

Workshop: Open-Source Software for Computational Thermodynamics and Kinetics Modeling

Course Description: This workshop will give a detailed introduction to CALPHAD-type computational thermodynamics and kinetics software within the PyCalphad ecosystem. It will feature hands-on exercises in an interactive cloud environment that will enable attendees to calculate phase diagrams, simulate solid-state precipitation of alloys, and to propagate uncertainty in thermodynamic calculations. **Attendees are encouraged to bring their laptop or computing device to follow along interactively.** Tables, power outlets, and WiFi will be provided.

Course Goal: After following along with the provided exercises, attendees will complete the course with new tools in-hand, ready to take home.

Course Audience: Engineers and practitioners interested in learning more about open-source materials design tools.

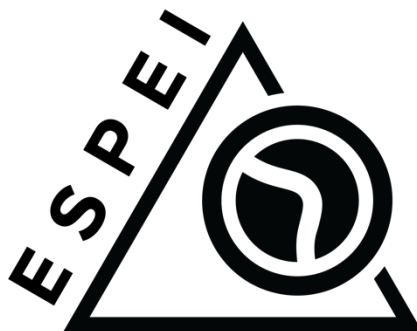
PyCalphad

PyCalphad is a free and open-source Python library for calculating phase diagrams, designing thermodynamic models, and investigating phase equilibria within the CALPHAD method. It provides routines for reading thermodynamic databases and solving the multi-component, multi-phase Gibbs energy minimization problem. All Gibbs energy and property models in PyCalphad are described symbolically allowing the models to be customized or overridden by users at runtime without changing any of the PyCalphad source code. Calculation results from PyCalphad are returned as multidimensional xarray datasets that make it easy to incorporate PyCalphad into any tool or workflow. New support for an imperative API, Jansson derivatives, and phase diagram mapping algorithms will be emphasized.



ESPEI

The Extensible Self-optimizing Phase Equilibria Infrastructure (ESPEI) package is a tool for thermodynamic database development and uncertainty quantification within the CALPHAD method. It uses PyCalphad for the forward calculation of thermodynamic properties to solve the inverse of the parameter evaluation problem. ESPEI uses a two-step method to first parameterize thermodynamic models and then optimize and determine the uncertainty of the parameters using Markov Chain Monte Carlo (MCMC). This workshop will highlight new capabilities in ESPEI for Calphad-type property modeling and for generating and optimizing mobility models from tracer and interdiffusivity data via Kawin.



Kawin

Kawin is a new open-source package providing support for Calphad-based precipitation and diffusion models. An overview of the organization and capabilities of the program is provided, along with an outline of the constituent physics. Kawin can simulate the bulk precipitation behavior of multiphase, multicomponent systems in response to complex heat treatments through the Kampmann-Wagner Numerical model. The inclusion of native strain calculations enables Kawin to predict the influence of internal or external stress fields on precipitation, as well as track the evolution of precipitate geometry throughout the course of a heat treatment. Kawin also provides multi-component support for single-phase diffusion and a homogenization model for multi-phase diffusion.

Kawin

The new property API decouples model parameters from the model implementation, which exposes implementation details, such as nucleation rate (precipitation models) or the mobility averaging functions (homogenization model), as well as allowing for easy initialization of multiple model instances by re-using defined parameter sets. As part of the new API, the single-phase diffusion and homogenization model supports custom mesh geometries, allowing users to go beyond a 1-D cartesian mesh and even to define their own meshes. Examples will be provided to show how precipitation and diffusion calculations can be set up and performed, as well as model coupling and creating custom parameters.

Agenda

Sunday, June 7

- 13:00 Opening and Introductions
- 13:15 PyCalphad
- 14:15 ESPEI
- 15:15 Break
- 15:30 Kawin
- 16:30 Discussion and Q&A
- 17:00 Closing