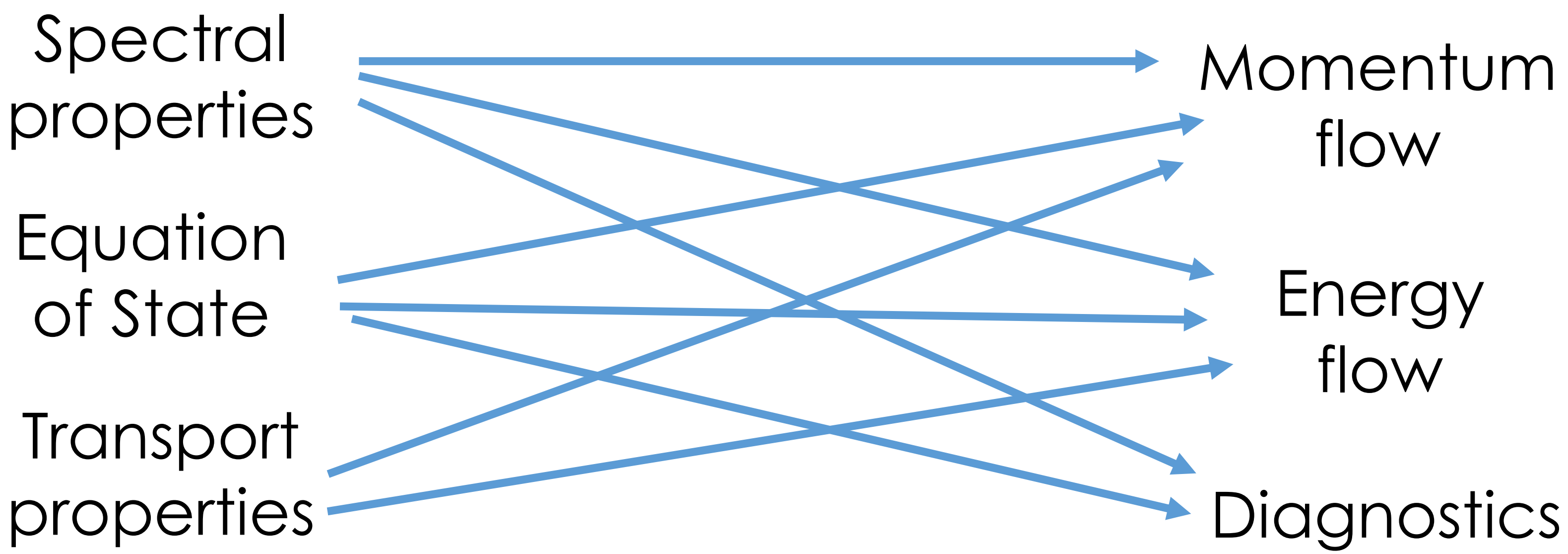
Self-consistent microphysics models for materials at high energy density

Adam R. Fraser[1,2], Dr Nicolas Niasse[2],
Dr Aidan Crilly[1], Dr James Pecover[2],
Dr Dave Chapman[2], **Prof. Jeremy Chittenden**[1].

1. Imperial College London
2. First Light Fusion Ltd

Numerical modelling of HEDP experiments

- Successful ability to model and interpret experiments dependent on the provision of accurate data for material properties



Radiation hydrodynamics

- Electron energy balance equation

$$\frac{\partial E_e}{\partial t} = \nabla \cdot \kappa_e \nabla T_e - 4\chi_P \sigma T_e^4 + c\chi_P E_r - p_e dV + \eta j^2 + Q(T_e - T_i)$$

- Ion energy balance equation

$$\frac{\partial E_i}{\partial t} = \nabla \cdot \kappa_i \nabla T_i - p_i dV - Q(T_e - T_i)$$

- Radiation energy balance equation

$$\frac{\partial E_r}{\partial t} + \nabla \cdot \mathbf{F}_r = 4\chi_P \sigma T_e^4 - c\chi_P E_r$$

Radiative properties

Transport properties

Equation of state

Saha equation → electronic partition function

- The electronic partition function can be separated into contributions from each ionisation stage

$$\mathcal{Z}_{e,tot} = \frac{\mathcal{Z}_e^{N_e}}{N_e!} \cdot \prod_{\alpha=0}^{Z} \frac{\mathcal{Z}_\alpha^{N_\alpha}}{N_\alpha!}$$

- The Saha equation relates the number densities of ionisation stages to their partition functions

$$\frac{N_{\alpha+1} N_e}{N_\alpha} = \frac{\mathcal{Z}_{\alpha+1} \mathcal{Z}_e}{\mathcal{Z}_\alpha}$$

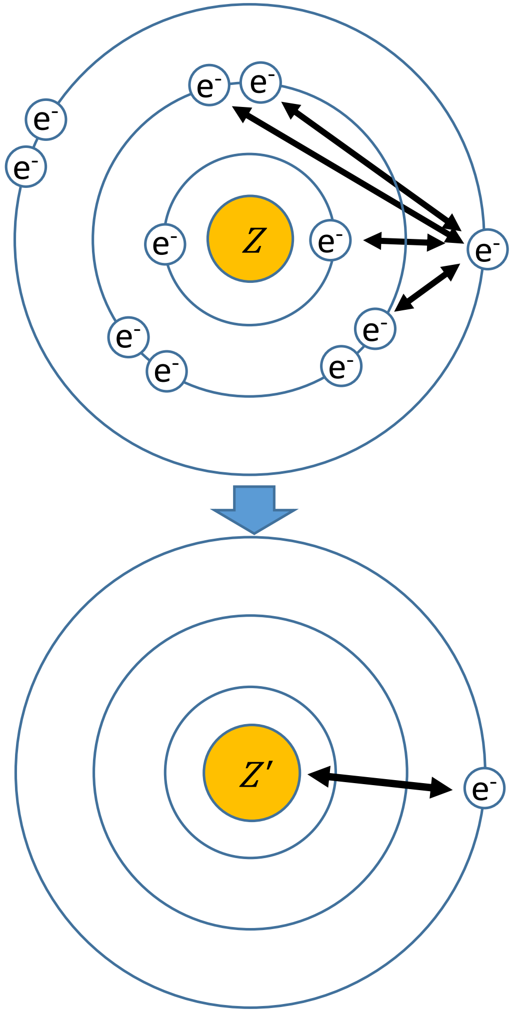
- Opacities and thermodynamic state functions can then be computed

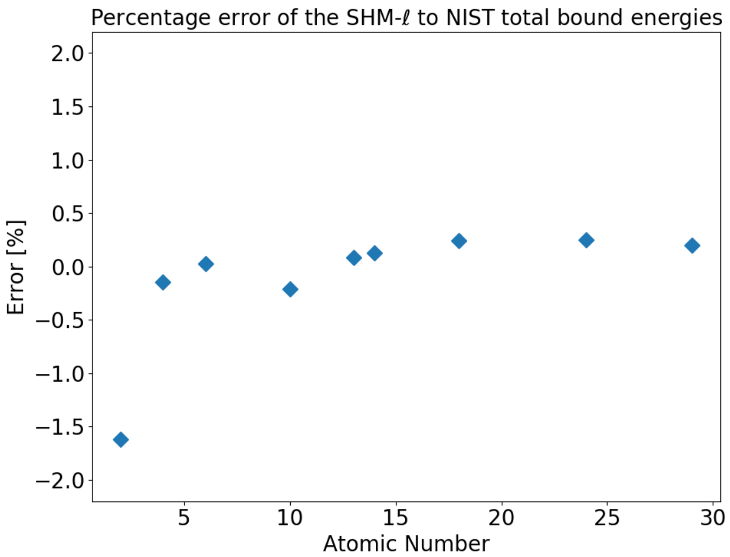
$$F = -k_{\mathrm{B}} T \ln \mathcal{Z}$$

- Requires knowledge of electronic energy levels and non-ideal physics

Energy levels can be obtained from NIST database - gaps filled in by SHM-ℓ

- Screened hydrogenic model with ℓ-splitting (SHM-ℓ) developed into an electronic EoS by Gerald Faussurier
- Used to calculate unknown bound state energies
- Reasonable agreement against NIST data
- Similar formalism can be applied to Saha equation





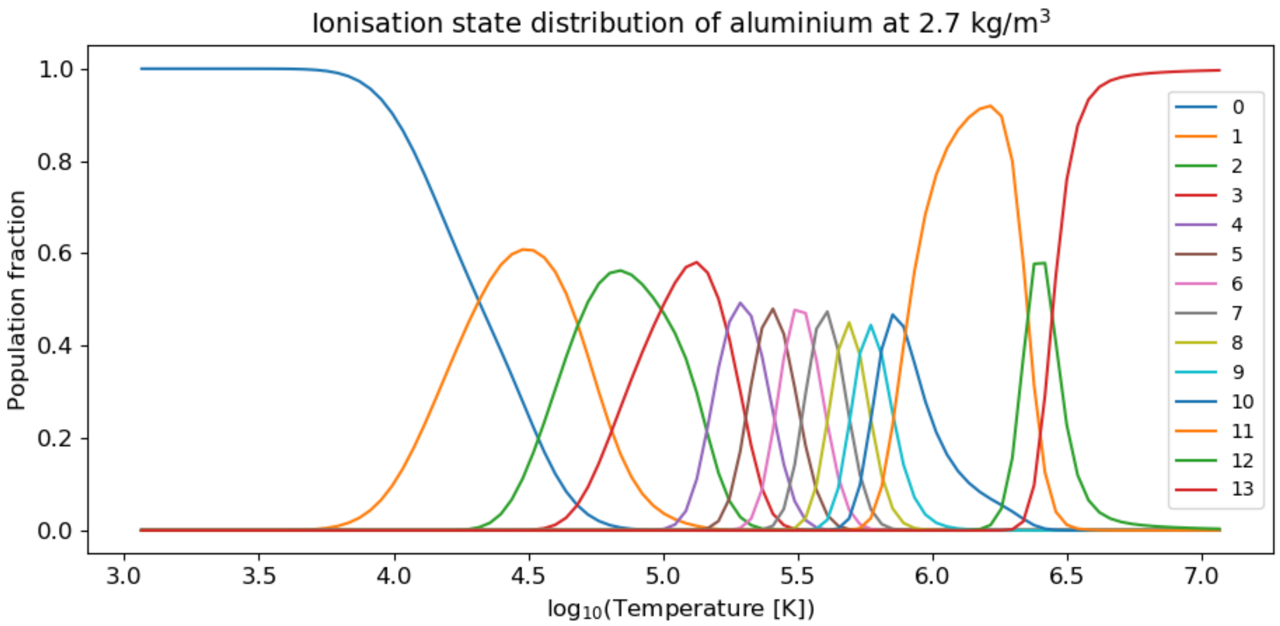
SpK – Saha solver and opacity calculations complete

- First developed by Dr Nicolas Niasse

- Full multi-species ionisation equilibrium calculations up to n = 10

  → Distribution of ionisation states

  + level populations



SpK – Saha solver and opacity calculations complete

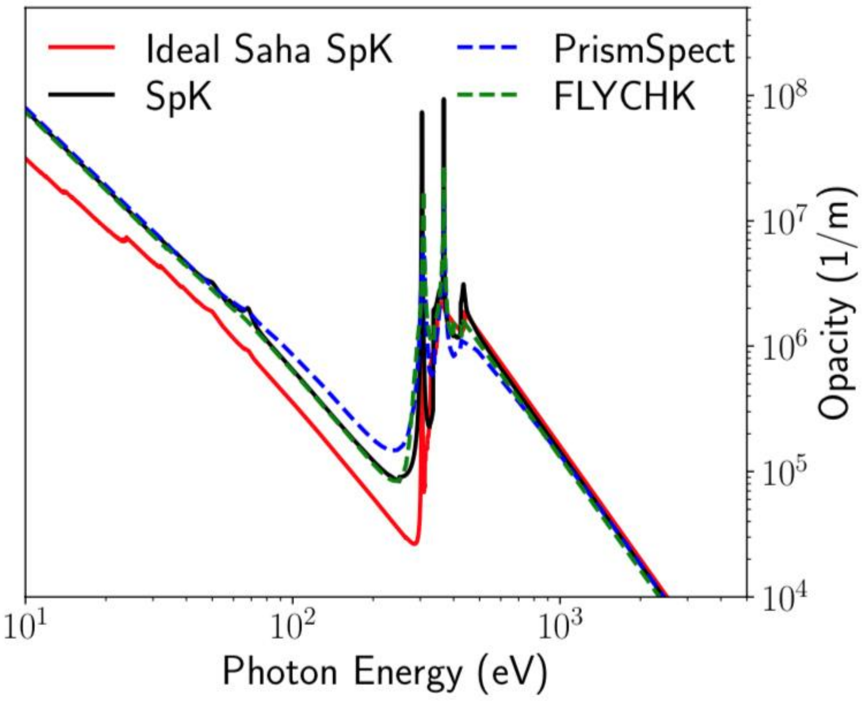
- First developed by Dr Nicolas Niasse

- Full multi-species ionisation equilibrium calculations up to n = 10
  - → Distribution of ionisation states + level populations

- Non-ideal contributions to partition function through IPD and plasma microfields

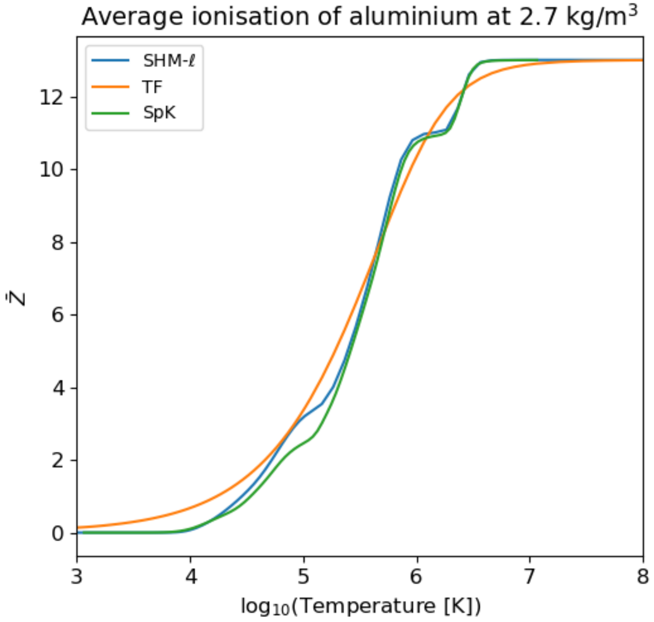
- Performs well relative to other commercial codes

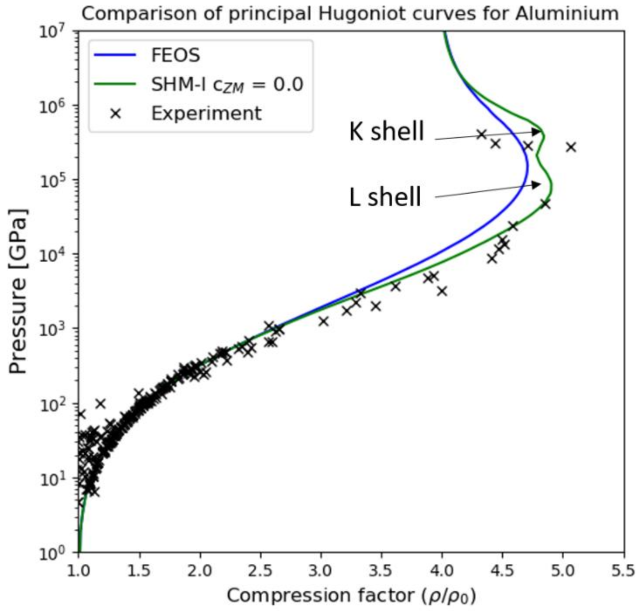
Carbon opacity at 1,000 kg/m^3 and 100 eV



SHM-ℓ – EoS already implemented

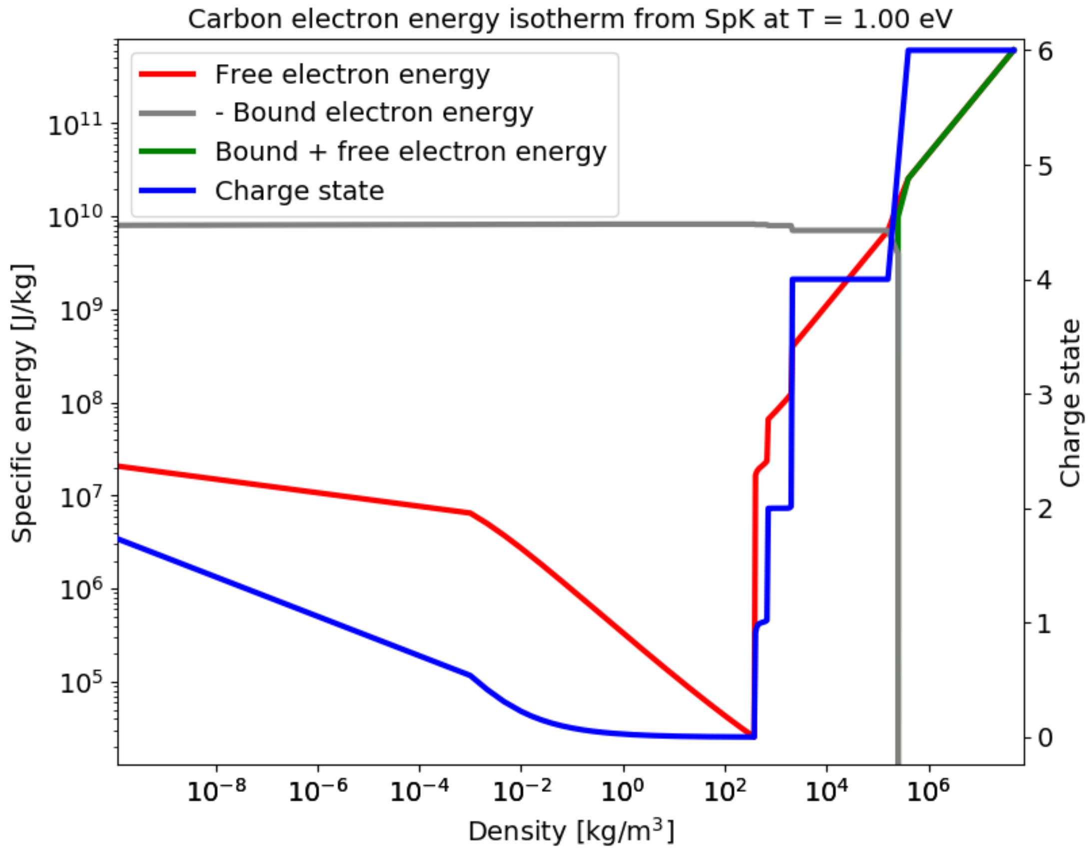
- $F_e = F_{free} + F_{bound} + F_{IPD}$
- Cowan model for ions
- Hugoniot calculations performed with clear demonstration of shell structure
- Issues: mono-elemental, blended with FEOS at low T, partial occupations
- Similar formalism can be used to develop SpK further





SpK – EoS progress

- $F_e = F_{free} + F_{bound} + F_{IPD}$
- F_{free} complete
- F_{bound} in progress
  - Need to establish thermodynamic contribution of plasma microfields
- Need to derive the contribution to the EoS by the bound states and the IPD, ensuring thermodynamic consistency.

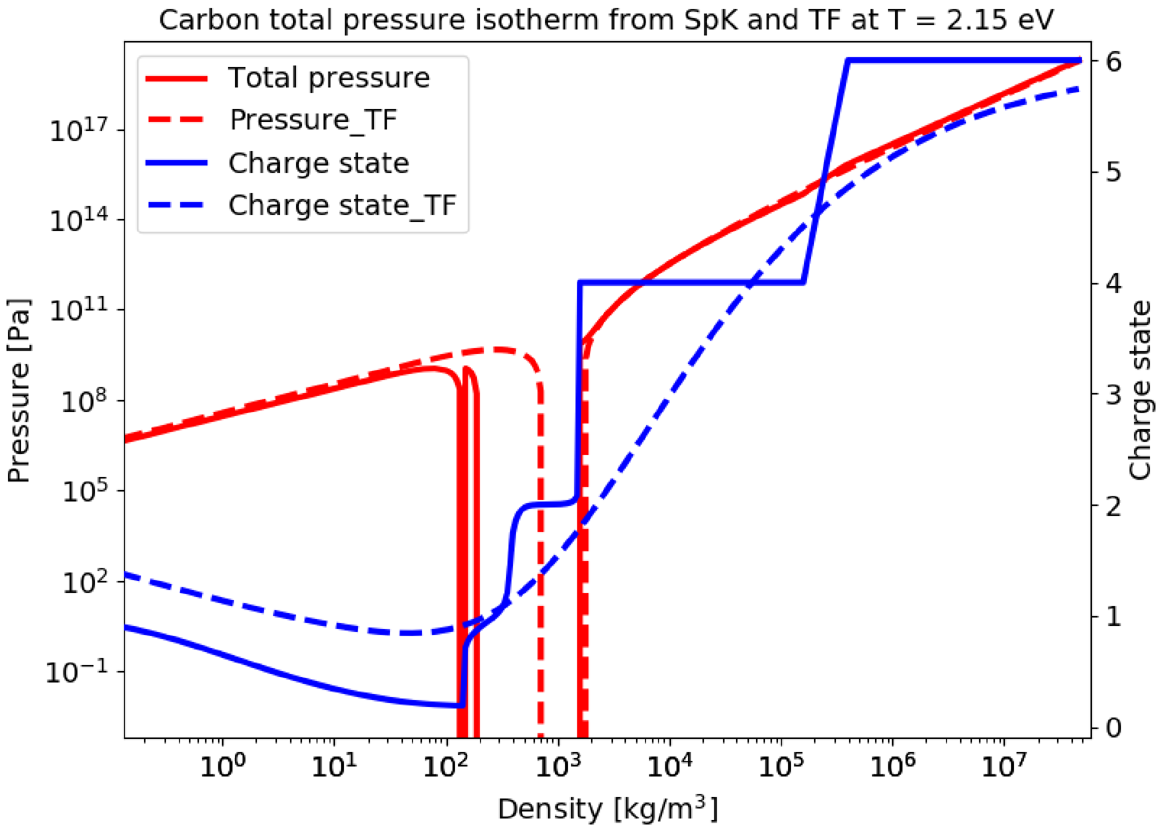


SpK – challenges

- Want to attempt to create full EoS table spanning all material phases

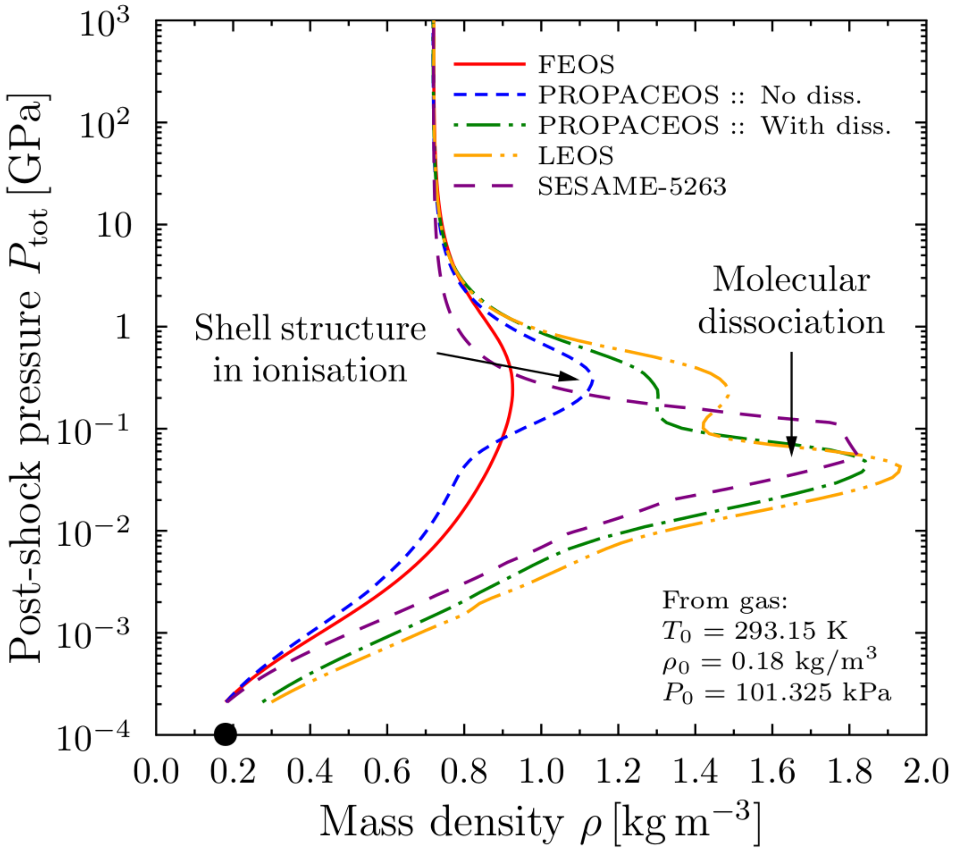
- Introduced bonding correction from FEOS:
  - Discontinuous jumps in pressure arising from shell structure lead to multiple spinodal curve solutions

- This will make performing a Maxwell construction difficult



Next stages – Maxwell construction and molecular dissociation

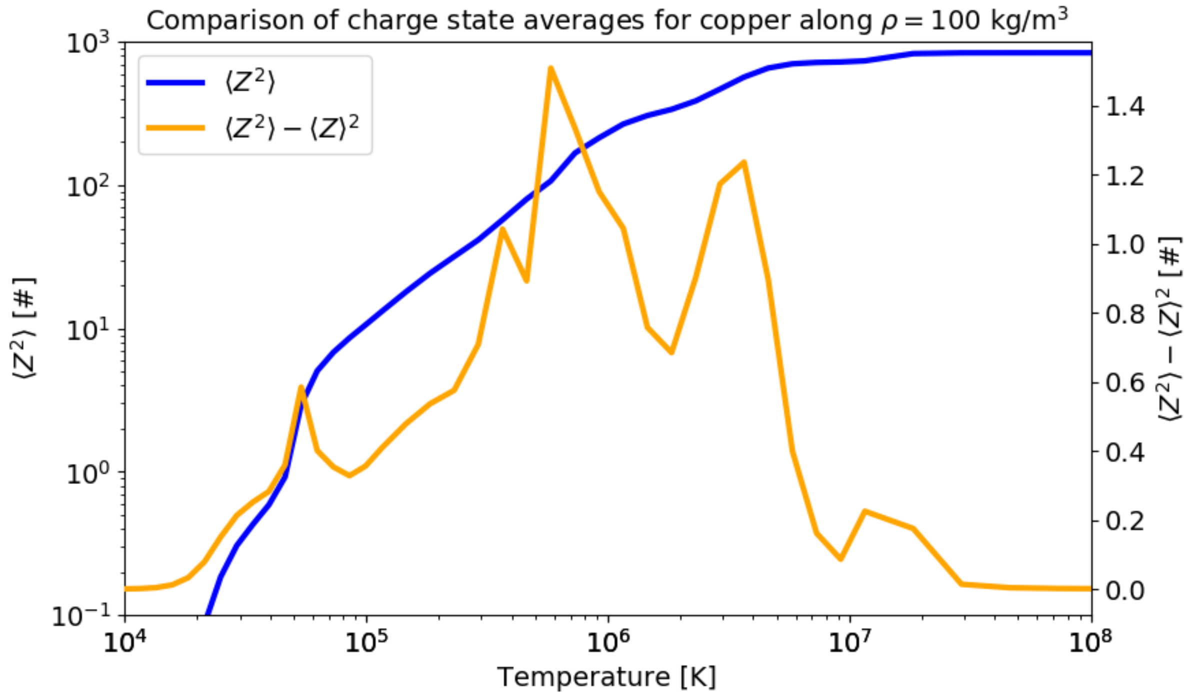
- Full thermodynamic consistency for all partition function components
- Improved bonding correction + Maxwell construction (if possible)
- Inclusion of molecular + dissociation physics
- Transport tables using appropriate ensemble averages of charge states
  (See Dave Chapman et al., TM12.00003)
- Implementing HNC to develop improved ion EoS



Chapman, D., *et al.*
FLF Internal report 0333 (2019).

Next stages – Maxwell construction and molecular dissociation

- Full thermodynamic consistency for all partition function components
- Improved bonding correction + Maxwell construction (if possible)
- Inclusion of molecular + dissociation physics
- Transport tables using appropriate ensemble averages of charge states
  (See Dave Chapman et al., TM12.00003)
- Implementing HNC to develop improved ion EoS



Summary

- Multiple physical processes at play in HEDP experiments
  - ➢ Requires self-consistent calculation for accuracy and epistemological purposes

- Development of SpK in progress to satisfy these requirements:
  - ➢ Saha solver including non-ideal physics
  - ➢ Corresponding opacity calculations
  - ➢ EoS development in progress
  - ➢ Access to full distribution of ionisation states for use in transport calculations