

Introduction to pycalphad

Richard Otis

Materials Genome Foundation

June 28-29, 2021

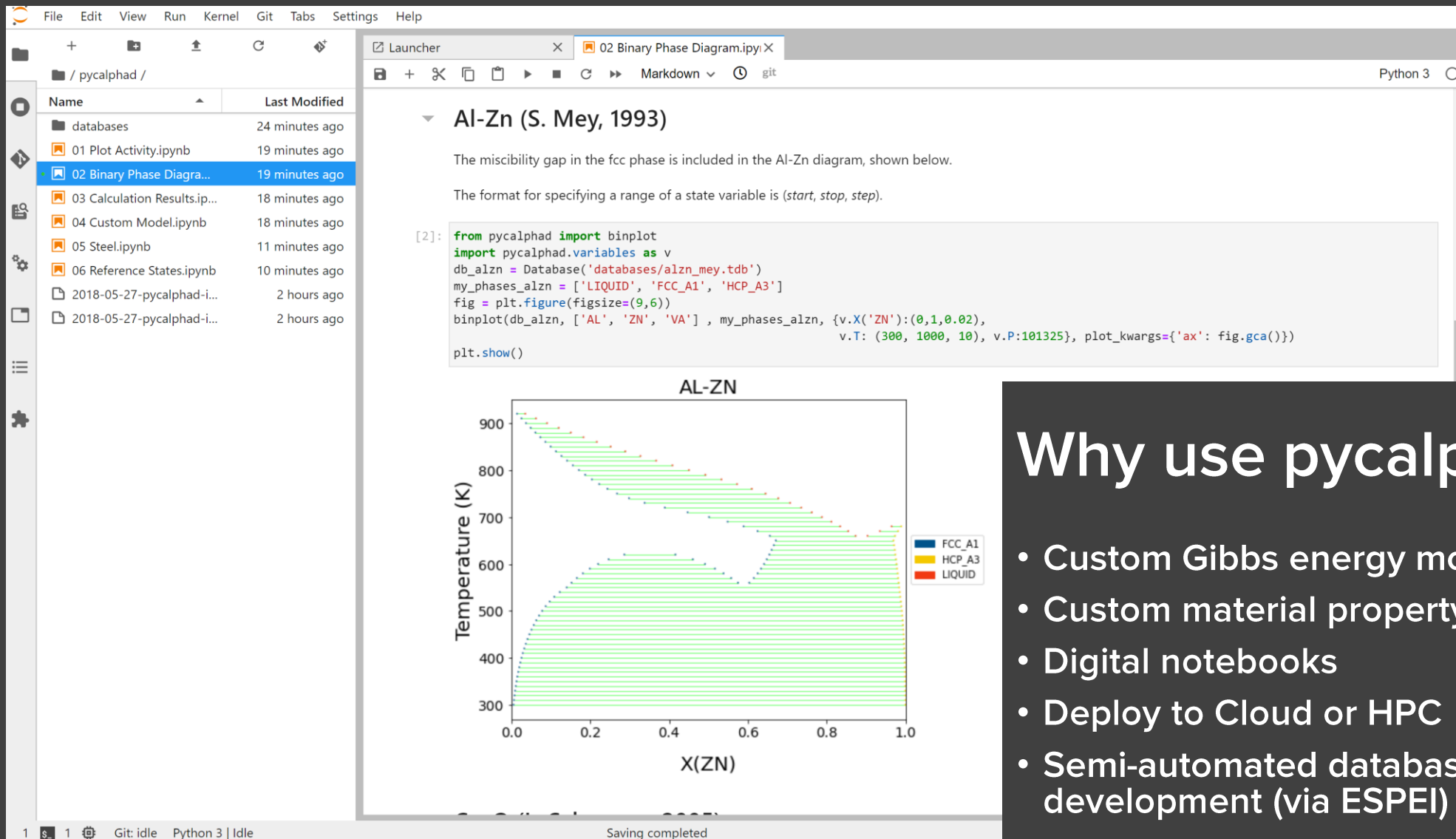
PyCalphad/ESPEI Virtual Workshop



pycalphad = Python + CALculation of PHAse Diagrams

- pycalphad is software for designing thermodynamic models, calculating phase diagrams and investigating phase equilibria.
- Using CALPHAD-based models, pycalphad predicts properties of materials, including
 - Transition (e.g., melt) temperatures, phase fractions, solidification, degradation, corrosion, etc.
 - Anything that can be connected to a chemical or thermodynamic process
- Free and open source at pycalphad.org





Why use pycalphad

- Custom Gibbs energy models
- Custom material property models
- Digital notebooks
- Deploy to Cloud or HPC
- Semi-automated database development (via ESPEI)

Notable Features in pycalphad 0.9

- Improved performance, nearly zero calculation start time
- Preliminary support for ‘local’ equilibrium calculations
- User-specified reference states
- Binary and ternary phase diagram plotting
- T , P , μ_i , x_i conditions with multiple components
- Step/map calculation, global minimization
- Support for associates and ionic liquids
- IHJ and Xiong magnetic models
- Order-disorder model, Two-state model, Einstein model
- Windows, Mac, and Linux support



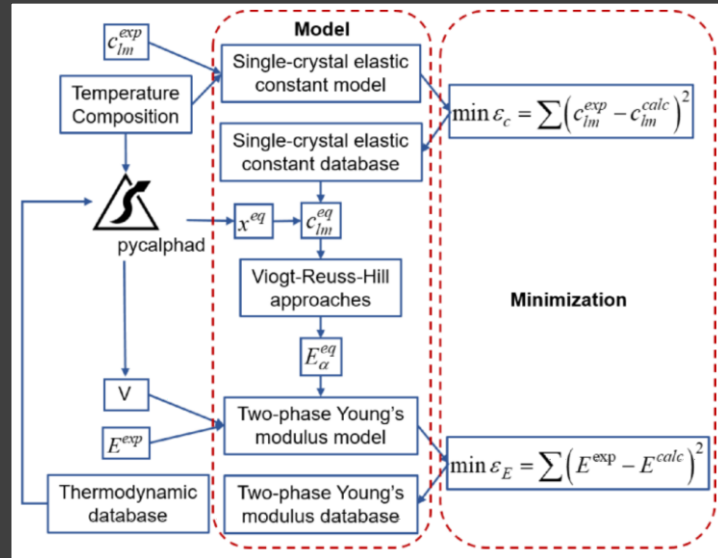
Current Limitations in pycalphad 0.9

- In progress: “Advanced” conditions (e.g., amount of a phase)
- In progress: Quasichemical model
- A few TDB features are unsupported (Option “B”, Option “F”, STATUS_BITS, etc...)
 - Contact us: we can usually help you work around the issue



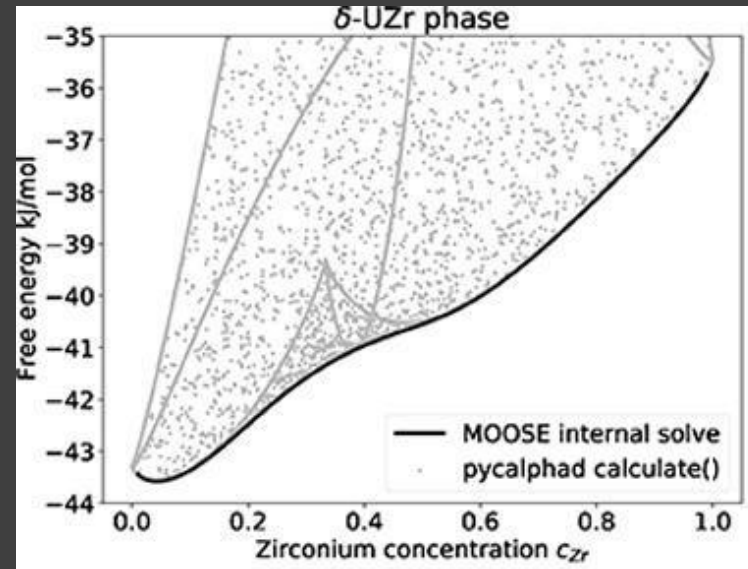
PyCalphad Community Selected Use Cases

Two-phase Elastic Constants



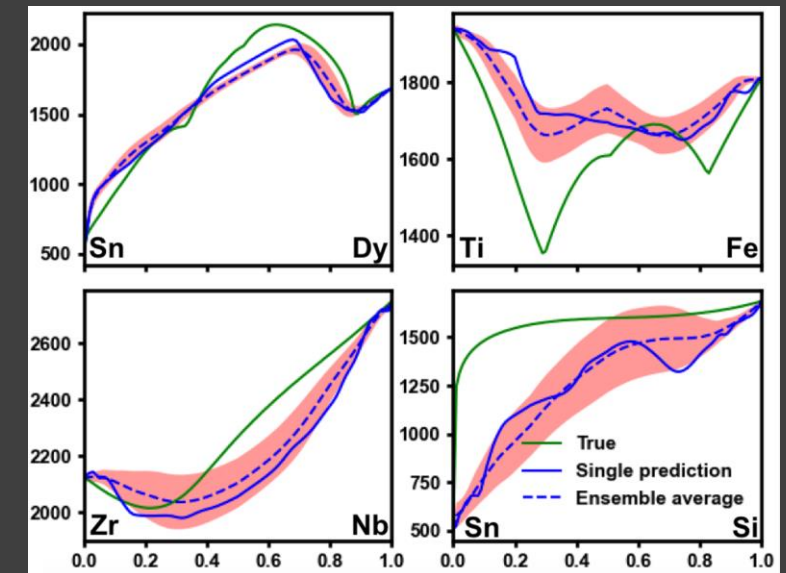
Y. Shang, et al., *Materialia* **8**, 100500 (2019)
doi: 10.1016/j.mtla.2019.100500

Multi-scale Coupling



D. Schwen, et al., *Comp. Mat. Sci.* **195** (2021)
doi: 10.1016/j.commatsci.2021.110466

Machine Learning



P. Guan and V. Viswanathan (2020)
arXiv:2010.14048v1



Agenda

- Plot thermodynamic activities
- Binary phase diagrams
- Manipulating calculation results
- Custom models
- 'Local' equilibrium computation
- Liquidus temperature
- Scheil solidification
- Setting reference states
- Q&A



Contact Us

richard.otis@materialsgenomefoundation.org

pycalphad.org

Chat with us on Gitter!

gitter.im/pycalphad/pycalphad

