BurnMan $\leftrightarrow$ ENKI?

Interdisciplinary thermodynamic modelling

ENKI Workshop, May 25th 2017

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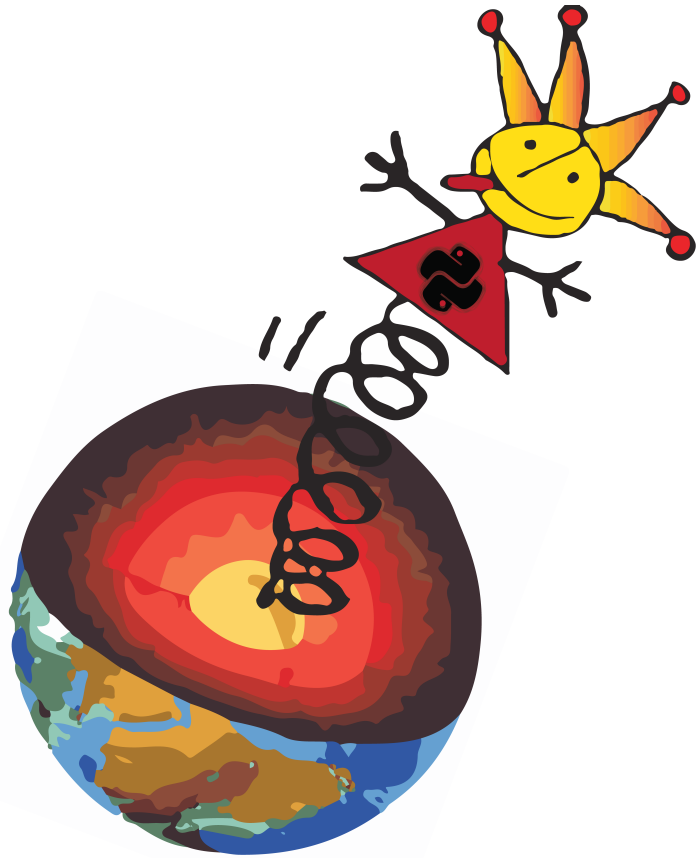
What is BurnMan?

- Open-source, peer-reviewed thermoelastic and thermodynamic toolkit, written in Python (Cottaar et al., 2014)
- Over 100 unit tests, ca. 30 examples and thorough database benchmarks
- Modular, readable, fully commented, every line of code reviewed



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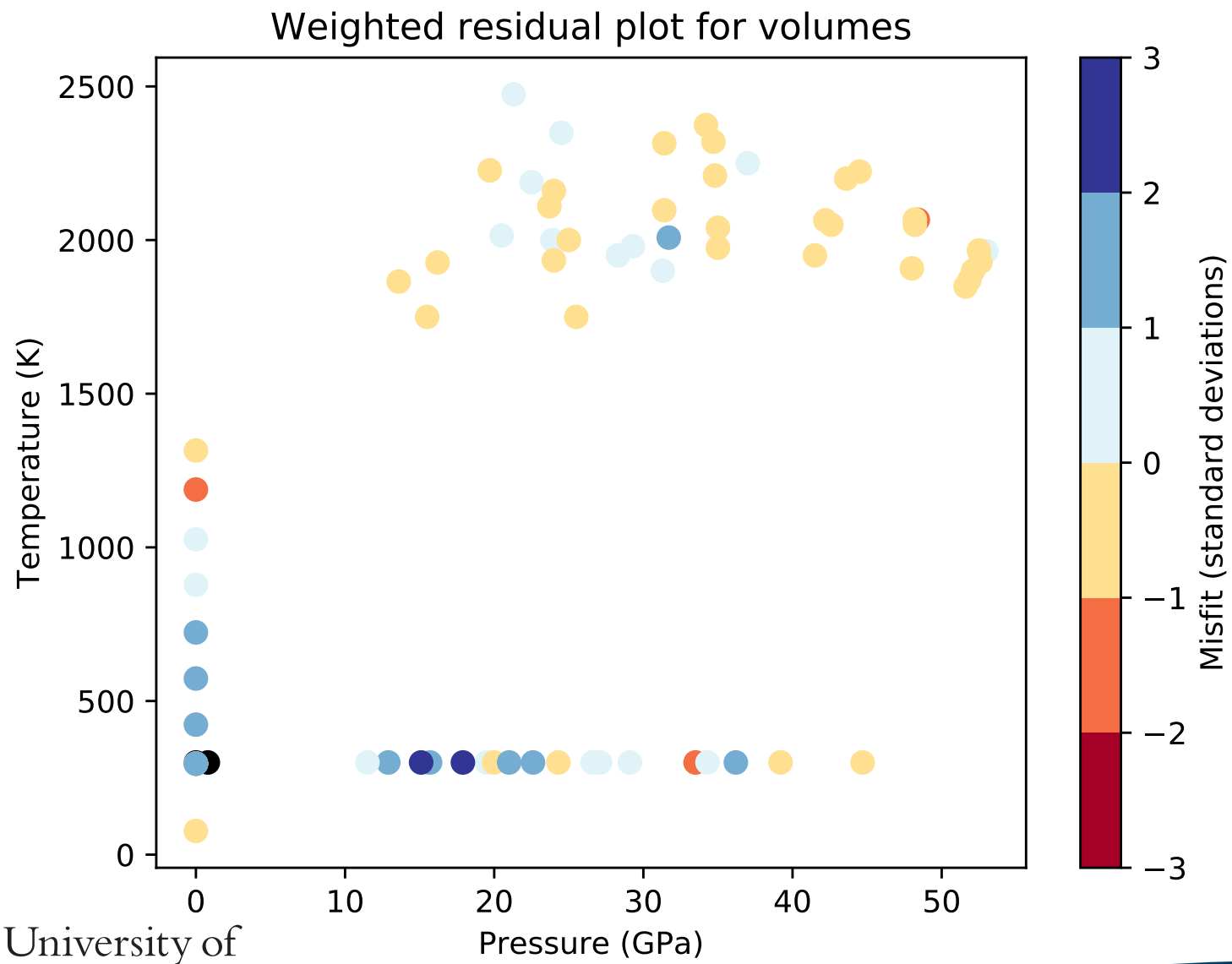
Some examples

- Initiation of endmembers, solutions and rocks
- Phase diagram construction
- EoS fitting with any measured variables (including enthalpy data)
- Output for geodynamics software

EoS fitting; the need for good visual tools



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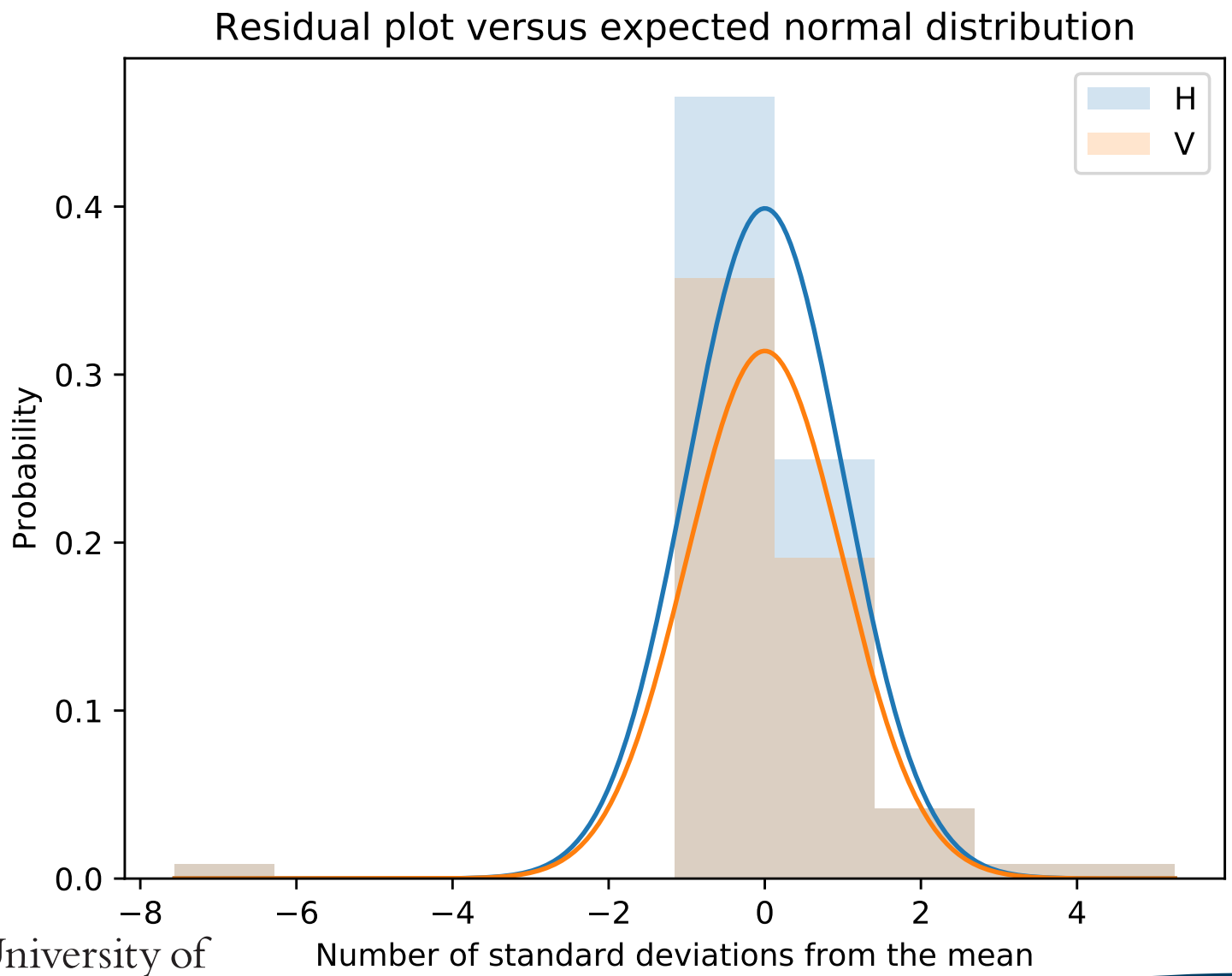

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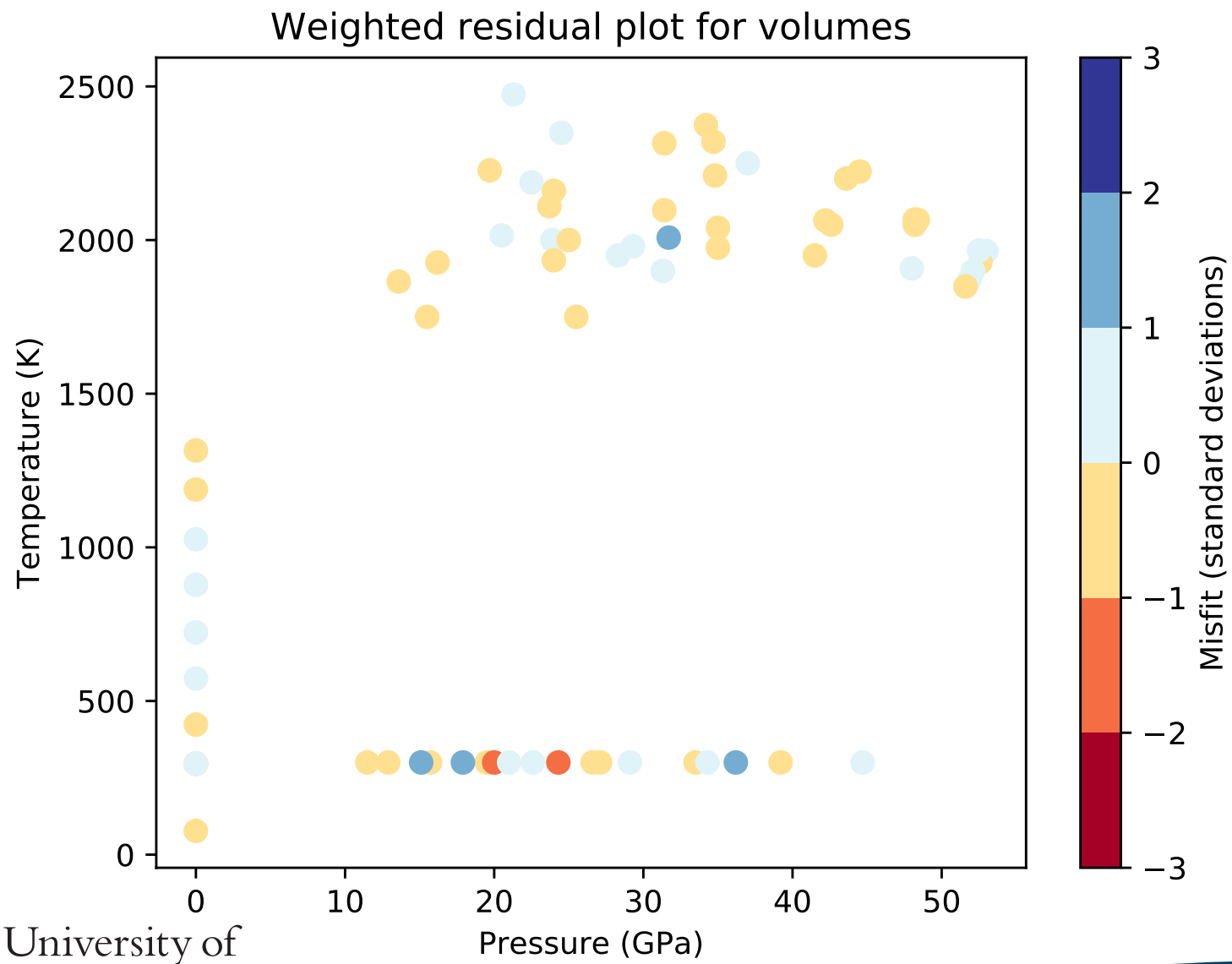
EoS fitting; dealing with bad data



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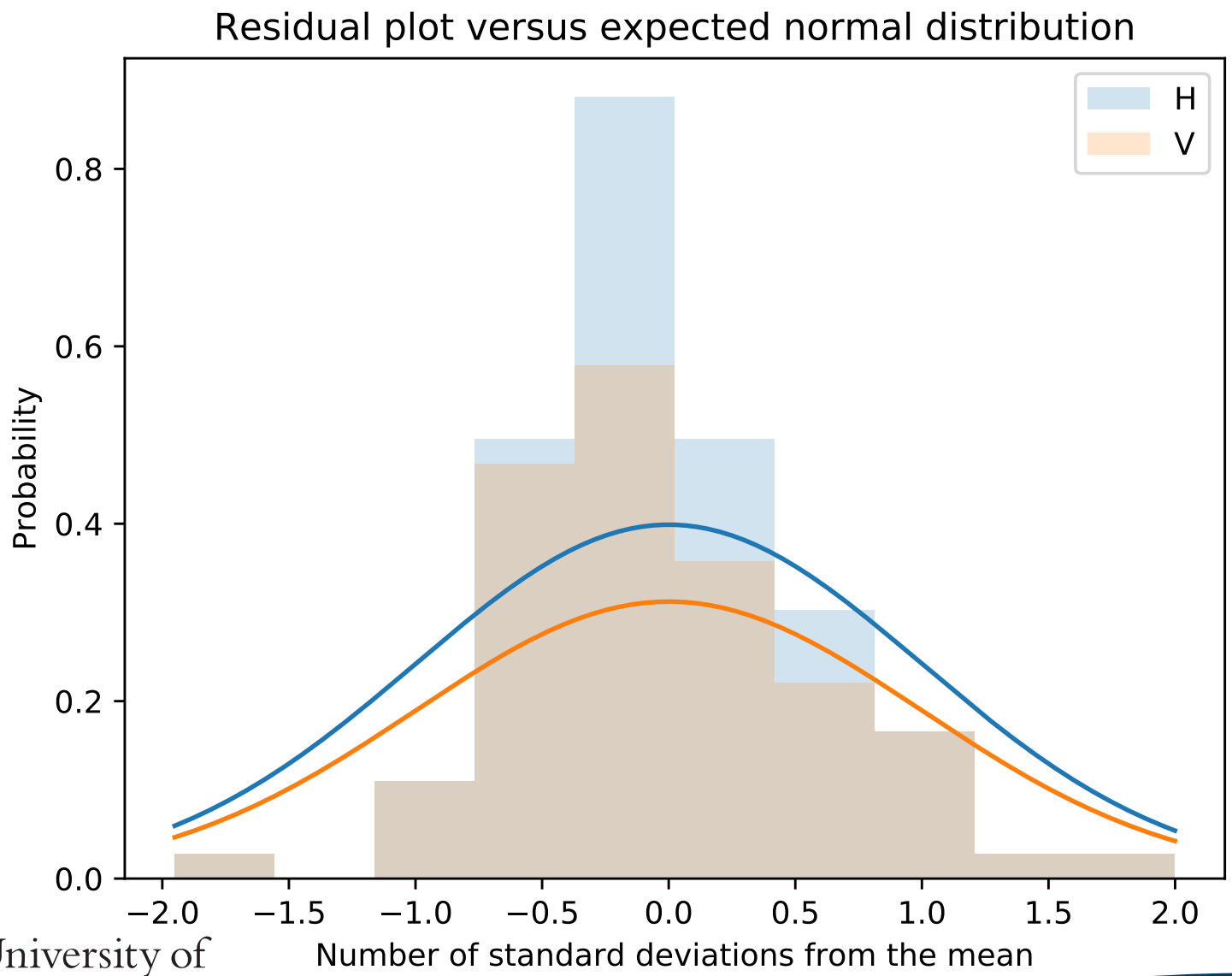

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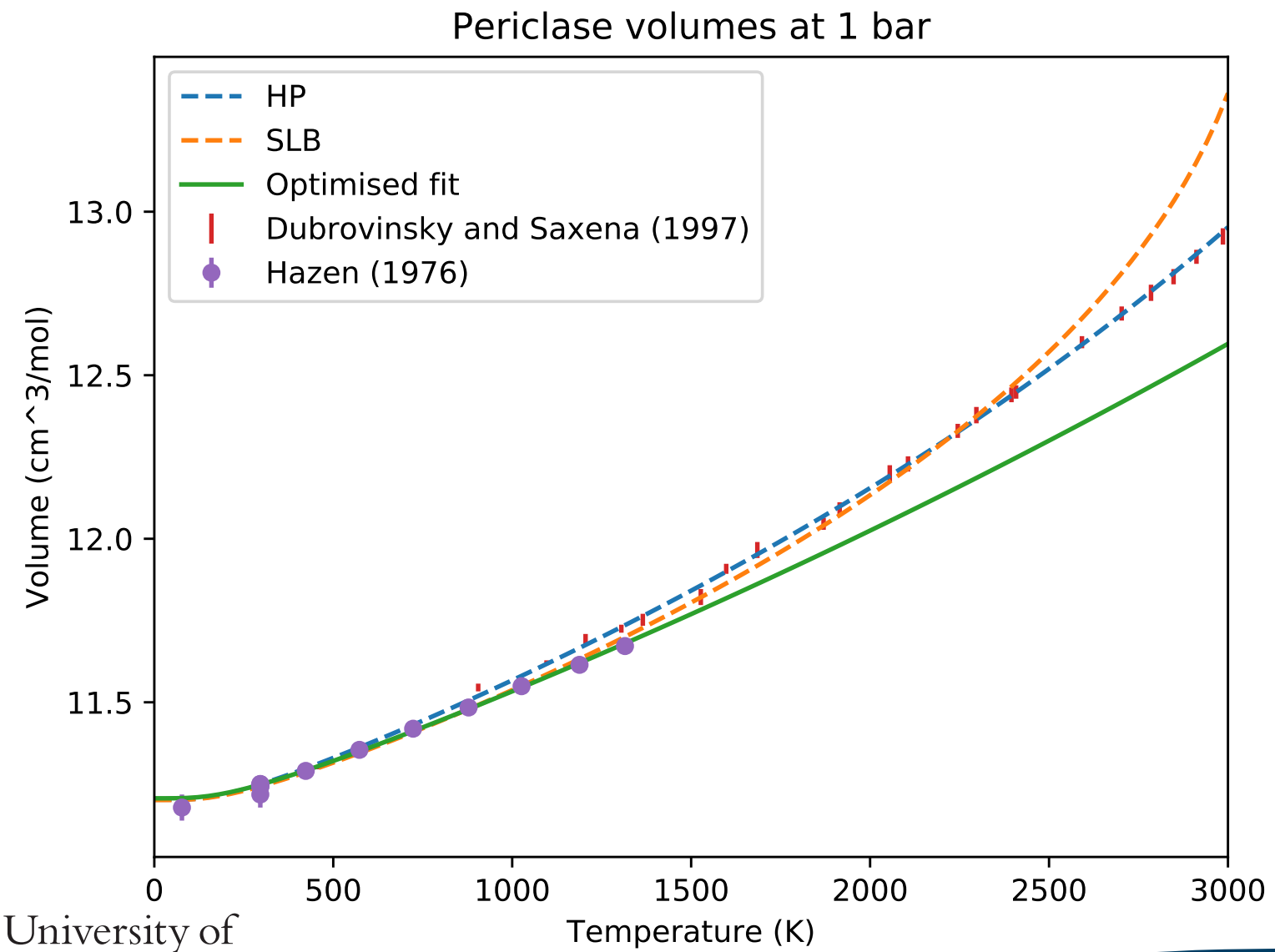
EoS fitting; a view to better results



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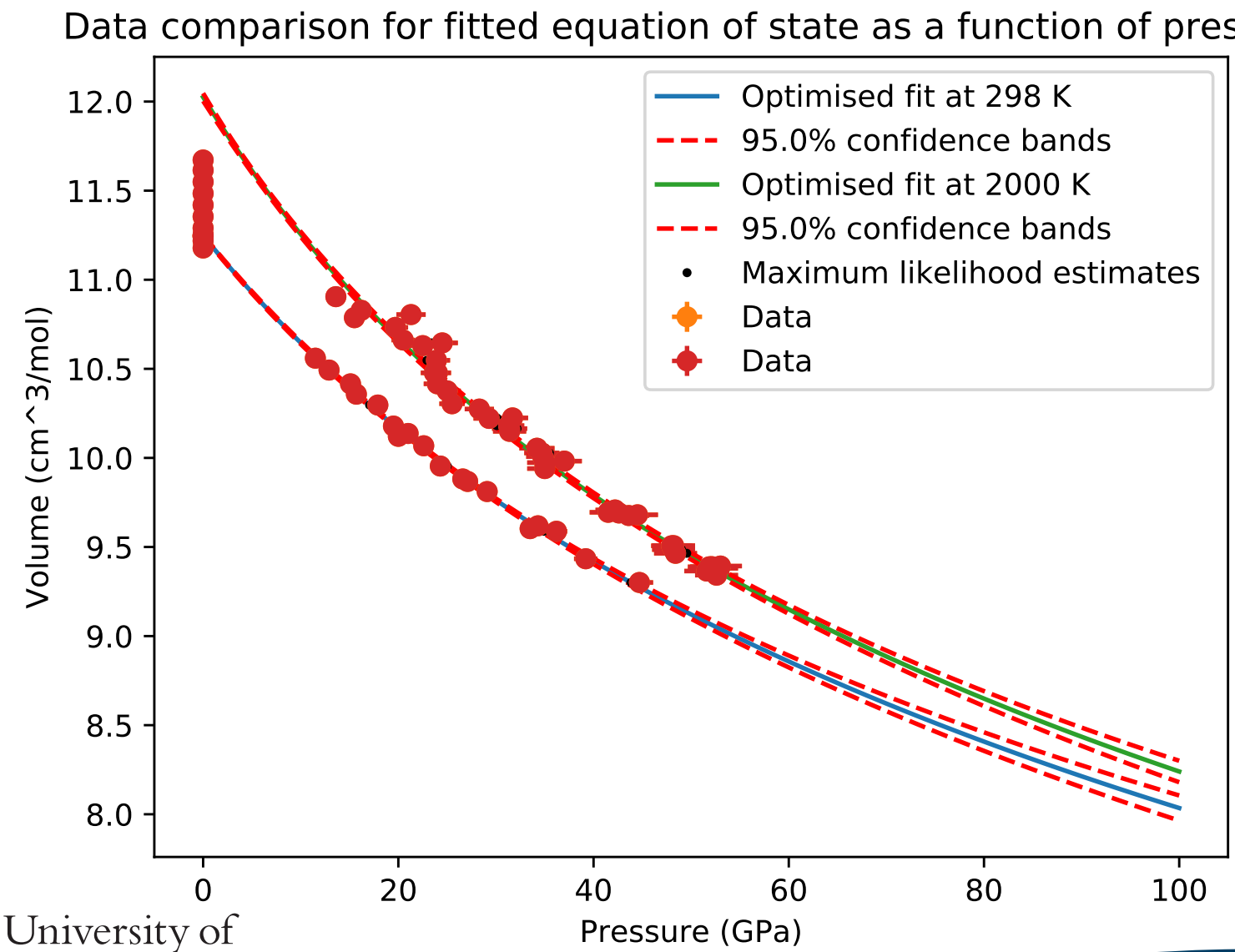

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The future?

Work in progress:

- Quasichemical and associated liquid solution models
  (because FactSAGE is $6000/license)
- Intracrystalline relaxation
  (for spin transitions, rapid order-disorder transitions)
- Output to seismic synthetics codes (DSM, AxiSEM, SpecFEM)

The future with ENKI:

- Use of low level libraries (to improve speed)
- Continued development of high level functions?