Pycalphad and ESPEI Workshop and Tutorial

Brandon Bocklund and Richard Otis

Sunday, May 27, 2018

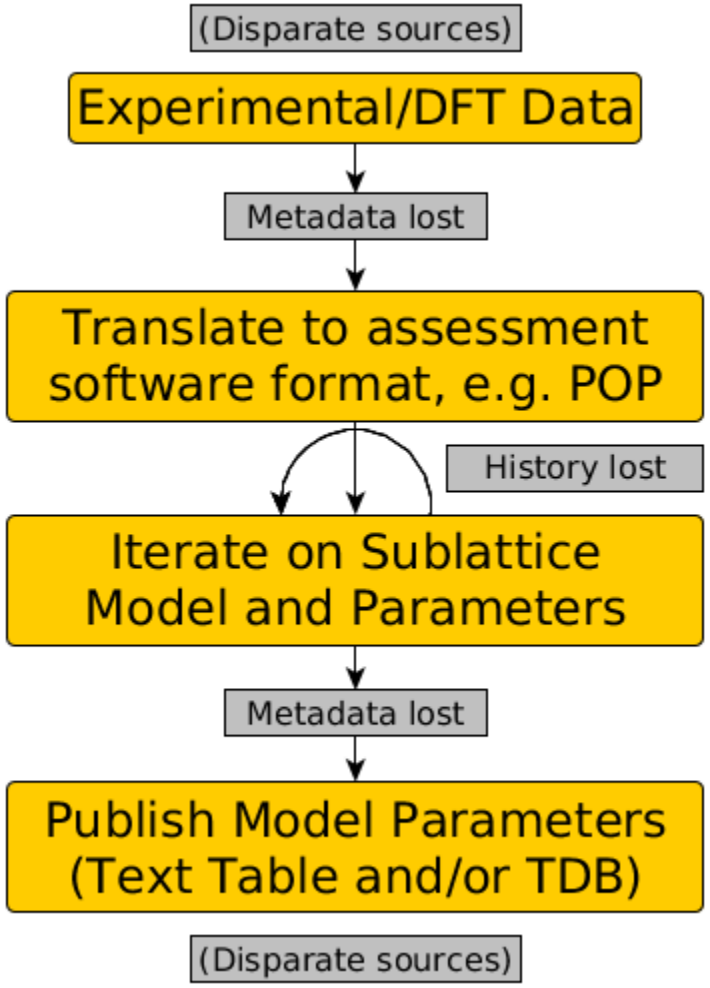
CALPHAD XLVII

Agenda

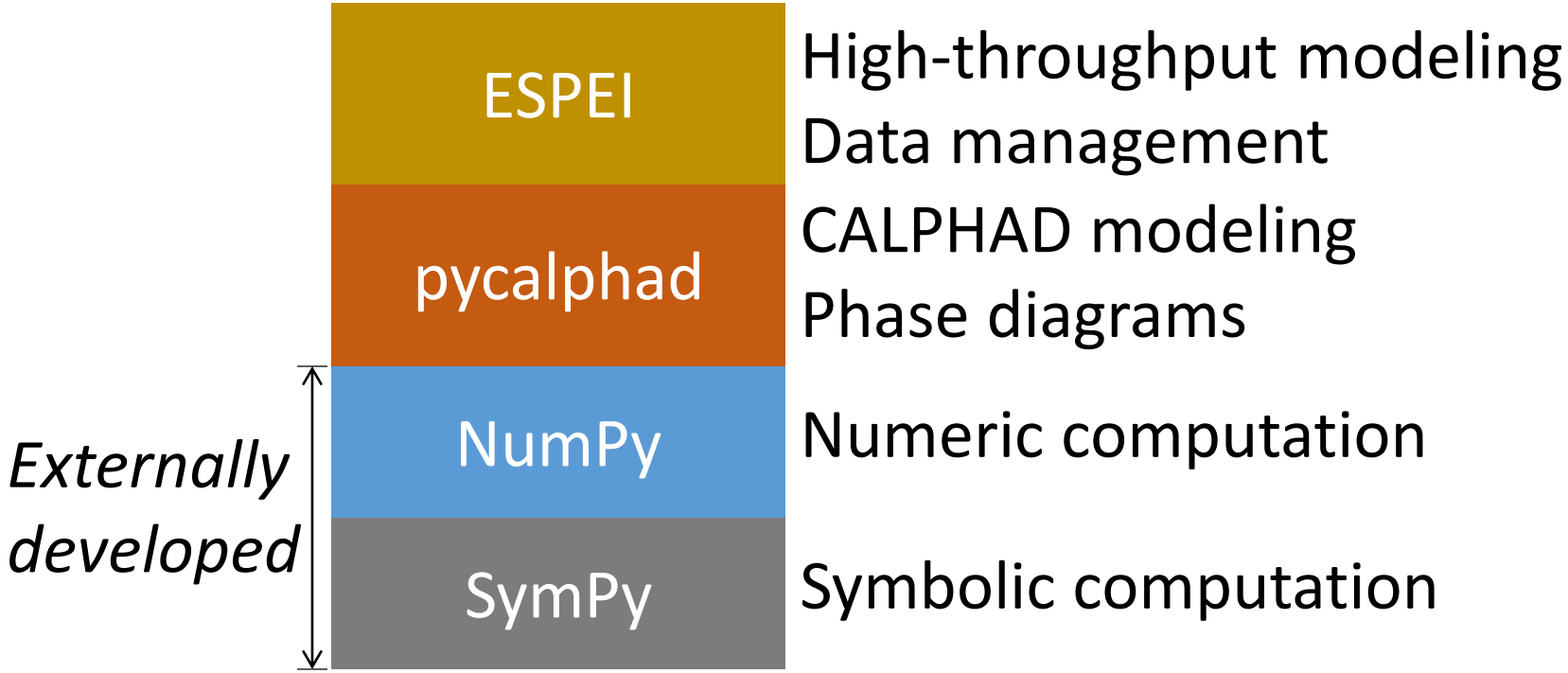
- 9:00 – 9:10: Introduction and Welcome
- 9:10 – 9:40: Software Installation
- 9:40 – 10:00: Python Crash Course
- 10:00 – 10:55: pycalphad Tutorial
- 10:55 – 11:10: Coffee Break
- 11:10 – 11:55: ESPEI Tutorial
- 11:55 – 12:00: Participant Feedback

CALPHAD Data Challenges

- Data fragmentation
- Data standards
- Workflow tools
- Uncertainty quantification
- **Reproducibility**



The ESPEI (Simplified) Software Stack



Team and Project History

- Richard Otis created pycalphad in 2014, under a NASA Space Technology Research Fellowship. He graduated Penn State in 2016.

- Brandon Bocklund (PSU) joined the team in 2016. He is the lead developer of ESPEI and a co-developer of pycalphad.

- Prof. Zi-Kui Liu (PSU) advises on both projects and leads public outreach efforts.

Goals for Workshop

- Interactively learn the basics of how to use the ESPEI stack
  - Not expert-level, but enough to ask good questions!
- Learn how to make your CALPHAD workflow more shareable and reproducible
- Understand how pycalphad and ESPEI fit into the materials modeling ecosystem

Software Installation

- 1. Download from https://app.box.com/folder/49757976049 or copy from USB
- 2. Double-click to run and follow installation instructions
  - Accept license agreement and use default options
- 3. Copy the workshop files to somewhere in your HOME directory
- Linux users: You may need to add `$HOME\workshop-installer` to your PATH manually before the next step
- 4. Open command prompt or terminal and
  - Windows: Run `jupyter-notebook %USERPROFILE%`
  - `Linux/Mac:` Run `jupyter-notebook $HOME`

If you need help, please ask!