Introduction to pycalphad

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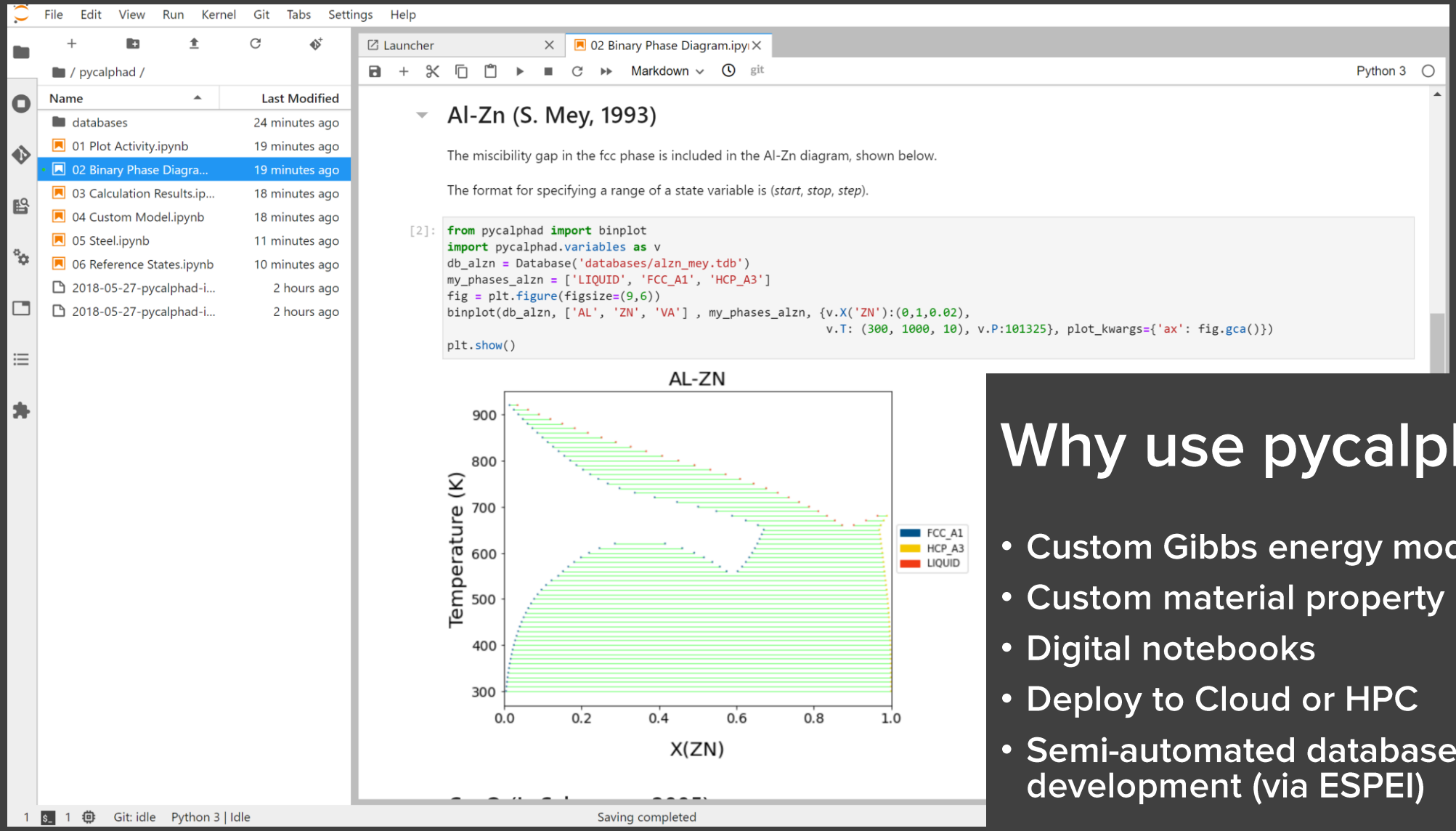
pycalphad = Python + CALculation of PHAse Diagrams

- 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)

R. Otis and Z-K. Liu, “pycalphad: CALPHAD-based computational thermodynamics in Python”, *Journal of Open Research Software*, 5: 1 (2017)

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

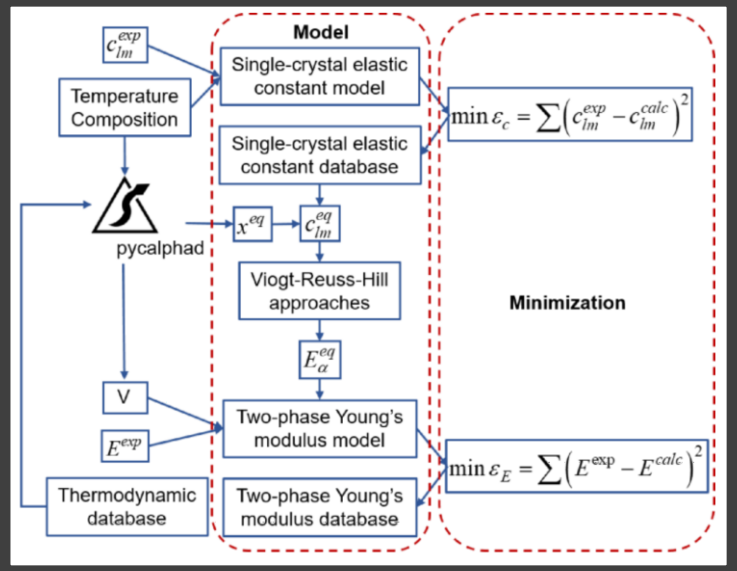
R. Otis, M. Emelianenko, Z. K. Liu, “An improved sampling strategy for global energy minimization of multi-component systems”, Comp. Mat. Sci. 130 (2017) 282–291.

Current Limitations in pycalphad 0.8

- 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

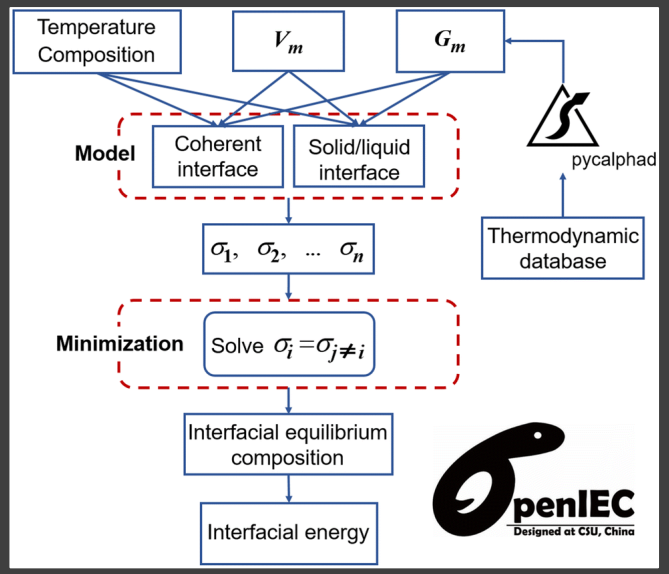
PyCalphad Community Selected Use Cases

Two-phase Elastic Constants



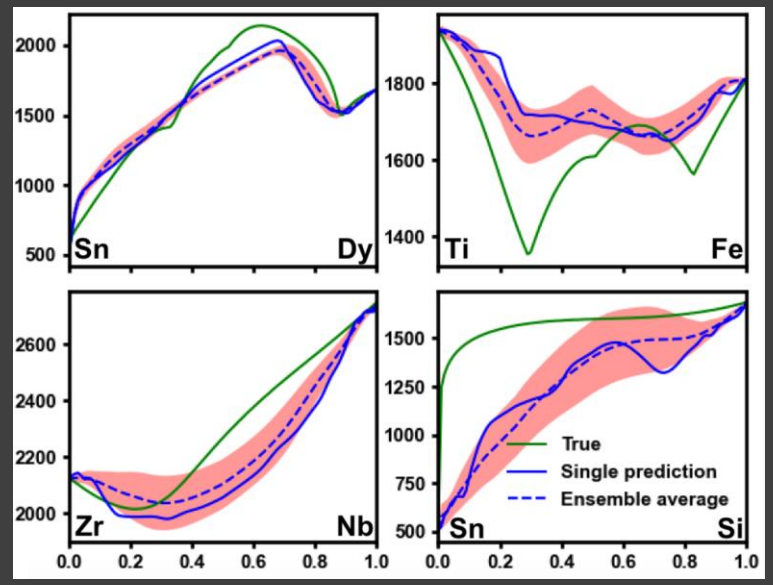
Y. Shang, et al., *Materialia* **8**, 100500 (2019)
doi: 10.1016/j.mtla.2019.100500

Interfacial Energy



S. Yang, et al., *J. Mat. Sci.* **54**, 10297–10311 (2019)
doi: 10.1007/s10853-019-03639-w

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

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pycalphad.org

Chat with us on Gitter!

gitter.im/pycalphad/pycalphad