialess electron response via Ohm's law (under development)
  - **Particles:**

    Momentum-conserving advance or energy-conserving advance

    Eulerian-Lagrangian particle remap
- **Range of applicability (by example):**
  - **Laser-foil interaction (relativistic electron beam generation and ion generation, LULI experiment)**
  - **Wave-particle, wave-wave interactions (Landau damping, streaming instabilities, drift cyclotron instabilities, Bernstein modes, etc.)**
  - **Charged particle beam transport (NDCX experiment, electron-beam pumping of gas lasers, etc.)**
  - **Relativistic charged-particle beam propagation in energetic jets emerging from the cores of active galactic nuclei!**

LSP simulation of longitudinal beam compression in NDCX



285-keV 26-mA K^+ beam injected at z = -27 cm with a 1.9-cm outer radius, -22 mrad angle, and 0.21-eV temperature

Density Functional Theory/QMD codes (e.g., VASP, ABINIT, …) (summary provided by Mike Desjarlais)

DFT: Density Functional Theory is formally exact, but is in practice an accurate approximate solution to the N electron Schrödinger equations. Accuracy dependent on choice of exchange/correlation functional, quality of pseudopotential, …. Hierarchy of functionals: LDA, GGA, meta-GGA, Exact Exchange (EXX), EXX + non-local correlation, ….

QMD: The **Kohn-Sham* DFT** equations are solved for a given atomic configuration (fixed in the Born-Oppenheimer approximation) and the **quantum mechanical forces** on all the atoms are calculated from the wavefunctions following the Feynman-Hellmann theorem, **the atomic positions are advanced classically,** and a new solution to the DFT equations is calculated.

Kubo-Greenwood linear response: Quantum analog of the classical current-current autocorrelation formulation of the conductivity. Uses only the wavefunctions and eigenvalues from the DFT calculation to produce optical conductivities. Kramers-Kronig relations for complete (low energy) optical properties.

Density Functional Theory/QMD codes (cont.)

Primary purpose is to simulate atomic scale processes and compute equation of state and transport properties. Used to build physics models.

Well suited to quasi-equilibrium WDM conditions: 0.01 to 10 eV, 0.01 ρ_0 to ~5 ρ_0

Limitations:

Size <~ 1000 atoms

Timescale <~ 20 picoseconds

Compression: pseudopotential dependent, need for inner shell electrons at higher compressions

Expansion: poor statistics for very large supercells (fewer atoms); increasing density of states requires more bands

Born-Oppenheimer approximation: No energy exchange between electronic and ionic degrees of freedom. Thermal ground state properties only. (T_e .ne. T_i okay)

Approximate functionals: Local density functionals contain some self-interaction error. This leads to lowered metalization densities, increased polarizabilities, and weakened electron affinities.

XEOS (description provided by P. Sterne)

Physics Models	Based on empirical data and global electron & ion thermal model. Uses Thomas-Fermi or Purgatorio data for electron-thermal contribution to EOS
Numerical techniques	GUI-driven EOS synthesizer and visualized built on Python/Tcl-Tk/C code
Regime of Applicability	Wide density-temperature range [10^{-10} - 10^{4} gm/cc, 1K - 100keV or more]
Purpose	Synthesize global equation of state from models for cold, electron-thermal and ion-thermal components using graphical comparison with experimental data
Benchmarking	Compared with experimental data during EOS table construction.
Availability	Not currently available for distribution. May be made available as EOS browser and/or EOS generator in the future.
Limits/Plans/ Goals	Limited to physics contained in the implemented models. Future plans include more flexibility in including new models (e.g. molecular model, Grueneisen variation at densities below normal density), better ion model, better treatment of foams.
Accuracy/Speed	Accuracy ~ 6 / 10 Limited by quality of models and availability of experimental data Speed ~ 9 / 10 Highly interactive and responsive

Purgatorio (description provided by P. Sterne)

Physics Models	Relativistic Dirac equation code to solve for an atom in jellium at finite temperature, providing EOS electron-thermal data
Numerical techniques	Density functional theory; radial Dirac equation solver. Adaptive refinement integration for electron energy integration
Regime of Applicability	Low density/large radius atomic limit to high denisty limit; temperatures from 1K to over 100keV
Purpose	Compute electron-thermal energy, entropy, effective charge (Z*) and conductivity for elements
Benchmarking	Comparisons with other atomic codes; comparisons with ACTEX; comparisons with solid state physics codes; comparisons with experiment
Availability	Not currently available for distribution
Limits/Plans/ Goals	Limited by single-atom approximation, density functional theory. Potential plans include response function calculations - optical properties, stopping powers. Limited by lack of atom-atom effects (lattice structure; molecules)
Accuracy/Speed	Accuracy ~ 7 / 10 Not as good as QMD, but wider applicability; much better than TF. Speed ~ 7 / 10 Much faster than QMD; slower than TF.

CRANGE (Description provided by P. Stoltz)

- The CRANGE code calculates stopping power as a function of energy for any ion in a variety of solid targets.

  The code uses tabulated experimental values of proton stopping scaled by semi-empirical estimates of effective charge to calcualte the stopping of heavy ions.

  The targets available are limited to those for which tabulated experimental protonic stopping values are available, and currently include aluminum, copper, iron, gold, lead, air, and water, among others.
- The semi-empirical estimates of heavy ion effective charge are based on parameterized fits by Ziegler and are also used in the SRIM code.

CRANGE (cont.)

- The range of projectile ion velocity for which CRANGE is most accurate is the Bohr velocity (scaled by the projectile atomic number) to approximately one GeV/amu.
- The CRANGE code is most accurate for cold targets. Calculations for targets of temperature an eV or greater should be used with caution.
- We have benchmarked CRANGE against SRIM for a few projectiles and targets, including potassium and sodium projectiles hitting aluminum targets. The codes agree to within a few percent.
- The CRANGE code is written in C, is available freely and is open-source.
- Future plans for CRANGE include expanding the number of targets and modifying the algorithms to include effects of warmer target temperature.

HYDRA, a 1,2,3-D multi-physics ICF hydrodynamics (fluid) code [description by M. Marinak; see also his talk]

- **Physical models**
  - **Laser propagation & deposition**
  - **Ion beam propagation (3-D raytrace) & deposition**
  - **Electron transport (flux limited conduction; nonlocal multigroup)**
  - **Radiation transport (multigroup diffusion, implicit MC photonics)**
  - **Magnetic fields (resistive MHD at present)**
  - **Thermonuclear burn**
  - **Multigroup transport of charged particle products**
  - **Neutron deposition in free-streaming limit**
  - **Ion conduction, e-i coupling**
  - **Lagrangian hydrodynamics withh ALE capability**
  - **EOS's: analytic forms, LEOS, EOP, SESAME tables, inline QEOS**
  - **Opacities: online server, tables, inline LTE & NLTE XSN, linear response matrix NLTE**

HYDRA (2)

- Numerical techniques
  - Lagrangian / ALE
  - 2nd order accurate advection w/ material interface reconstruction
  - Block-structured mesh w/ ability to handle reduced and enhanced connectivity boundaries
  - Finite element techniques used for most transport algorithms
  - Scalable matrix solvers
  - Runs on workstations or distributed clustered SMP architectures, using a strategy based on POSIX threads, Open MP, & MPI library
  - Dynamic load balancing in certain packages
  - Designed for ease of use, high accuracy, and efficiency
  - Several options available for modeling each physical process

HYDRA (3)

- **Regimes of applicability:**
  - **Physical processes modeled, EOS, opacities, are generally globally applicable**
  - **Most frequently tested / used in regimes with:**
  - **laser intensity ~ 10^{14} W/cm^2, density ~ 0.001-1000's g/cm^3, Te ~ 10's-10,000's eV, P up to terabars**
- **Benchmarking:**
  - **Tested against a wide variety of laser-driven experiments, ranging from planar RT, integrated sim's of capsule implosions, complex hydrodynamic flow experiments, laser propagation experiments, drive symmetry experiments**
  - **Many comparisons are published in journals**
- **Postprocessing:**
  - **Many tools are available for data visualization (GUI or CLI); Yorick is a highly flexible postprocessing tool, freely available, used to generate simulated experimental data**

HYDRA (4)

- Availability
  - HYDRA is export-restricted. It can be made available to U.S. "persons"; these are U.S. citizens and most permanent resident aliens (with a green card).
  - Is used at several national laboratories
- Plans for Development
  - Will implement Desjarlais conductivities (electrical & thermal) soon
  - Will soon implement isotropic material strength
  - Will incorporate MC neutronics in next 2 years
  - Will benefit from new EOS tables with improved construction in WDM regime
  - Improvements to user interface are planned
  - Generalized Ohm's law in B-field package
  - Special requirements for simulation of WDM physics (see slide)

Special requirements for simulations of warm dense matter (from M. Marinak)

- Ion deposition model
  - Formulas for stopping power intended for IFE with higher energy per nucleon
- Electron beam heating
  - Can link deposition profile from ITS Monte Carlo code
- Thermal conductivity
  - Is it important on time scales of interest for a given experiment?
  - Lee and More σ is default, Desjarlais conductivities are to be implemented
- Electron-ion coupling
- Improved equations of state for WDM regime
  - Treat phase changes with sufficient resolution
  - Ensure thermodynamic derivatives from tables well behaved for WDM
- Material strength – isotropic strength being implemented
  - Include temperature dependence
  - Spallation model required?
- Surface tension could be implemented at material interfaces
  - Could model evaporation kinetics in non-equilibrium two phase fluids

Big-2 (V. Fortov; description courtesy N. Tahir)

- Based on Godunov-type scheme
- Arbitrary Lagrangian Eulerian (ALE) scheme
- 2D hydrodynamics
- 1 Temperature
- Tabulated EOS data (semi-empirical)
- Heat Conduction
- Tabulated ion stopping data from SRIM
- Takes beam geometry into account
- Complicated target geometry
- Two ion beams:
  - High intensity bunched beam for heating
  - Low intensity unbunched beam for diagnostics

MPQeos (description provided by W. Sharp)

- Authors: A. J. Kemp (MPQ, LLNL) and J. Meyer-ter-Vehn (MPQ)
- Based on published description of QEOS by R. More
- Purpose: calculate EOS for single ion species using QEOS formalism
- Numerical techniques:
  - semi-empirical analytic model for ions
  - table lookup and scaling for electrons
- Physics models:
  - generalized Cowan model for ions
  - Thomas-Fermi model with quantum corrections for electrons
  - chemical-bonding corrections
- Regime of applicability:
  - approximate but well-behaved output over wide parameter range
  - asymptotically correct and internally consistent

MPQeos (cont.)

- **Benchmarks:**
  - **visual comparison with selected QEOS published results**
  - **authors doubtless did more checking**

- **Limitations:**
  - **approximate results only**
  - **misses details of electronic structure and other quantum effects**

- **Availability:**
  - **free! open source! no export controls!**

- **Plans / goals:**
  - **will be generalized to handle multiple ion species**

Presentation by Philip Sterne (LLNL) to working group 3

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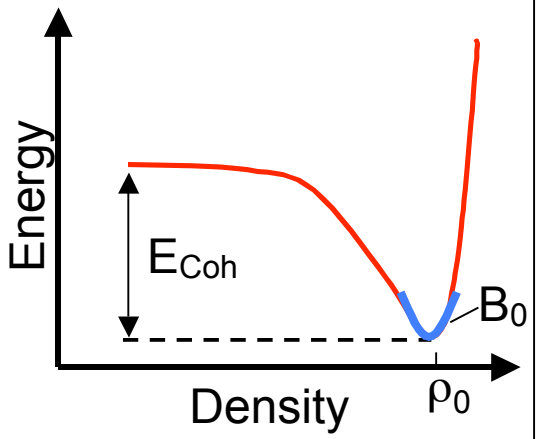
We write the global EOS in terms of three components

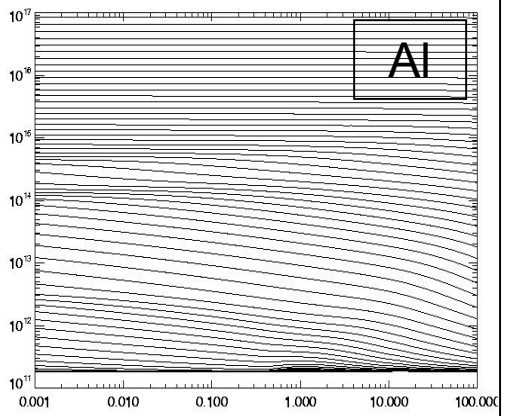
$$F[\rho,T] = E_{Cold}[\rho] + F_{Elec}[\rho,T] + F_{Ion}[\rho,T]$$

Cold Curve



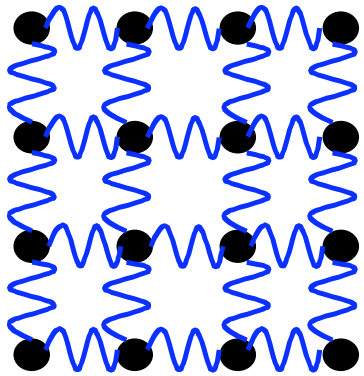
Cold curve may include additional parameters to modify $\rho < \rho_0$ and $\rho > \rho_0$ behavior

Electron-Thermal



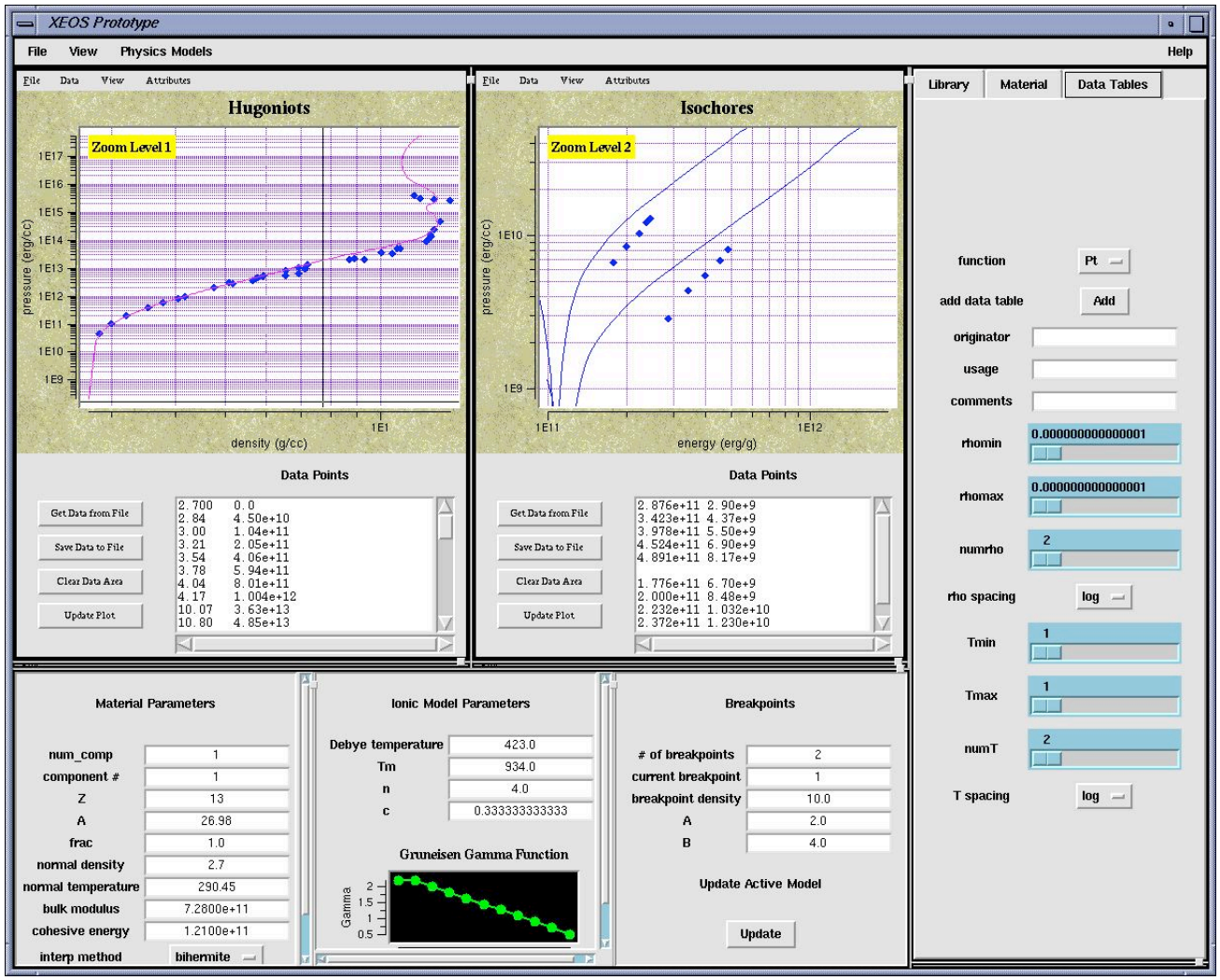
Ionization features seen in Purgatorio-based electron-thermal energy and entropy.

Ion-Thermal



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

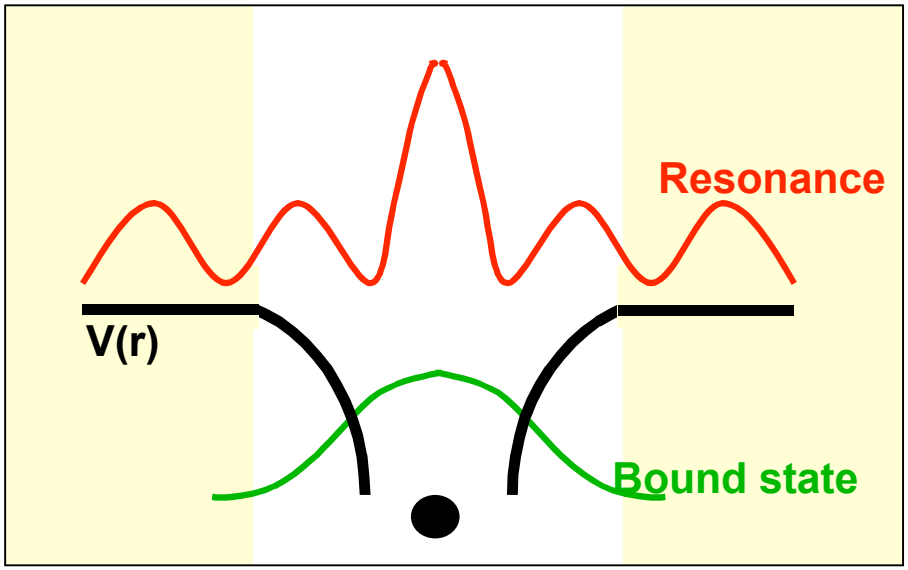
XEOS facilitates the interactive construction of new EOS tables



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

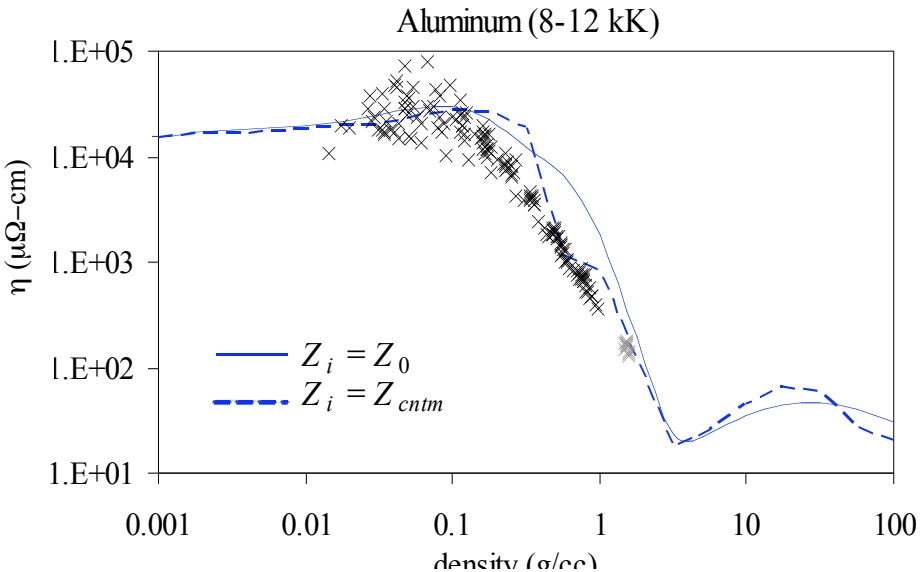


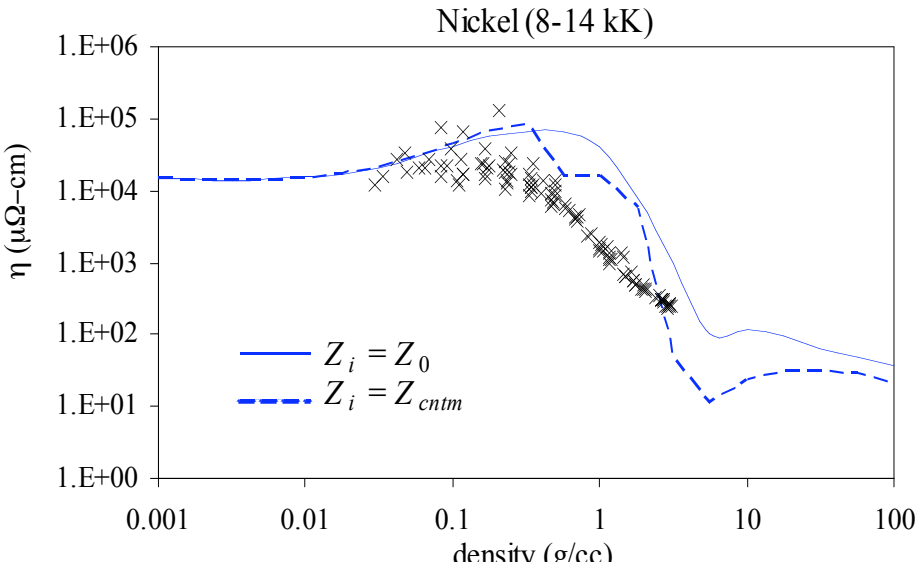
Our Purgatorio model is a modern reimplementation of David Liberman's Inferno Code :

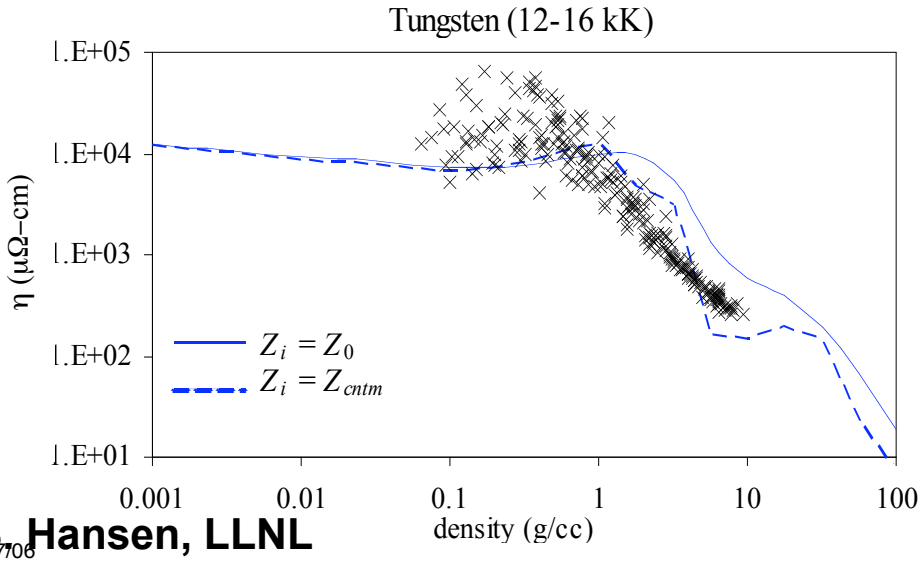
- Fully relativistic *ab initio* muffin-tin model of a single atom in jellium
- Charge neutrality enforced within atomic sphere
- Production code that works across the periodic table for a wide range of temperatures and densities
- Phase-amplitude method gives more accurate solutions for high energy,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

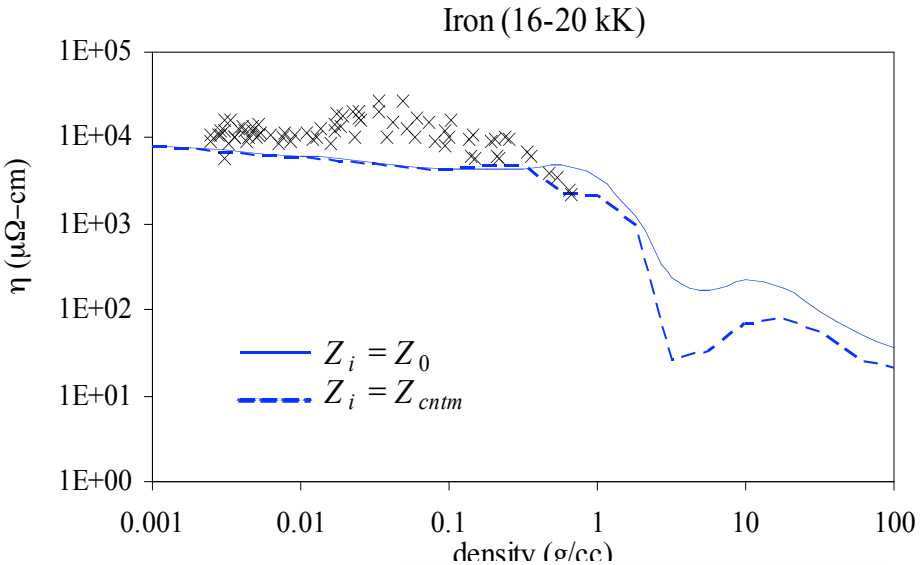
Purgatorio is an important enabling tool for future research since we can build on it to incorporate more physics. We have already extended it to calculated electron conductivities.

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



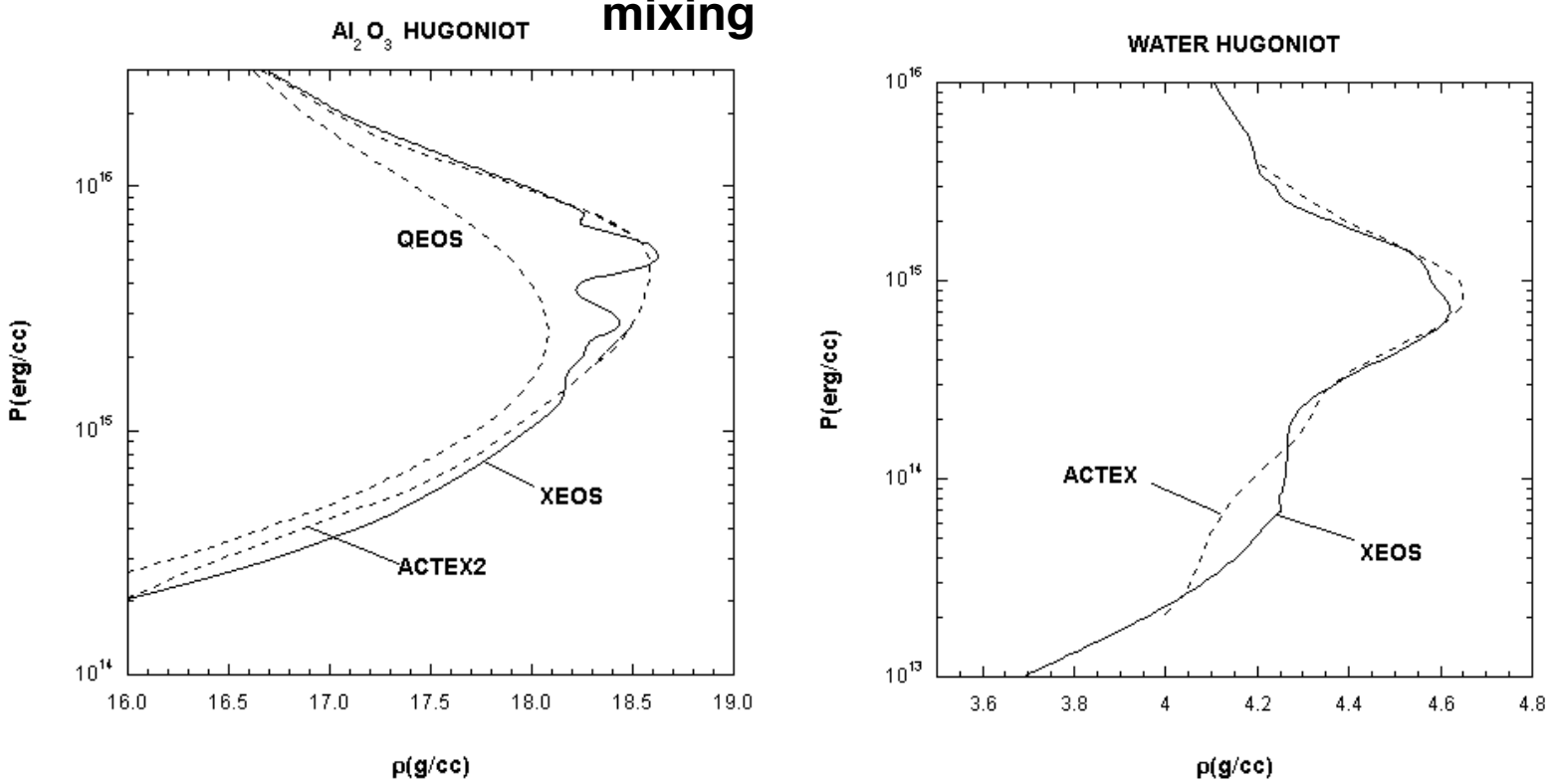






Mixtures

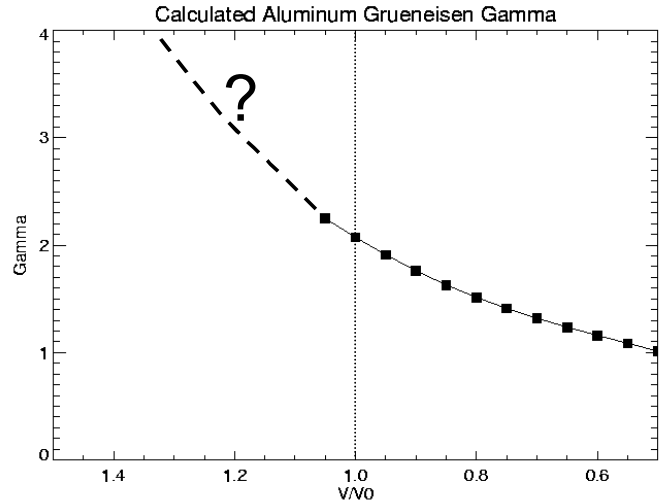
Constant-pressure mixing



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?