Introduction to pycalphad

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About Materials Genome Foundation

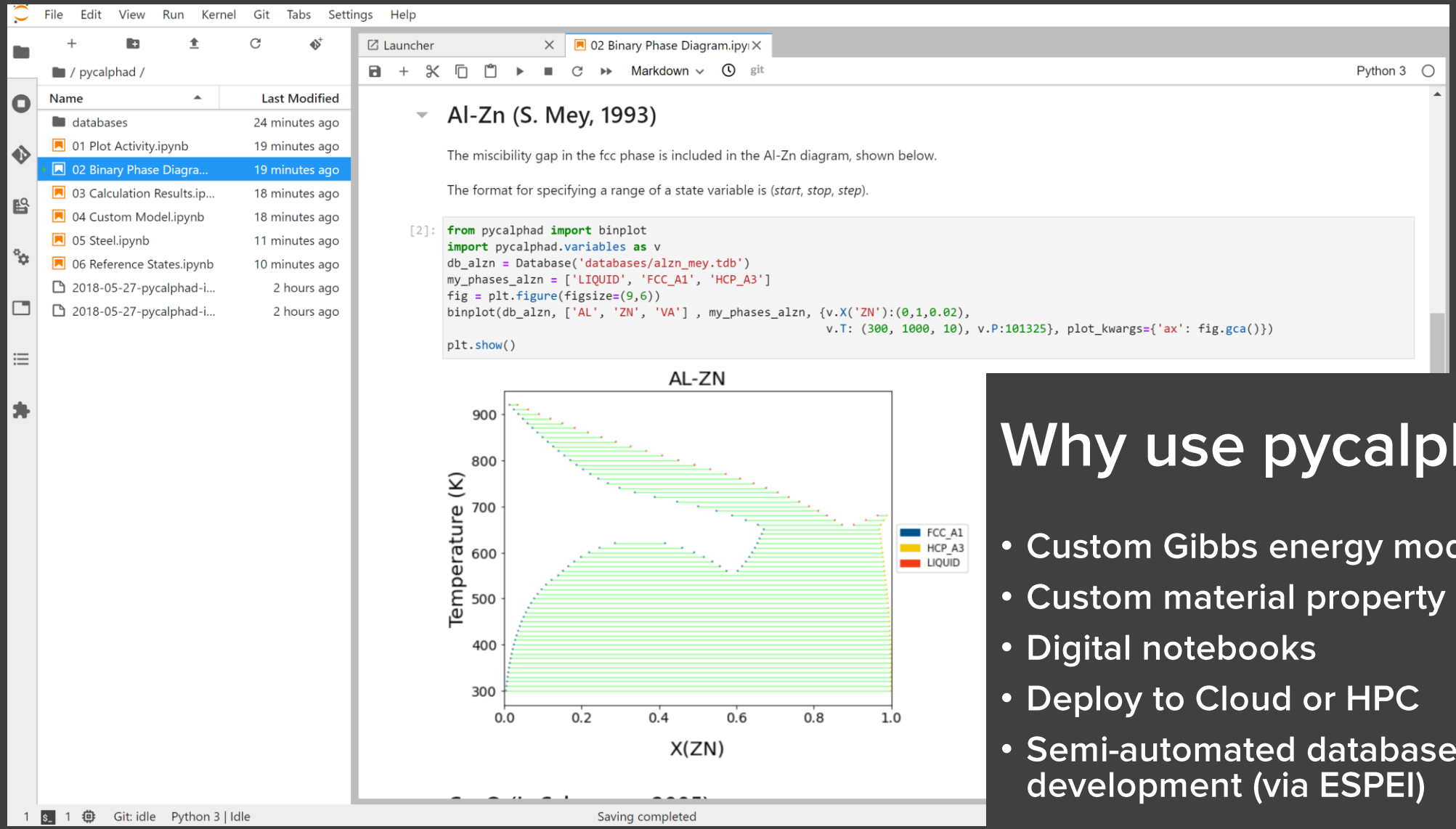
- A nonprofit organization founded in 2018 to promote development and evolution of software tools in materials science and engineering
- Key Goal: Bridge the gap between “one-off” academic scripts and software products
  - Documentation, Tests, Infrastructure / Continuous Integration, etc.
- Current activities focus on cloud-based interactive workshops and tutorials

Instructions for Cloud Environment

1. Go to https://workshop.mgfcloud.org/
2. Enter your email address. A code will be sent to that address.
3. Enter the code in the login form.
4. You will be redirected to an interactive cloud environment.
5. Note: Storage is persistent for the duration of the 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)

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 0.10

- Improved performance, nearly zero calculation start time
- Preliminary support for ‘local’ equilibrium calculations
- T, P, μ_i, x_i conditions with multiple components
- Step/map calculation, global minimization
- Support for associates and ionic liquids
- Support for solid phases with charged species
- Support for modified quasichemical model and DAT files
- Phases with symmetry (‘Option B/F’)
- Windows, Mac, and Linux support

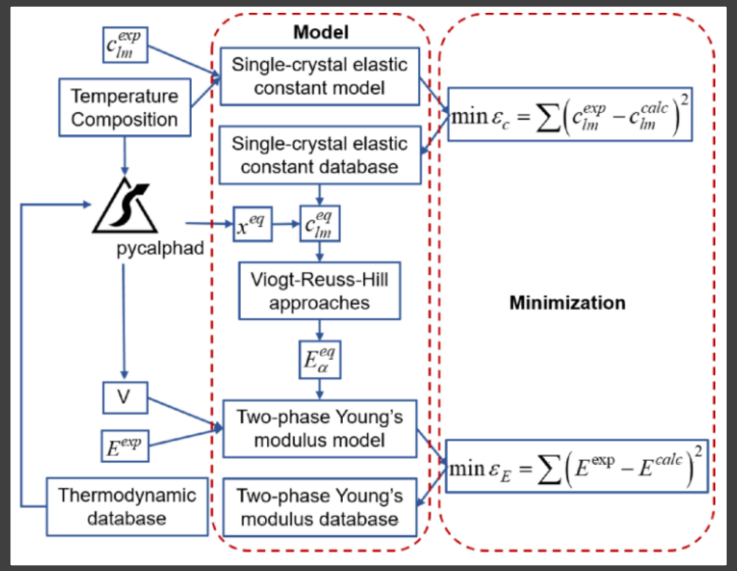
R. Otis, M. Emelianenko, Z. K. Liu, “An improved sampling strategy for global energy minimization of multi-component systems”, Comp. Mat. Sci. 130 (2017) 282–291.

Current Limitations in pycalphad 0.10

- In progress: Better phase diagram mapping
  - Will improve resolution of narrow phase boundaries, ternary isotherms, and isopleths
- In progress: DAT file writing
- In progress: Derivatives of thermodynamic properties (liquidus slopes, etc.)
- In progress: T0 calculation
- In progress: New “Computable Property Framework”
  - Simplify calculation and visualization of any property, including custom properties
  - Better support for metastability (driving force calculation, etc.)
  - Physical units and automatic unit conversion (temperature scales, gram-to-mole, etc.)

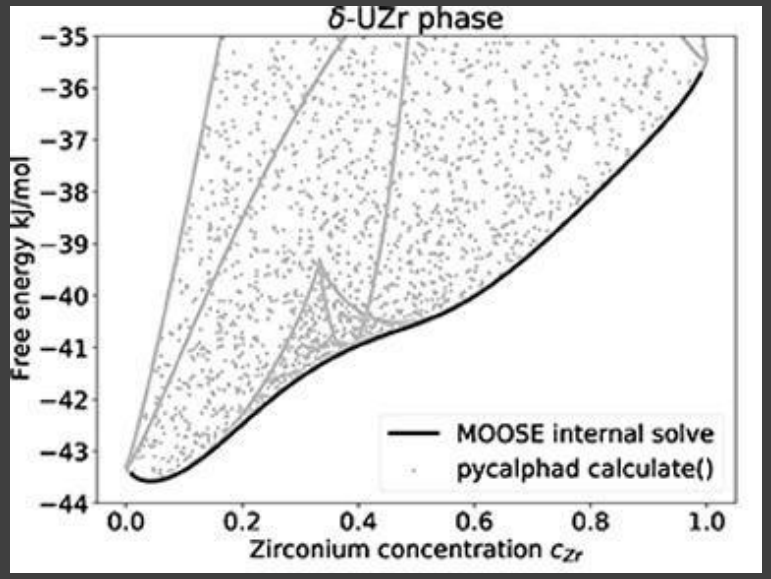
PyCalphad Community Selected Use Cases

Two-phase Elastic Constants



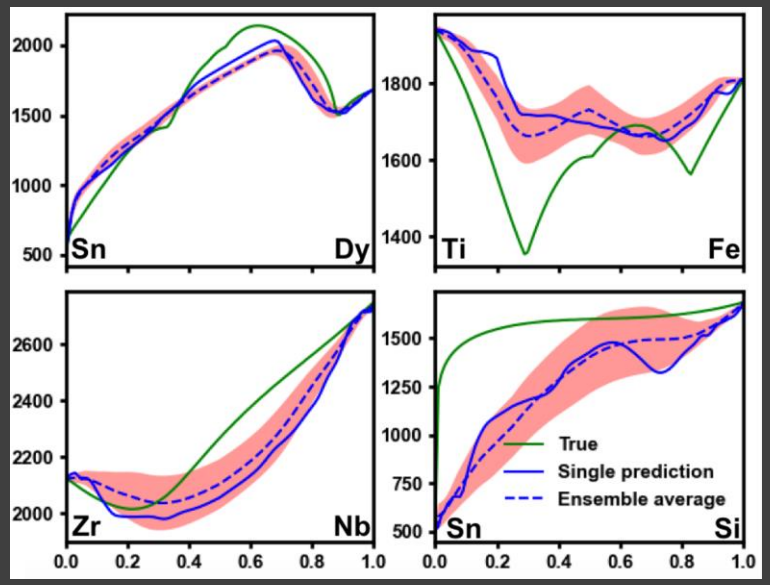
Y. Shang, et al., *Materialia* **8**, 100500 (2019)
doi: 10.1016/j.mtla.2019.100500

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
- Charged species
- Q&A

Contact Us

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pycalphad.org

Chat with us on Gitter!

gitter.im/pycalphad/pycalphad