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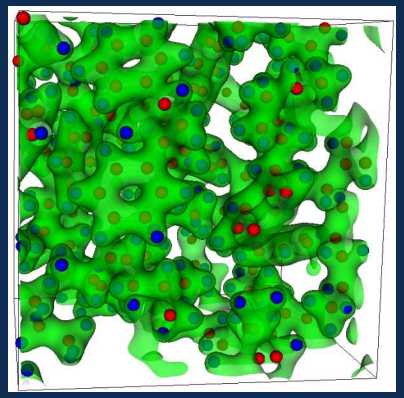

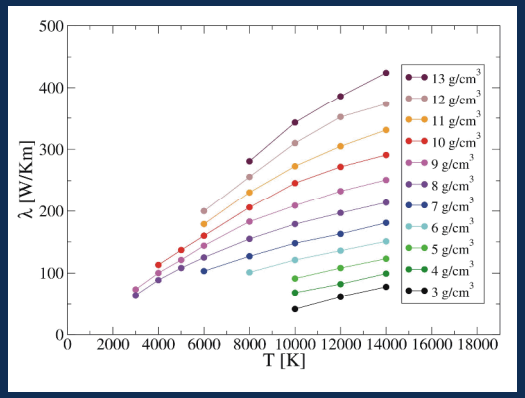

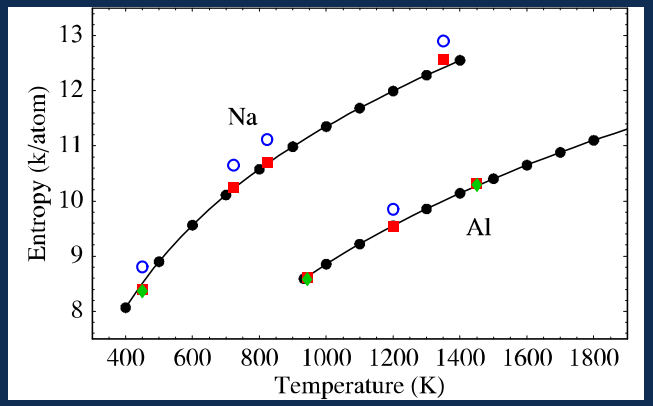

Sandia ASC/PEM/EOS 2014 to 2020 and beyond – new methods and new material models

Thomas R. Mattsson

Sandia National Laboratories

PEM tri-lab workshop March 2014, Sandia National Laboratories

U.S. DEPARTMENT OF ENERGY | NNSA

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Material models determine the outcome of radiation-magneto-hydrodynamic simulations

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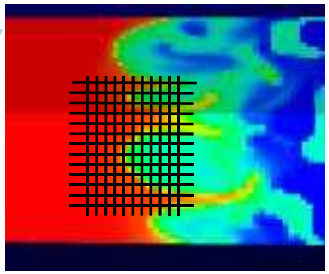
Hydrodynamics

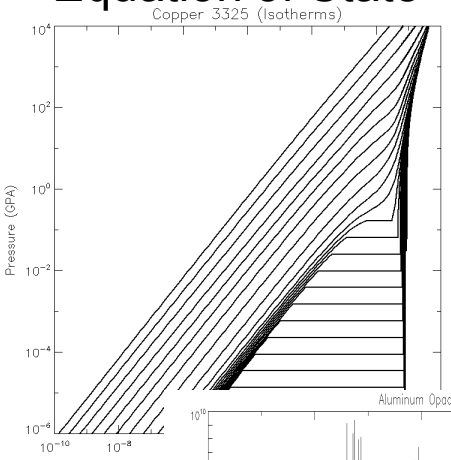


Tom Haill, SNL

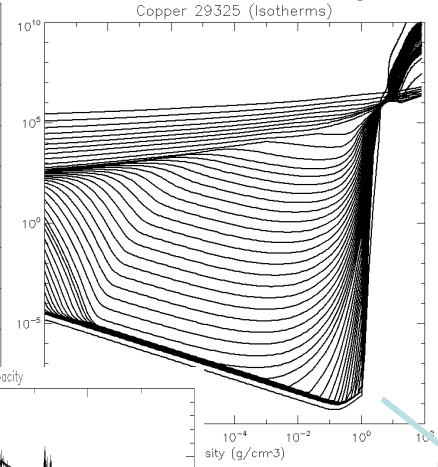
Most simulation codes will tally the total energy in each cell and, based on that energy and the density, compute a new pressure and temperature in preparation for the next hydrodynamic step.

The hydrodynamics moves material based on the material properties.

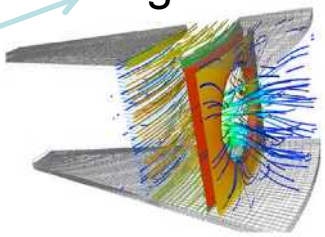
Equation of State



Conductivity

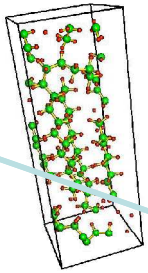


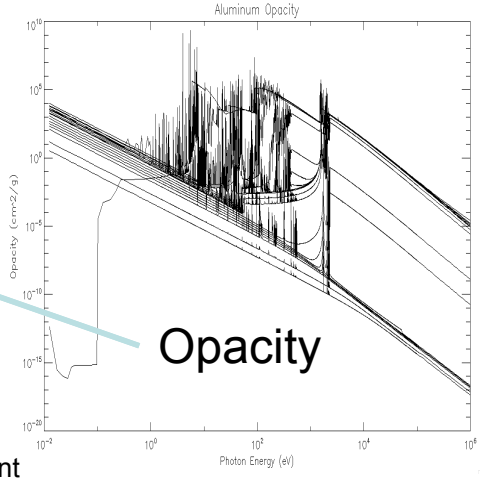
Magnetics



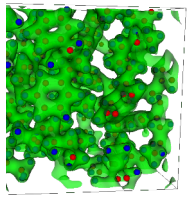
Chris Garasi, SNL

Conductivity determines magnetic field diffusion.

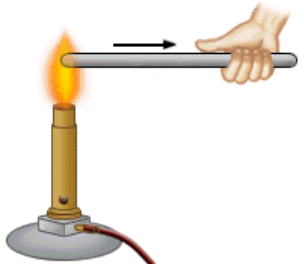




Opacity

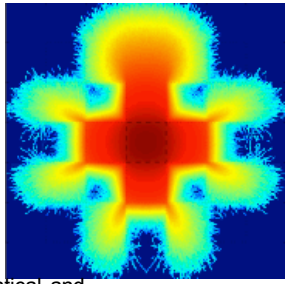


Conduction



Thermal conduction is used to augment the movement of energy in a simulation.

Radiation

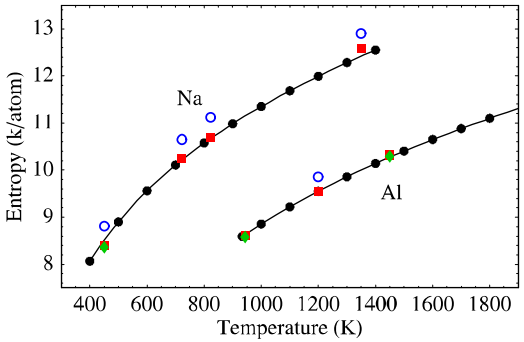


Tom Brunner, LLNL

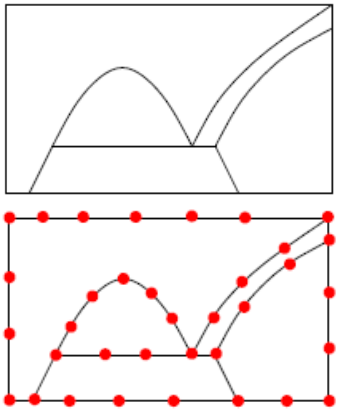
Radiation is an important energy transfer mechanism for hot systems

Nuclear Mathematical and Computational Sciences: A Century in Review, A Century anew

Present focus and results in the EOS subelement – deliver materials models of high fidelity



Absolute entropy for liquid metals



UQ enabled topological adaptive mesh for EOS tables

Gaps/challenges

- Predictive modeling of phase transitions
  - *Solid/solid and solid/liquid*
  - *Kinetics of phase transitions*
- Integrated consistent description of EOS and transport properties
  - *All models from one framework*
- Modeling of all materials, also those challenging for DFT/QMD
  - *Quantum Monte Carlo*
- EOS tables supporting uncertainty analysis
  - *EOS tables with unstructured adaptive mesh – on triangular grid*
  - *Bayesian analysis of sensitivity*

Results after FY13 restart

- Method for calculating entropy of a liquid
- Implemented DFT/QMD calculation of viscosity
- Developed Utri and integrated EOS uncertainty quantification in the ALEGRA MHD code

We have systematically investigated Quantum Monte Carlo for materials – pioneering solid benchmarks

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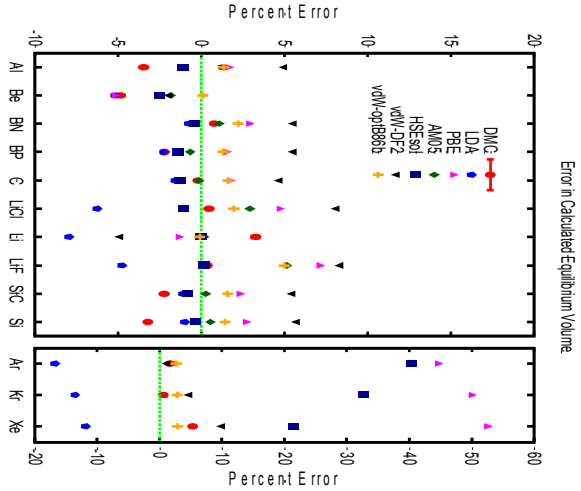
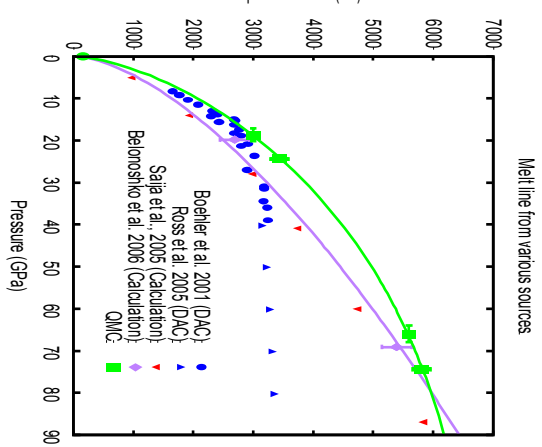


Benchmarking a broad set of solids using QMC – comparing to state-of-the-art DFT methods



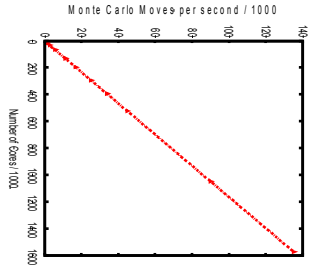
QMC high-pressure melt line of xenon

Benchmarked QMC for solids

- QMC has uniform excellent performance for ionic solids, metals, covalent solids, and van-der Waals solids
- L. Shulenburger, T.R. Mattsson, PRB **88** 245117 (2013).

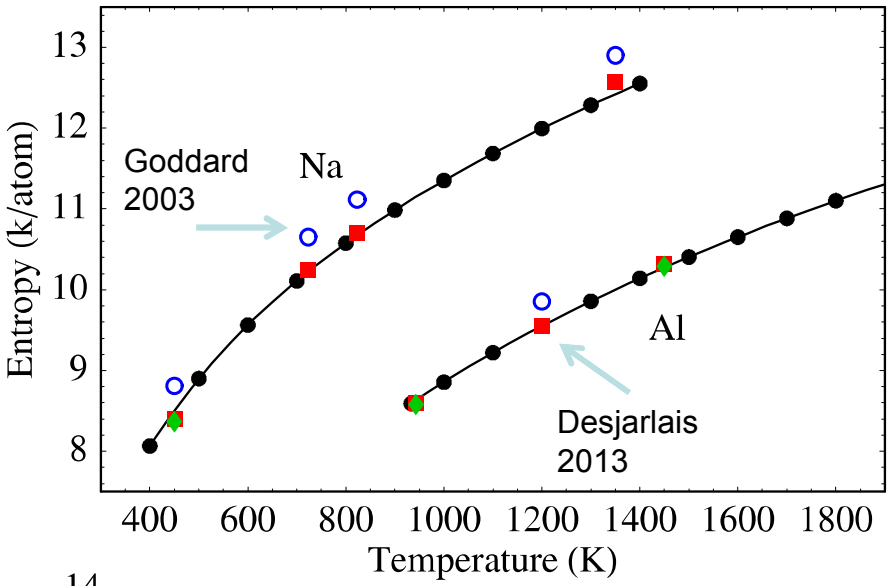
Key applications

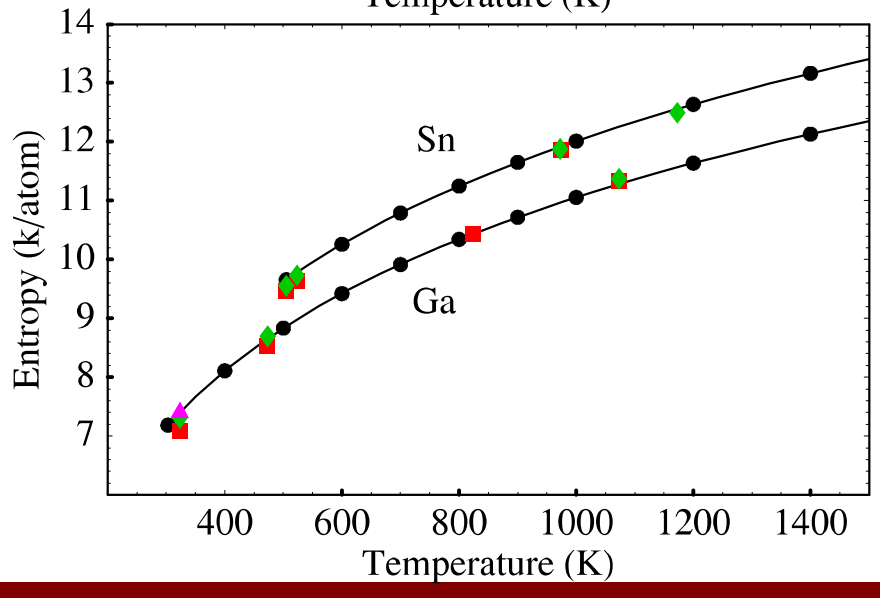
- Phase structure/boundaries
  - *LiD, Be, Li*
- Phase transitions
  - *Xenon melting under pressure*
- Fundamental van der Waals bonding
  - *Xe, Kr, Ellipticine + DNA*



Linear scaling to 1.5 M cores on Sequoia w qmcpack

We have developed a quantitative method for calculating absolute entropies of liquid metals





Absolute entropy from DFT/QMD

- Density Functional Theory (DFT) based molecular dynamics (QMD)
- Provides the missing link in first-principles thermodynamics:
  - *Internal energy, pressure, entropy*
- M.P. Desjarlais PRE **88** 062145 (2013)

Key applications

- Improved accuracy for calculations of liquid/solid phase transition at pressure
  - *Beryllium, steel, tantalum*
- High accurate calculations of release-adiabats from shock states

A deliberate way of adaptive mesh refinement and topological equivalence – beyond square tables

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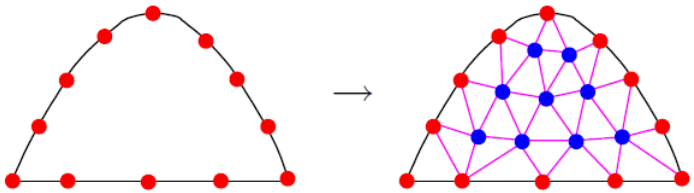
N sample tables with consistent topologies are used to make tables that are all consistent with data, but showing the spread in eigenmodes in the table

Boundary point locations on each phase line segment are related by a linear mapping.



$$\frac{1}{\sqrt{g}}\frac{\partial}{\partial \xi^\alpha}\left(\sqrt{g}g^{\alpha\beta}\frac{\partial x^i}{\partial \xi^\alpha}\right) = 0$$

Laplace-Beltrami smoother

Phase boundary information explicitly included in the table – allowing consistency between EOS and transport properties.
Interior boundary point locations are smoothed to control noise.

Governing questions, gaps, and scientific innovation are cornerstones steer our work

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Multi-phase descriptions of all materials where it matters – and a reliable description of mix and heterogeneous materials.

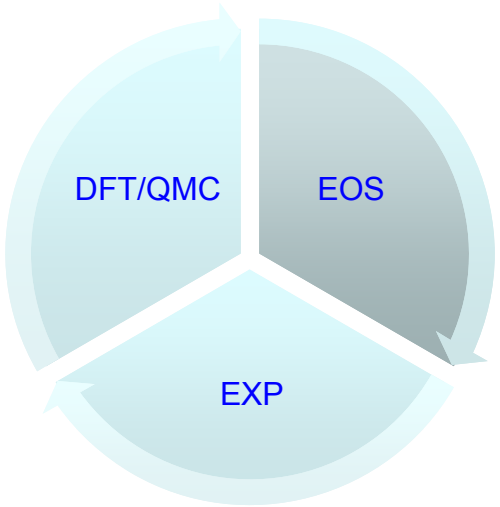
R&D dimension remains the most demanding – old methods don't die, instead they become routine with less efforts needed to maintain

Flexibility and agility to quickly address also complex questions for all materials

- 1,2,4 Need in 10 years to become predictive and remove knobs?
  - Consistent sets of material models
    - Including chemistry/dissociation & solid-solid phase transitions
  - It is possible to "solve" a problem/material, and that should be our firm ambition. *Model X for material Y is done*
  - It is important to realize that we need PEM also to maximize today's often integrated experimental platforms, Z, NIF, Omega.
- 3 Skill sets needed – *change is constant*
  - DFT a routine method also for complex systems; new hires are in Quantum Monte Carlo, GW and TD-DFT for electron/ion dynamics [attoseconds] and are adapt in visualization
- 6 New aspects
  - Transition to adaptive EOS tables
  - An extensive library of UQ enabled EOS tables coupled to hydro codes with UQ – reporting uncertainties

Future work in the EOS subelement is focused on removing gaps on multiple timescales

Integrated effort including developing methodology, delivering tables – and doing so in response to material needs for a broad range of applications: science campaigns C1,C2,AC,ICF



- 2015 - 19
  - Consistent set of material models based on DFT/QMD
    - Including chemistry/dissociation
    - Solid-solid phase transitions
  - Advance advanced electronic structure methods
    - Quantum Monte Carlo for high-fidelity phase transitions; Path-Integral MC for high-temperature structure and dynamics
    - Employ GW and TD-DFT for electron/ion dynamics [attoseconds]
  - Transition to adaptive EOS tables
    - Deliver Al and quartz EOSs within UQ framework
- 2020 – 24
  - QMC for *all materials* as a validated method
  - Transport properties beyond DFT linear response
    - GW and TD-DFT used routinely
- 2025 -30
  - Flexibility and agility to quickly address also complex questions for all materials
  - An extensive library of UQ enabled EOS tables coupled to hydro codes with UQ – reporting uncertainties

Extra slides – for Q and discussiun

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Multiphase Tabular Representation is flexible and allows for UQ aware EOS tables

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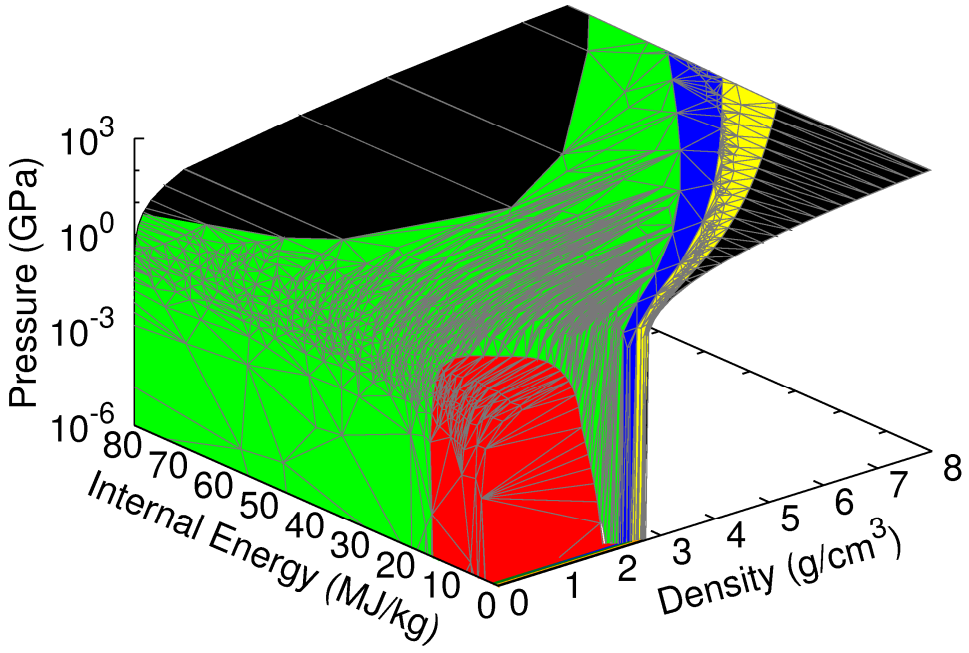
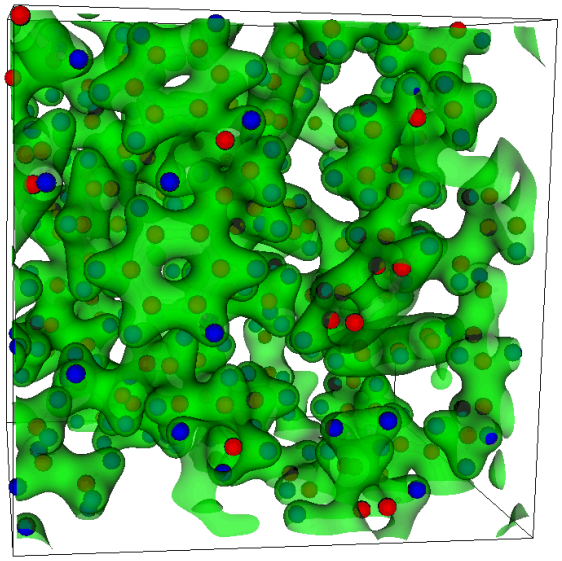
- We now build multiphase EOS tables with unstructured triangular grids.

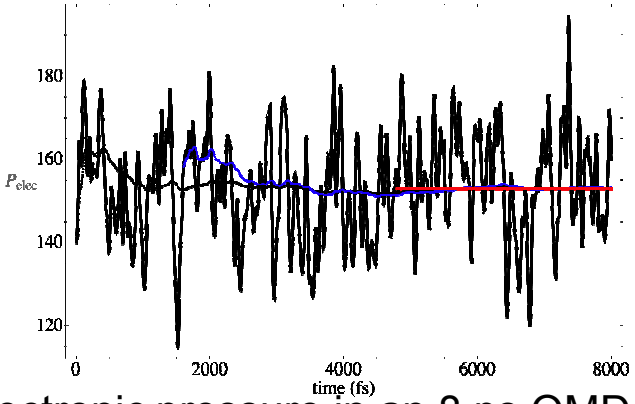
  - Wide-range EOS features, such as phase boundaries, are easily followed.
  - Grid adaptation allows for reduction of table size.
  - Use principal component analysis (PCA) on tabular samples to provide a compressed tabular representation with random coefficients and mode shapes.



Describing the electronic structure of materials from first principles – the power of DFT



GDP ion structure and electron density



Electronic pressure in an 8 ps QMD simulation

Density Functional Theory (DFT)

- Founded on quantum mechanics
  - Walter Kohn '98 Nobel prize in chemistry
- Includes molecular binding, ionization by pressure and/or temperature
- Now well-established in shock physics
  - Mike Desjarlais' work on D_2 in 2003
  - *Convergence is key*
  - Electrons with finite temperature k_BT and a Fermi distribution
- Efficient codes and fast computers allow following hundreds of atoms for tens of ps in "normal" simulations

First-principles thermodynamics

- Internal energy, pressure, entropy, and structure/phases

Transport properties

- Conductivity, diffusion, viscosity