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Spot Checking EOS with Ab Initio Calculations

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What are the most useful spot checks of EOS from ab initio calculations?

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- Direct comparison of experimental observables
  - Hugoniot
  - Isentropes
  - Vapor dome
  - Compressibility
  - Vapor dome
  - Phase boundaries
- Calculated model parameters
  - Gruneisen gamma
  - Heat capacity
  - Cold curve parameters
  - Debye temperature

Where are ab initio calculations deemed trustworthy and why?

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- What is required to validate results from a given approximation for use elsewhere?
- How can ab initio results be integrated into EOS when inconsistent with experimentally known data
  - For instance the ambient density is wrong but the Hugoniot and phase boundaries look good?
- How are grids of calculated P/T/rho/E points integrated into consistent models?
- What calculations would you like to see?

Moving from warm dense to high temperatures

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- The Mermin-DFT calculations that are currently relied on require calculation of enough quantum states to satisfy the Fermi-Dirac distribution
  - Kohn-Sham DFT (typical implementations) scale like $O(N^3)$ with states or equivalently $O(T^{4.5})$ at high temperatures
- Other methods are often used at higher temperatures
  - Average atom
  - Thomas-Fermi-Dirac
  - Orbital-Free DFT
  - Path Integral Monte Carlo
- How can these be stitched together?
  - LANL has some interesting work on matching families of orbital free functionals to standard low T approximations
  - Zhang et al., Phys. Plasmas **23**, 042707 (2016) – Combine analytic continuum states with typical low temperature approach