
ESPEI Documentation

Release 0.6.1

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Contents

I	Introduction	1
1	Installation	3
2	Quickstart	5
3	Goals	9
4	History	11
5	Change log	13
II	Tutorials	19
6	Cu-Mg example	21
7	Making ESPEI datasets	33
III	Reference	39
8	YAML input files	41
9	Theory	47
10	Recipes	49
11	Advanced Schedulers	51
IV	Developer	85
12	Contributing to ESPEI	87
13	Software design	91

V	Appendix	95
14	Appendices	97
	Python Module Index	99

Part I

Introduction

1.1 Anaconda (recommended)

ESPEI does not require any special compiler, but several dependencies do. Therefore it is suggested to install ESPEI from conda-forge.

```
conda install -c pycalphad -c msys2 -c conda-forge --yes espei
```

After installation, you must turn off dask's work stealing. Change the work stealing setting to `distributed.scheduler.work-stealing: False` in `~/.config/dask/distributed.yaml`. See [configuration](#) below for more details.

1.2 PyPI

Before you install ESPEI via PyPI, be aware that `pycalphad` and `emcee` must be compiled and `pycalphad` requires an external dependency of `lpopt`.

```
pip install espei
```

After installation, you must turn off dask's work stealing. Change the work stealing setting to `distributed.scheduler.work-stealing: False` in `~/.config/dask/distributed.yaml`. See [configuration](#) below for more details.

1.3 Development versions

You may install ESPEI however you like, but here we suggest using Anaconda to download all of the required dependencies. This method installs ESPEI with Anaconda, removes specifically the ESPEI package, and replaces it with the package from GitHub.

```
git clone https://github.com/phasesresearchlab/espei.git
cd espei
conda install espei
conda remove --force espei
pip install -e .
```

Upgrading ESPEI later requires you to run `git pull` in this directory.

After installation, you must turn off dask's work stealing. Change the work stealing setting to `distributed.scheduler.work-stealing: False` in `~/.config/dask/distributed.yaml`. See [configuration](#) below for more details.

1.4 Configuration

ESPEI uses dask-distributed to parallelize ESPEI.

After installation, you must turn off dask's work stealing! Change the file at `~/.config/dask/distributed.yaml` to look something like:

```
distributed:
  version: 2
  scheduler:
    work-stealing: False
```

See the [dask-distributed documentation](#) for more.

ESPEI has two different fitting modes: single-phase and multi-phase fitting. You can run either of these modes or both of them sequentially.

To run either of the modes, you need to have a phase models file that describes the phases in the system using the standard CALPHAD approach within the compound energy formalism. You also need to describe the data that ESPEI should fit to. You will need single-phase and multi-phase data for a full run. Fit settings and all datasets are stored as JSON files and described in detail at the [Making ESPEI datasets](#) page. All of your input datasets should be validated by running `espei --check-datasets my-input-datasets`, where `my-input-datasets` is a folder of all your JSON files.

The main output result is going to be a database (defaults to `out.tdb`), an array of the steps in the MCMC trace (defaults to `trace.npy`), and the an array of the log-probabilities for each iteration and chain (defaults to `lnprob.npy`).

2.1 Single-phase only

If you have only heat capacity, entropy and enthalpy data and mixing data (e.g. from first-principles), you may want to see the starting point for your MCMC calculation.

Create an input file called `espei-in.yaml`.

```
system:
  phase_models: my-phases.json
  datasets: my-input-datasets
generate_parameters:
  excess_model: linear
  ref_state: SGTE91
```

Then ESPEI can be run by running

```
espei --input espei-in.yaml
```

2.2 Multi-phase only

If you have a database already and just want to do a multi-phase fitting, you can specify a starting TDB file (named `my-tdb.tdb`) with

```
system:
  phase_models: my-phases.json
  datasets: my-input-data
mcmc:
  iterations: 1000
  input_db: my-tdb.tdb
```

The TDB file you input must have all of the degrees of freedom you want as `FUNCTIONs` with names beginning with `VV`.

2.3 Restart from previous run-phase only

If you've run an MCMC fitting already in ESPEI and have a trace file called `my-previous-trace.npy`, then you can resume the calculation with the following input file

```
system:
  phase_models: my-phases.json
  datasets: my-input-data
mcmc:
  iterations: 1000
  input_db: my-tdb.tdb
  restart_trace: my-previous-trace.npy
```

2.4 Full run

A minimal full run of ESPEI with single phase fitting and MCMC fitting is done by the following

```
system:
  phase_models: my-phases.json
  datasets: my-input-data
generate_parameters:
  excess_model: linear
  ref_state: SGTE91
mcmc:
  mcmc_steps: 1000
```

2.5 Input Customization

ESPEI lets you control many aspects of your calculations with the input files shown above. See *ESPEI YAML input files* for a full description of all possible inputs.

2.6 FAQ

2.6.1 Q: There is an error in my JSON files

A: Common mistakes are using single quotes instead of the double quotes required by JSON files. Another common source of errors is misaligned open/closing brackets.

Many mistakes are found with ESPEI's `check-datasets` utility. Run `espei check-datasets my-input-datasets` on your directory `my-input-datasets`.

2.6.2 Q: How do I analyze my results?

A: By default, ESPEI will create `trace.npy` and `lnprob.npy` for the MCMC chain at the specified save interval and according to the save interval (defaults to every iteration). These are created from arrays via `numpy.save()` and can thus be loaded with `numpy.load()`. Note that the arrays are preallocated with zeros. These filenames and settings can be changed using in the input file. You can then use these chains and corresponding log-probabilities to make corner plots, calculate autocorrelations, find optimal parameters for databases, etc.. Finally, you can use `py:mod:espei.plot` functions such as `multiplot` to plot phase diagrams with your input equilibria data and `plot_parameters` to compare single-phase data (e.g. formation and mixing data) with the properties calculated with your database.

2.6.3 Q: Can I run ESPEI on a supercomputer supporting MPI?

A: Yes! ESPEI has MPI support. See the [Advanced Schedulers](#) page for more details.

ESPEI, or Extensible Self-optimizing Phase Equilibria Infrastructure, is a tool for automated thermodynamic database development within the CALPHAD method. It uses `pycalphad` for calculating Gibbs free energies of thermodynamic models.

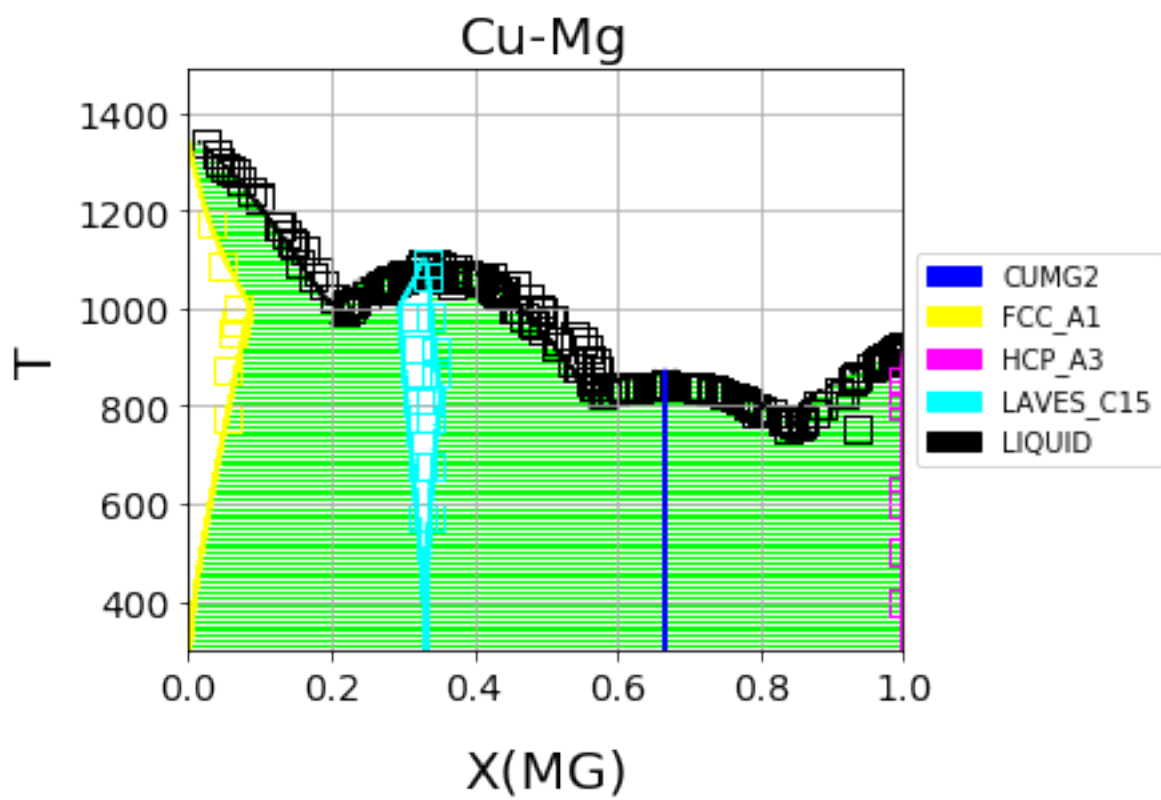


Fig. 1: Cu-Mg phase diagram from a database created with and optimized by ESPEI. See the [Cu-Mg Example](#).

Goals

1. Offer a free and open-source tool for users to develop multicomponent databases with quantified uncertainty
2. Enable development of CALPHAD-type models for Gibbs energy, thermodynamic or kinetic properties
3. Provide a platform to build and apply novel model selection and optimization methods

The implementation for ESPEI involves first fitting single-phase data by calculating parameters in thermodynamic models that are linearly described by the single-phase input data. Then Markov Chain Monte Carlo (MCMC) is used to optimize the candidate models from the single-phase fitting to multi-phase zero-phase fraction data. The benefit of this approach is the automated, simultaneous fitting for many parameters that yields uncertainty quantification, as shown in Otis and Liu High-Throughput Thermodynamic Modeling and Uncertainty Quantification for ICME. [Jom 69, \(2017\)](#). Single-phase and multi-phase fitting methods are described in Chapter 3 of [Richard Otis's thesis](#).

CHAPTER 4

History

The ESPEI package is based on a fork of [pycalphad-fitting](#). The name and idea of ESPEI are originally based off of Shang, Wang, and Liu, ESPEI: Extensible, Self-optimizing Phase Equilibrium Infrastructure for Magnesium Alloys *Magnes. Technol.* 2010 617-622 (2010).

5.1 What's New

5.1.1 0.6.1 (2018-08-28)

This a major release with several important features and bug fixes

- Enable use of ridge regression alpha for parameter selection via the `parameter_generation.ridge_alpha` input parameter.
- Add ternary parameter selection. Works by default, just add data.
- Set memory limit to zero to avoid dask killing workers near the dask memory limits.
- Remove ideal mixing from plotting models so that `plot_parameters` gives the correct entropy values.
- Add *recipes documentation* <<https://github.com/PhasesResearchLab/ESPEI/blob/master/docs/recipes.rst>> that contains some Python code for common utility operations.
- Add documentation for running custom distributed schedulers in ESPEI

5.1.2 0.6 (2018-07-02)

This is a update including *breaking changes to the input files* and several minor improvements.

- Update input file schema and Python API to be more consistent so that the `trace` always refers to the collection of chains and `chain` refers to individual chains. Additionally removed some redundancy in the parameters nested under the `mcmc` heading, e.g. `mcmc_steps` is now `iterations` and `mcmc_save_interval` is now `save_interval` in the input file and Python API. See [Writing Input](#) documentation for all of the updates.
- The default save interval is now 1, which is more reasonable for most MCMC systems with significant numbers of phase equilibria.
- Bug fixes for plotting and some better plotting defaults for plotting input data
- Dataset parsing and cleaning improvements.

- Documentation improvements (see the [PDF!](#))

5.1.3 0.5.2 (2018-04-28)

This is a major bugfix release for MCMC multi-phase fitting runs for single phase data.

- Fixed a major issue where single phase thermochemical data was always compared to Gibbs energy, giving incorrect errors in MCMC runs.
- Single phase errors in ESPEI incorrectly compared values with ideal mixing contributions to data, which is excess only.
- Fixed a bug where single phase thermochemical data with that are dependent on composition and pressure and/or temperature were not fit correctly.
- Added utilities for analyzing ESPEI results and add them to the Cu-Mg example docs.

5.1.4 0.5.1 (2018-04-17)

This is a minor bugfix release.

- Parameter generation for phases with vacancies would produce incorrect parameters because the vacancy site fractions were not being correctly removed from the contributions due to their treatment as `Species` objects in `pycalphad >=0.7`.

5.1.5 0.5 (2018-04-03)

- Parameter selection now uses the corrected AIC, which further prevents overparameterization where there is sparse training data.
- Activity and single phase thermochemical data can now be included in MCMC fitting runs. Including single phase data can help anchor metastable phases to DFT data when they are not on the stable phase diagram. See the [Gathering input data](#) documentation for information on how to input activity data.
- Dataset checking has been improved. Now there are checks to make sure sublattice interactions are properly sorted and mole fractions sum to less than 1.0 in ZPF data.
- Support for fitting phases with arbitrary `pycalphad` Models in MCMC, including (charged and neutral) species and ionic liquids. There are several consequences of this:
 - ESPEI requires support on `pycalphad >=0.7`
 - ESPEI now uses `pycalphad Model` objects directly. Using the JIT compiled Models has shown up to a *50% performance improvement* in MCMC runs.
 - Using JIT compiled `Model` objects required the use of `cloudpickle` everywhere. Due to challenges in overriding `pickle` for upstream packages, we now rely solely on `dask` for scheduler tasks, including `mpi` via `dask-mpi`. Note that users must turn off `work-stealing` in their `~/.dask/config.yaml` file.
- [Developers] Each method for calculating error in MCMC has been moved into a module for that method in an `error_functions` subpackage. One top level function from each module should be imported into the `mcmc.py` and used in `lnprob`. Developers should then just customize `lnprob`.
- [Developers] Significant internal docs improvements: all non-trivial functions have complete docstrings.

5.1.6 0.4.1 (2018-02-05)

- Enable plotting of isothermal sections with data using `dataplot` (and `multiplot`, etc.)
- Tielines are now plotted in `dataplot` for isothermal sections and T-x phase diagrams
- Add a useful `ravel_conditions` method to unpack conditions from datasets

5.1.7 0.4 (2017-12-29)

- MCMC is now deterministic by default (can be toggled off with the `mcmc.deterministic` setting).
- Added support for having no scheduler (running with no parallelism) with the `mcmc.scheduler` option set to `None`. This may be useful for debugging.
- Logging improvements
 - Extraneous warnings that may be confusing for users and dirty the log are silenced.
 - A warning is added for when there are no datasets found.
 - Fixed a bug where logging was silenced with the dask scheduler
- Add `optimal_parameters` utility function as a helper to get optimal parameter sets for analysis
- Several improvements to plotting
 - Users can now plot phase diagram data alone with `dataplot`, useful for checking datasets visually. This changes the API for `dataplot` to no longer infer the conditions from an equilibrium `Dataset` (from `pycalphad`). That functionality is preserved in `eqdataplot`.
 - Experimental data points are now plotted with unique symbols depending on the reference key in the dataset. This is for both phase diagram and single phase parameter plots.
 - Options to control plotting parameters (e.g. symbol size) and take user supplied Axes and Figures in the plotting functions. The symbol size is now smaller by default.
- Documentation improvements for API and separation of theory from the Cu-Mg example
- Fixes a bug where elements with single character names would not find the correct reference state (which are typically named GHSERCC for the example of C).
- [Developer] All MCMC code is moved from the `paramselect` module to the `mcmc` module to separate these tasks
- [Developer] Support for arbitrary user reference states (so long as the reference state is in the `refdata` module and follows the same format as SGTE91)

5.1.8 0.3.1.post2 (2017-10-31)

- Propagate the new entry point to `setup.py`

5.1.9 0.3.1.post1 (2017-10-31)

- Fix for module name/function conflict in entry point

5.1.10 0.3.1 (2017-10-31)

- ESPEI is much easier to run interactively in Python and in Jupyter Notebooks
- Reference data is now included in ESPEI instead of in pycalphad
- Several reference data fixes including support for single character elements ('V', 'B', 'C', ...)
- Support for using multiprocessing to parallelize MCMC runs, used by default (@olivia-higgins)
- Improved documentation for installing and developing ESPEI

5.1.11 0.3.post2 (2017-09-20)

- Add input-schema.yaml file to installer

5.1.12 0.3.post1 (2017-09-20)

- Add LICENSE to manifest

5.1.13 0.3 (2017-09-20)

- **ESPEI input is now described by a file.** This change is breaking. Old command line arguments are not supported. See [Writing input files](#) for a full description of all the inputs.
- New input options are supported, including modifying the number of chains and standard deviation from the mean
- ESPEI is now available on conda-forge
- TinyDB 2 support is dropped in favor of TinyDB 3 for conda-forge deployment
- Allow for restarting previous mcmc calculations with a trace file
- Add Cu-Mg example to documentation

5.1.14 0.2.1 (2017-08-17)

Fixes to the 0.2 release plotting interface

- `multiplot` is renamed from `multi_plot`, as in docs.
- Fixed an issue where phases in datasets, but not in equilibrium were not plotted by `dataplot` and raised an error.

5.1.15 0.2 (2017-08-15)

- New `multiplot` interface for convenient plotting of phase diagrams + data. `dataplot` function underlies key data plotting features and can be used with `eqplot`. See their API docs for examples. Will break existing code using `multiplot`.
- MPI support for local/HPC runs. Only single node runs are explicitly supported currently. Use `--scheduler='MPIPool'` command line option. Requires `mpi4py`.
- Default debug reporting of acceptance ratios
- Option (and default) to output the log probability array matching the trace. Use `--probfile` option to control.

- Optimal parameters are now chosen based on lowest error in chain.
- Bug fixes including
 - py2/3 compatibility
 - unicode datasets
 - handling of singular matrix errors from pycalphad's `equilibrium`
 - reporting of failed conditions

5.1.16 0.1.5 (2017-08-02)

- Significant error checking of JSON inputs.
- Add new `--check-datasets` option to check the datasets at path. It should be run before you run ESPEI fittings. All errors must be resolved before you run.
- Move the `espei` script module from `fit.py` to `run_espei.py`.
- Better docs building with mocking
- Google docstrings are now NumPy docstrings

5.1.17 0.1.4 (2017-07-24)

- Documentation improvements for usage and API docs
- Fail fast on JSON errors

5.1.18 0.1.3 (2017-06-23)

- Fix bad version pinning in `setup.py`
- Explicitly support Python 2.7

5.1.19 0.1.2 (2017-06-23)

- Fix dask incompatibility due to new API usage

5.1.20 0.1.1 (2017-06-23)

- Fix a bug that caused logging to raise if bokeh isn't installed

5.1.21 0.1 (2017-06-23)

ESPEI is now a package! New features include

- Fork <https://github.com/richardotis/pycalphad-fitting>
- Use `emcee` for MCMC fitting rather than `pymc`
- Support single-phase only fitting
- More control options for running ESPEI from the command line

- Better support for incremental saving of the chain
- Control over output with logging over printing
- Significant code cleanup
- Better usage documentation

See [what's new!](#)

Part II

Tutorials

6.1 Cu-Mg Example

The Cu-Mg binary system is an interesting and simple binary subsystem for light metal alloys. It has been modeled in the literature by Coughanowr et al.¹, Zuo and Chang² and Zhou et al.³ and was featured as a case study in Computational Thermodynamics The Calphad Method by Lukas, Fries, & Sundman⁴.

Here we will combine density functional theory and experimental calculations of single-phase data to generate a first-principles phase diagram. Then that database will be used as a starting point for a Markov Chain Monte Carlo (MCMC) Bayesian optimization of the parameters to fit zero-phase fraction data.

6.1.1 Input data

All of the input data for ESPEI is stored in a public [ESPEI-datasets](#) repository on GitHub. The data in this repository is Creative Commons Attribution 4.0 (CC-BY-4.0) licensed and may be used, commercialized or reused freely.

In order to run ESPEI with the data in ESPEI-datasets, you should clone this repository to your computer. Files referred to throughout this tutorial are found in the *CU-MG* folder. The input files will be very briefly explained in this tutorial so that you are able to know their use. A more detailed description of the files is found on the [Making ESPEI datasets](#) page.

If you make changes or additions, you are encouraged to share these back to the ESPEI-datasets repository so that others may benefit from this data as you have. You may then add your name to the CONTRIBUTORS file as described in the README.

¹ Coughanowr, C. A., Ansara, I., Luoma, R., Hamalainen, M. & Lukas, H. L. Assessment of the Cu-Mg system. *Zeitschrift für Met.* 82, 574–581 (1991).

² Zuo, Y. U. E. & Chang, Y. A. Thermodynamic calculation of the Mg-Cu phase diagram. *Zeitschrift für Met.* 84, 662–667 (1993).

³ Zhou, S. et al. Modeling of Thermodynamic Properties and Phase Equilibria for the Cu-Mg Binary System. *J. Phase Equilibria Diffus.* 28, 158–166 (2007). doi:10.1007/s11669-007-9022-0

⁴ Lukas, H., Fries, S. G. & Sundman, B. Computational Thermodynamics The Calphad Method. (Cambridge University Press, 2007). doi:10.1017/CBO9780511804137

6.1.2 Phases and CALPHAD models

The Cu-Mg system contains five stable phases: Liquid, disordered fcc and hcp, the C15 Laves phase and the CuMg₂ phase. All of these phases will be modeled as solution phases, except for CuMg₂, which will be represented as a stoichiometric compound. The phase names and corresponding sublattice models are as follows:

```
LIQUID:      (CU, MG) 1
FCC_A1:      (CU, MG) 1 (VA) 1
HCP_A3:      (CU, MG) 1 (VA) 1
LAVES_C15:   (CU, MG) 2 (CU, MG) 1
CUMG2:       (CU) 1 (MG) 2
```

These phase names and sublattice models are described in the JSON file *Cu-Mg-input.json* file as seen below

```
{
  "components": ["CU", "MG", "VA"],
  "phases": {
    "LIQUID": {
      "sublattice_model": [["CU", "MG"]],
      "sublattice_site_ratios": [1]
    },
    "CUMG2": {
      "sublattice_model": [["CU"], ["MG"]],
      "sublattice_site_ratios": [1, 2]
    },
    "FCC_A1": {
      "sublattice_model": [["CU", "MG"], ["VA"]],
      "sublattice_site_ratios": [1, 1]
    },
    "HCP_A3": {
      "sublattice_site_ratios": [1, 0.5],
      "sublattice_model": [["CU", "MG"], ["VA"]]
    },
    "LAVES_C15": {
      "sublattice_site_ratios": [2, 1],
      "sublattice_model": [["CU", "MG"], ["CU", "MG"]]
    }
  }
}
```

6.1.3 ESPEI

ESPEI has two types of fitting – parameter generation and MCMC optimization. The parameter generation step uses experimental and first-principles data of the derivatives of the Gibbs free energy to parameterize the Gibbs energies of each individual phase. The MCMC optimization step fits the generated parameters to experimental phase equilibria data. These two fitting procedures can be used together to fully assess a given system. For clarity, we will preform these steps separately to fit Cu-Mg. The next two sections are devoted to describing ESPEI's parameter generation and optimization.

Though it should be no problem for this case, since the data has already been used, you should get in the habit of checking datasets before running ESPEI. ESPEI has a tool to help find and report problems in your datasets. This is automatically run when you load the datasets, but will fail on the first error. Running the following command (assuming from here on that you are in the CU-MG folder from [ESPEI-datasets](#)):

```
espei --check-datasets input-data
```

The benefit of this approach is that all of the datasets will be checked and reported at once. If there are any failures, a list of them will be reported with the two main types of errors being `JSONError`, for which you should read the JSON section of *Making ESPEI datasets*, or `DatasetError`, which are related to the validity of your datasets scientifically (matching conditions and values shape, etc.). The `DatasetError` messages are designed to be clear, so please open an [issue on GitHub](#) if there is any confusion.

6.1.4 First-principles phase diagram

By using the `Cu-Mg-input.json` phase description for the fit settings and passing all of the input data in the `input-data` folder, we can first use ESPEI to generate a phase diagram based on single-phase experimental and DFT data. Currently all of the input datasets must be formation properties, and it can be seen that the formation enthalpies are defined from DFT and experiments for the Laves and CuMg2 phases. Mixing enthalpies are defined for the fcc, hcp, and Laves phases from DFT and for liquid from experimental measurements.

The following command will generate a database named `cu-mg_dft.tdb` with parameters selected and fit by ESPEI:

```
espei --input espei-in.yaml
```

where `espei-in.yaml` is a *ESPEI input file* with the following contents

```
system:
  phase_models: Cu-Mg-input.json
  datasets: input-data
generate_parameters:
  excess_model: linear
  ref_state: SGTE91
output:
  output_db: cu-mg_dft.tdb
```

The calculation should be relatively quick, on the order of a minute of runtime. With the above command, only minimal output (warnings) will be reported. You can increase the verbosity to report info messages by setting the `output.verbosity` key to 1 or debug messages with 2.

With the following code, we can look at the generated phase diagram and compare it to our data.

```
# First-principles phase diagram
from pycalphad import Database, variables as v
from espei.datasets import load_datasets, recursive_glob
from espei.plot import multiplot
import matplotlib.pyplot as plt

# load the experimental and DFT datasets
datasets = load_datasets(recursive_glob('input-data', '*.json'))

# set up the pycalphad phase diagram calculation
dbf = Database('cu-mg_dft.tdb')
comps = ['CU', 'MG', 'VA']
phases = ['LIQUID', 'FCC_A1', 'HCP_A3', 'CUMG2', 'LAVES_C15']
conds = {v.P: 101325, v.T: (300, 1500, 10), v.X('MG'): (0, 1, 0.01)}

# plot the phase diagram and data
multiplot(dbf, comps, phases, conds, datasets)
plt.savefig('cu-mg_dft_phase_diagram.png')
```

Which should result in the following figure

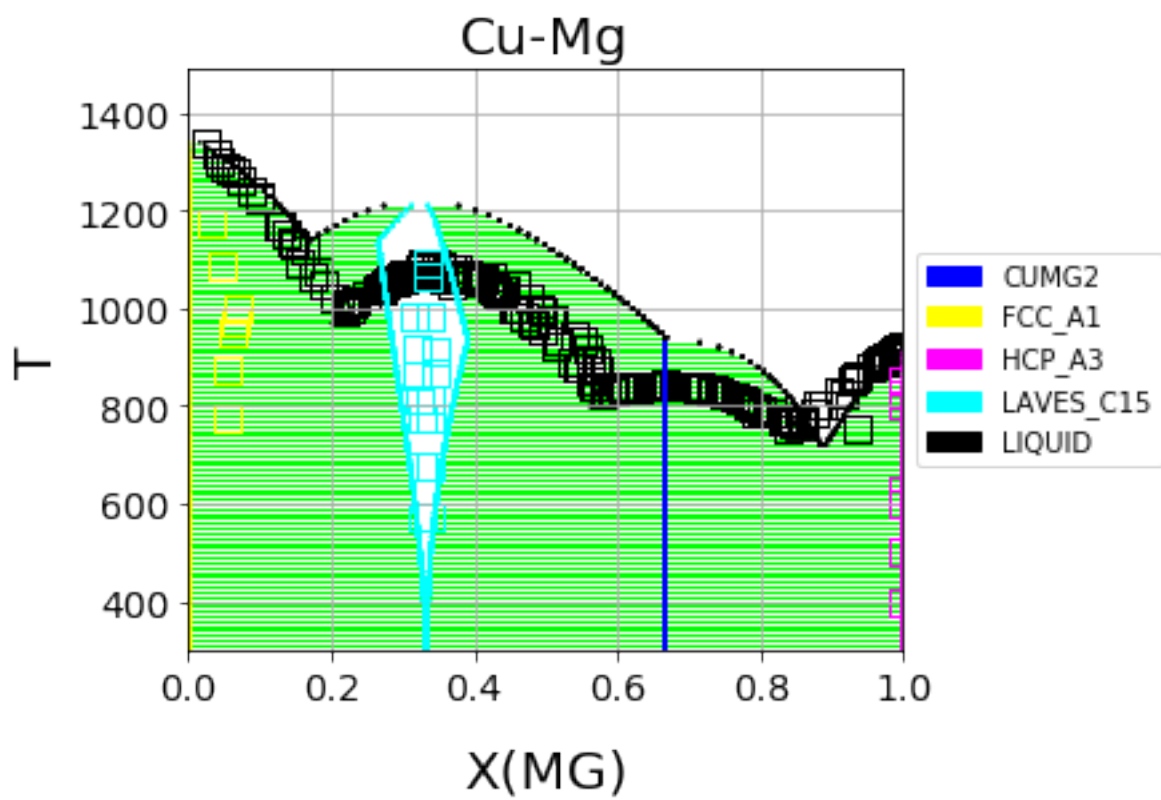


Fig. 1: First-principles Cu-Mg phase diagram from the single-phase fitting in ESPEI

We can see that the phase diagram is already very reasonable compared to the experimental points. The liquidus temperatures and the solubilities of the fcc and Laves phases are the key differences between the equilibrium data and our first-principles phase diagram. The next section will discuss using ESPEI to optimize the parameters selected and calculated based on the single-phase data to these multi-phase equilibria.

6.1.5 MCMC optimization

With the data in the CU-MG input data, ESPEI generated 18 parameters to fit. For systems with more components, solution phases, and input data, may more parameters could be required to describe the thermodynamics of the specific system well. Because they describe Gibbs free energies, parameters in CALPHAD models are highly correlated in both single-phase descriptions and for describing equilibria between phases. For large systems, global numerical optimization of many parameters simultaneously is computationally intractable.

To combat the problem of optimizing many parameters, ESPEI uses MCMC, a stochastic optimization method. For more details on how MCMC is used in ESPEI, see the [Theory](#) page.

Now we will use our zero phase fraction equilibria data to optimize our first-principles database with MCMC. The following command will take the database we created in the single-phase parameter selection and perform a MCMC optimization, creating a `cu-mg_mcmc.tdb`:

```
espei --input espei-in.yaml
```

where `espei-in.yaml` is an *ESPEI input file* with the following structure

```
system:
  phase_models: Cu-Mg-input.json
  datasets: input-data
mcmc:
  iterations: 1000
  input_db: cu-mg_dft.tdb
output:
  output_db: cu-mg_mcmc.tdb
```

ESPEI defaults to run 1000 iterations and depends on calculating equilibrium in pycalphad several times for each iteration and the optimization is compute-bound. Fortunately, MCMC optimizations are embarrassingly parallel and ESPEI allows for parallelization using [dask](#) or with MPI using [mpi4py](#) (single-node only at the time of writing - we are working on it).

Note that you may also see messages about convergence failures or about dropping conditions. These refer to failures to calculate the log-probability or in the pycalphad solver's equilibrium calculation. They are not detrimental to the optimization accuracy, but overall optimization may be slower because those parameter proposals will never be accepted (they return a log-probability of $-\infty$).

Finally, we can use the newly optimized database to plot the phase diagram

```
# Optimized phase diagram from ESPEI's multi-phase fitting
from pycalphad import Database, variables as v
from espei.datasets import load_datasets, recursive_glob
from espei.plot import multiplot
import matplotlib.pyplot as plt

# load the experimental and DFT datasets
datasets = load_datasets(recursive_glob('input-data', '*.json'))

# set up the pycalphad phase diagram calculation
dbf = Database('cu-mg_mcmc.tdb')
comps = ['CU', 'MG', 'VA']
```

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```

phases = ['LIQUID', 'FCC_A1', 'HCP_A3', 'CUMG2', 'LAVES_C15']
conds = {v.P: 101325, v.T: (300, 1500, 10), v.X('MG'): (0, 1, 0.01)}

# plot the phase diagram and data
multiplot(dbf, comps, phases, conds, datasets)
plt.savefig('cu-mg_mcmc_phase_diagram.png')

```

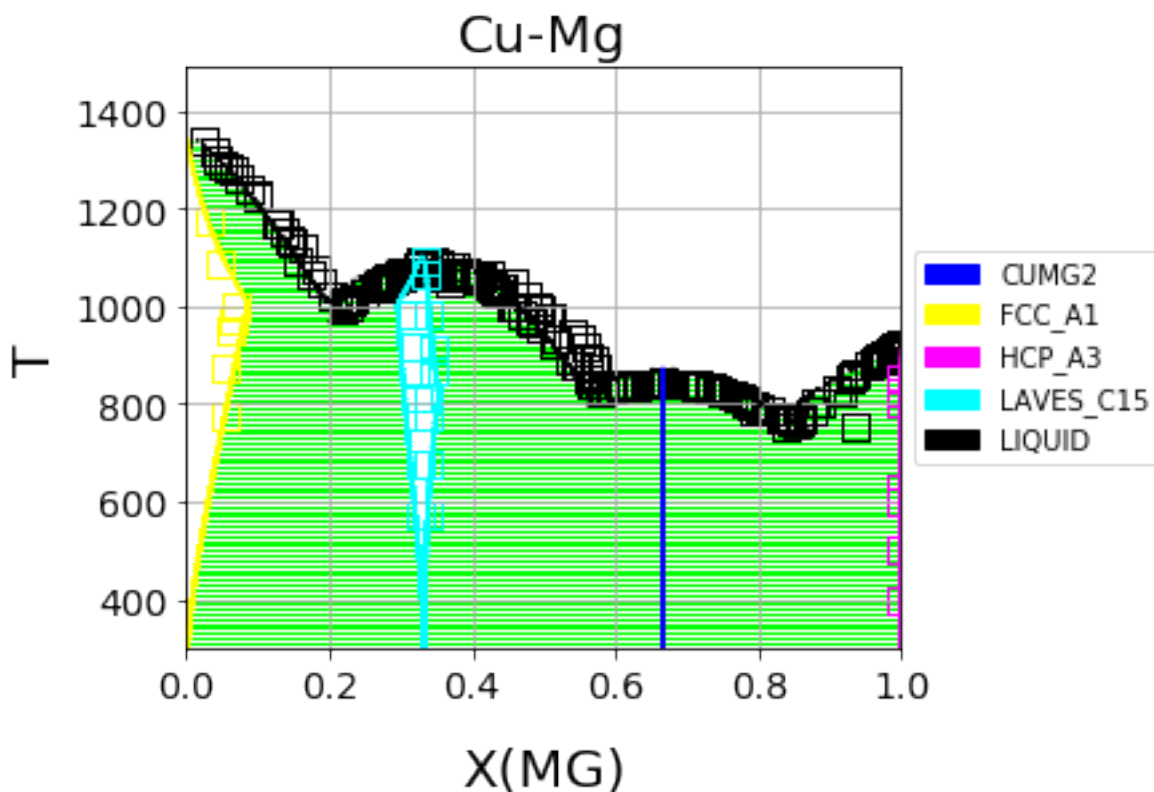


Fig. 2: Optimized Cu-Mg phase diagram from the multi-phase fitting in ESPEI

6.1.6 Analyzing ESPEI Results

After finishing a MCMC run, you will want to analyze your results.

All of the MCMC results will be maintained in two output files, which are serialized NumPy arrays. The file names are set in your `espei-in.yaml` file. The filenames are set by `output.tracefile` and `output.probfile` ([documentation](#)) and the defaults are `trace.npy` and `lnprob.npy`, respectively.

The `tracefile` contains all of the parameters that were proposed over all chains and iterations (the trace). The `probfile` contains all of calculated log probabilities for all chains and iterations (as negative numbers, by convention).

There are several aspects of your data that you may wish to analyze. The next sections will explore some of the options.

Probability convergence

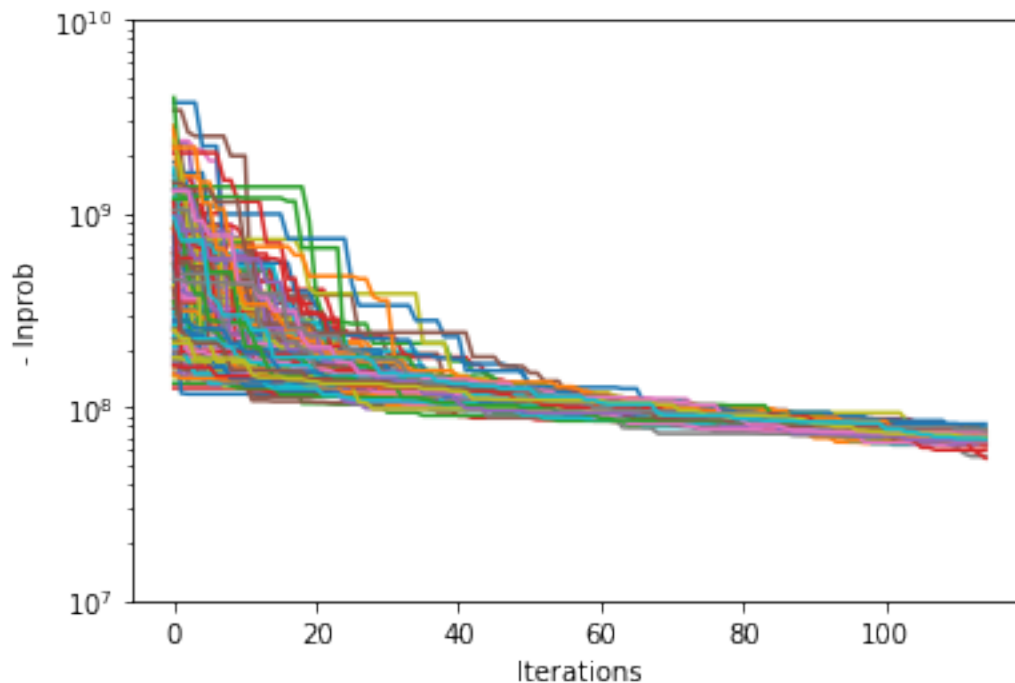
First we'll plot how the probability changes for all of the chains as a function of iterations. This gives a qualitative view of convergence. There are several quantitative metrics that we won't explore here, such as autocorrelation. Qualitatively, this run does not appear converged after 115 iterations.

```
# remove next line if not using iPython or Jupyter Notebooks
%matplotlib inline
import matplotlib.pyplot as plt
import numpy as np
from espei.analysis import truncate_arrays

trace = np.load('trace.npy')
lnprob = np.load('lnprob.npy')

trace, lnprob = truncate_arrays(trace, lnprob)

ax = plt.gca()
ax.set_yscale('log')
ax.set_ylim(1e7, 1e10)
ax.set_xlabel('Iterations')
ax.set_ylabel('- lnprob')
num_chains = lnprob.shape[0]
for i in range(num_chains):
    ax.plot(-lnprob[i,:])
plt.show()
```



Visualizing the trace of each parameter

We would like to see how each parameter changed during the iterations. For brevity in the number of plots we'll plot all the chains for each parameter on the same plot. Here we are looking to see how the parameters explore the space

and converge to a solution.

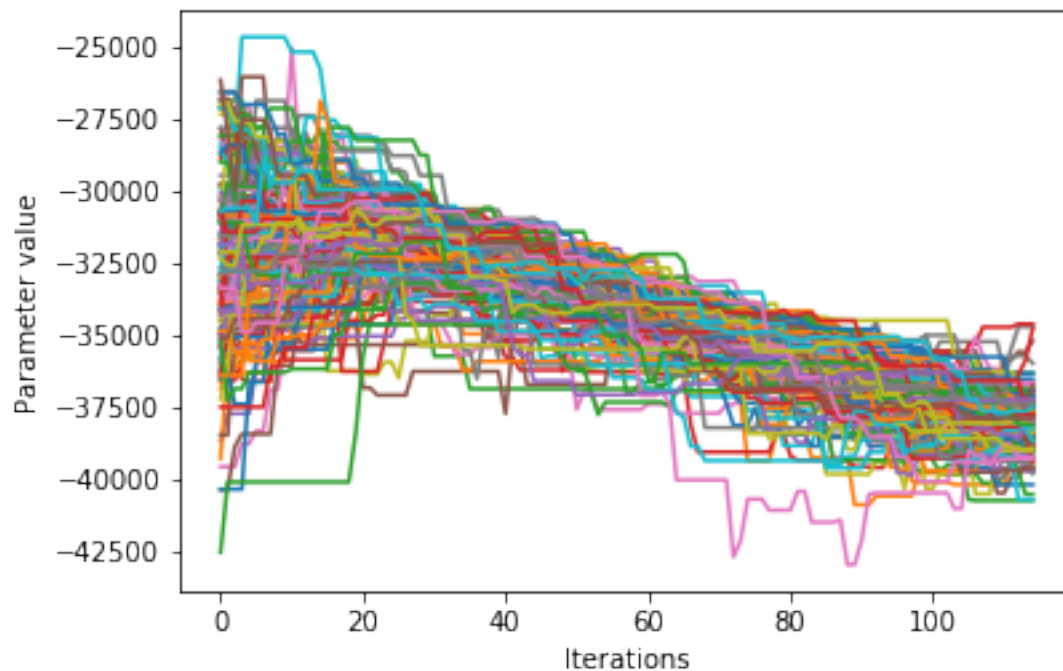
```
# remove next line if not using iPython or Jupyter Notebooks
%matplotlib inline
import matplotlib.pyplot as plt
import numpy as np

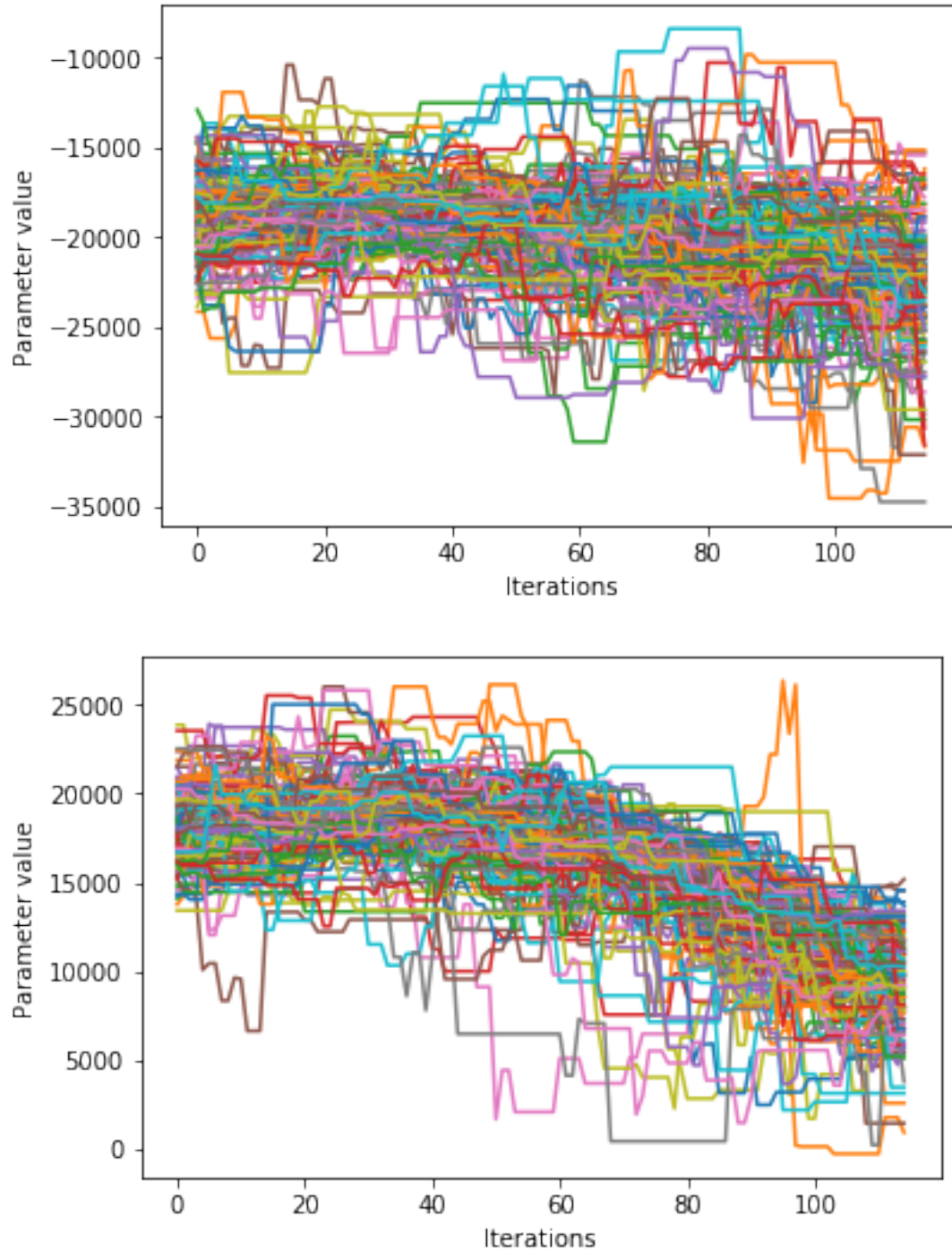
from espei.analysis import truncate_arrays

trace = np.load('trace.npy')
lnprob = np.load('lnprob.npy')

trace, lnprob = truncate_arrays(trace, lnprob)

num_chains = trace.shape[0]
num_parameters = 3 # only plot the first three parameter, for all of them use `trace.
                    # ↪ shape[2]`
for parameter in range(num_parameters):
    ax = plt.figure().gca()
    ax.set_xlabel('Iterations')
    ax.set_ylabel('Parameter value')
    for chain in range(num_chains):
        ax.plot(trace[chain, :, parameter])
plt.show()
```





Corner plots

Note: You must install the `corner` package before using it (`conda install corner` or `pip install corner`).

In a corner plot, the distributions for each parameter are plotted along the diagonal and covariances between them under the diagonal. A more circular covariance means that parameters are not correlated to each other, while elongated shapes

indicate that the two parameters are correlated. Strongly correlated parameters are expected for some parameters in CALPHAD models within phases or for phases in equilibrium, because increasing one parameter while decreasing another would give a similar error.

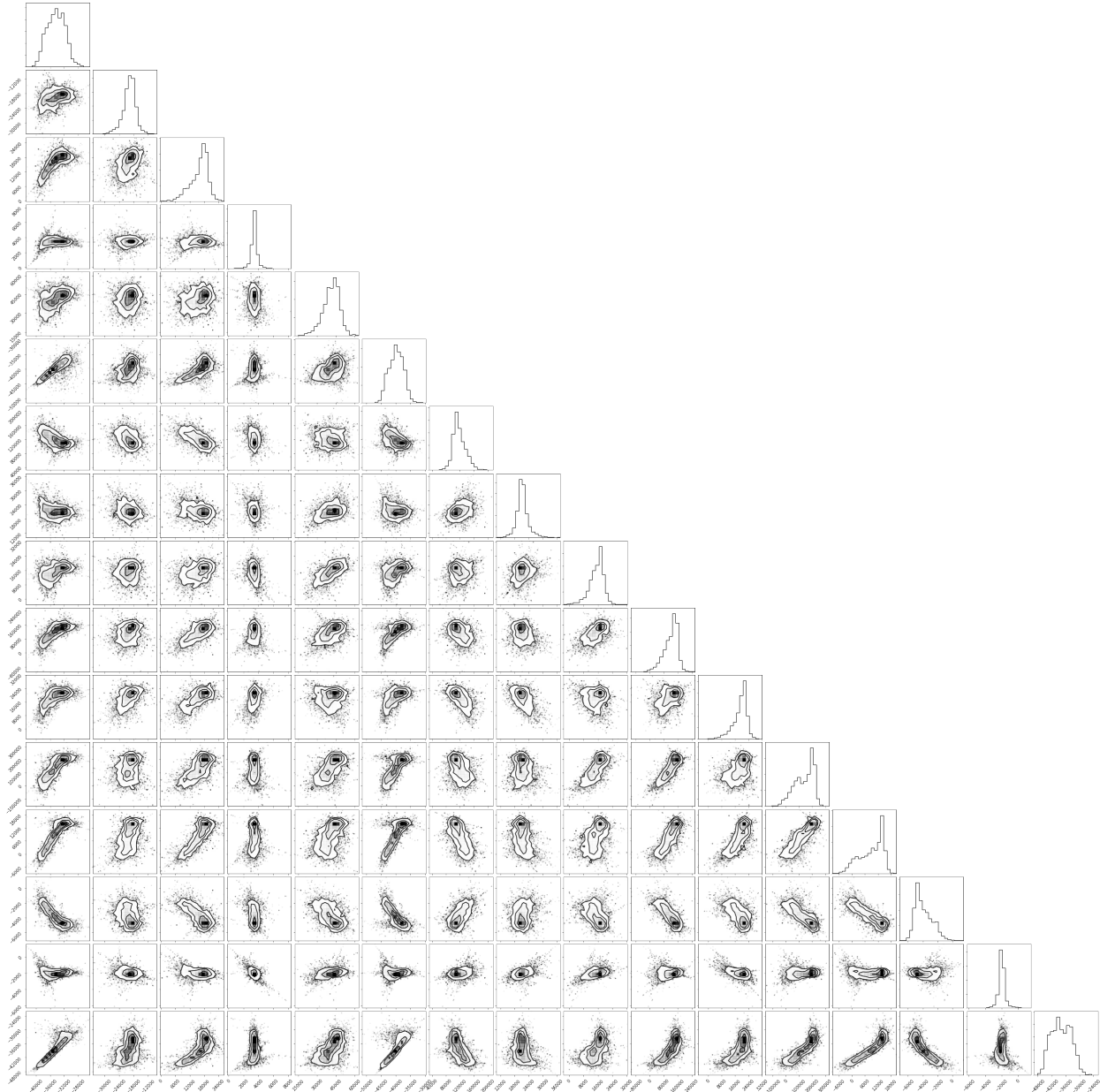
```
# remove next line if not using iPython or Jupyter Notebooks
%matplotlib inline
import matplotlib.pyplot as plt
import numpy as np
import corner

from espei.analysis import truncate_arrays

trace = np.load('trace.npy')
lnprob = np.load('lnprob.npy')

trace, lnprob = truncate_arrays(trace, lnprob)

# flatten the along the first dimension containing all the chains in parallel
fig = corner.corner(trace.reshape(-1, trace.shape[-1]))
plt.show()
```



Ultimately, there are many features to explore and we have only covered a few basics. Since all of the results are stored as arrays, you are free to analyze using whatever methods are relevant.

6.1.7 Summary

ESPEI allows thermodynamic databases to be easily reoptimized with little user interaction, so more data can be added later and the database reoptimized at the cost of only computer time. In fact, the existing database from estimates can be used as a starting point, rather than one directly from first-principles, and the database can simply be modified to match any new data.

6.1.8 References

6.1.9 Acknowledgements

Credit for initially preparing the datasets goes to Aleksei Egorov.

Making ESPEI datasets

7.1 Making ESPEI datasets

7.1.1 JSON Format

ESPEI has a single input style in JSON format that is used for all data entry. Single-phase and multi-phase input files are almost identical, but detailed descriptions and key differences can be found in the following sections. For those unfamiliar with JSON, it is fairly similar to Python dictionaries with some rigid requirements

- All string quotes must be double quotes. Use "key" instead of 'key'.
- Numbers should not have leading zeros. 00.123 should be 0.123 and 012.34 must be 12.34.
- Lists and nested key-value pairs cannot have trailing commas. {"nums": [1,2,3,],} is invalid and should be {"nums": [1,2,3]}.

These errors can be challenging to track down, particularly if you are only reading the JSON error messages in Python. A visual editor is encouraged for debugging JSON files such as [JSONLint](#). A quick reference to the format can be found at [Learn JSON in Y minutes](#).

ESPEI has support for checking all of your input datasets for errors, which you should always use before you attempt to run ESPEI. This error checking will report all of the errors at once and all errors should be fixed. Errors in the datasets will prevent fitting. To check the datasets at path `my-input-data/` you can run `espei --check-datasets my-input-data`.

7.1.2 Phase Descriptions

The JSON file for describing CALPHAD phases is conceptually similar to a setup file in Thermo-Calc's PARROT module. At the top of the file there is the `refdata` key that describes which reference state you would like to choose. Currently the reference states are strings referring to dictionaries in `pycalphad.refdata` only "SGTE91" is implemented.

Each phase is described with the phase name as they key in the dictionary of phases. The details of that phase is a dictionary of values for that key. There are 4 possible entries to describe a phase: `sublattice_model`,

sublattice_site_ratios, equivalent_sublattices, and aliases. sublattice_model is a list of lists, where each internal list contains all of the components in that sublattice. The BCC_B2 sublattice model is `[["AL", "NI", "VA"], ["AL", "NI", "VA"], ["VA"]]`, thus there are three sublattices where the first two have Al, Ni, and vacancies. sublattice_site_ratios should be of the same length as the sublattice model (e.g. 3 for BCC_B2). The sublattice site ratios can be fractional or integers and do not have to sum to unity.

The optional equivalent_sublattices key is a list of lists that describe which sublattices are symmetrically equivalent. Each sub-list in equivalent_sublattices describes the indices (zero-indexed) of sublattices that are equivalent. For BCC_B2 the equivalent sublattices are `[[0, 1]]`, meaning that the sublattice at index 0 and index 1 are equivalent. There can be multiple different sets (multiple sub-lists) of equivalent sublattices and there can be many equivalent sublattices within a sublattice (see FCC_L12). If no equivalent_sublattice key exists, it is assumed that there are none.

Finally, the aliases key is used to refer to other phases that this sublattice model can describe when symmetry is accounted for. Aliases are used here to describe the BCC_A2 and FCC_A1, which are the disordered phases of BCC_B2 and FCC_L12, respectively. Notice that the aliased phases are not otherwise described in the input file. Multiple phases can exist with aliases to the same phase, e.g. FCC_L12 and FCC_L10 can both have FCC_A1 as an alias.

```
{
  "refdata": "SGTE91",
  "components": ["AL", "NI", "VA"],
  "phases": {
    "LIQUID": {
      "sublattice_model": ["AL", "NI"],
      "sublattice_site_ratios": [1]
    },
    "BCC_B2": {
      "aliases": ["BCC_A2"],
      "sublattice_model": ["AL", "NI", "VA"], ["AL", "NI", "VA"], ["VA"],
      "sublattice_site_ratios": [0.5, 0.5, 1],
      "equivalent_sublattices": [[0, 1]]
    },
    "FCC_L12": {
      "aliases": ["FCC_A1"],
      "sublattice_model": ["AL", "NI"], ["AL", "NI"], ["AL", "NI"], ["AL", "NI"], [
↪ "VA"],
      "sublattice_site_ratios": [0.25, 0.25, 0.25, 0.25, 1],
      "equivalent_sublattices": [[0, 1, 2, 3]]
    },
    "AL3NI1": {
      "sublattice_site_ratios": [0.75, 0.25],
      "sublattice_model": ["AL"], ["NI"]
    },
    "AL3NI2": {
      "sublattice_site_ratios": [3, 2, 1],
      "sublattice_model": ["AL"], ["AL", "NI"], ["NI", "VA"]
    },
    "AL3NI5": {
      "sublattice_site_ratios": [0.375, 0.625],
      "sublattice_model": ["AL"], ["NI"]
    }
  }
}
```

7.1.3 Units

- Energies are in J/mol-atom (and the derivatives follow)
- All compositions are mole fractions
- Temperatures are in Kelvin
- Pressures in Pascal

7.1.4 Single-phase Data

Two example of ESPEI input file for single-phase data follow. The first dataset has some data for the formation heat capacity for BCC_B2.

The `components` and `phases` keys simply describe those found in this entry. Use the `reference` key for book-keeping the source of the data. In `solver` the sublattice configuration and site ratios are described for the phase.

`sublattice_configurations` is a list of different configurations, that should correspond to the sublattices for the phase descriptions. Non-mixing sublattices are represented as a string, while mixing sublattices are represented as a lists. Thus an endmember for BCC_B2 (as in this example) is `["AL", "NI", "VA"]` and if there were mixing (as in the next example) it might be `["AL", ["AL", "NI"], "VA"]`. Mixing also means that the `sublattice_occupancies` key must be specified, but that is not the case in this example. It is important to note that any mixing configurations must have any ideal mixing contributions removed. Regardless of whether there is mixing or not, the length of this list should always equal the number of sublattices in the phase, though the sub-lists can have mixing up to the number of components in that sublattice. Note that the `sublattice_configurations` is a *list* of these lists. That is, there can be multiple sublattice configurations in a single dataset. See the second example in this section for such an example.

The `conditions` describe temperatures (T) and pressures (P) as either scalars or one-dimensional lists. Most important to describing data are the `output` and `values` keys. The type of quantity is expressed using the `output` key. This can in principle be any thermodynamic quantity, but currently only CPM*, SM*, and HM* (where * is either nothing, _MIX or _FORM) are supported. Support for changing reference states planned but not yet implemented, so all thermodynamic quantities must be formation quantities (e.g. HM_FORM or HM_MIX, etc.).

The `values` key is the most complicated and care must be taken to avoid mistakes. `values` is a 3-dimensional array where each value is the `output` for a specific condition of pressure, temperature, and sublattice configurations from outside to inside. Alternatively, the size of the array must be `(len(P), len(T), len(subl_config))`. In the example below, the shape of the `values` array is (1, 12, 1) as there is one pressure scalar, one sublattice configuration, and 12 temperatures.

```
{
  "reference": "Yi Wang et al 2009",
  "components": ["AL", "NI", "VA"],
  "phases": ["BCC_B2"],
  "solver": {
    "sublattice_site_ratios": [0.5, 0.5, 1],
    "sublattice_configurations": [["AL", "NI", "VA"]],
    "comment": "NiAl sublattice configuration (2SL)"
  },
  "conditions": {
    "P": 101325,
    "T": [ 0, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 110]
  },
  "output": "CPM_FORM",
  "values": [[ [ 0 ],
               [-0.0173 ]]
```

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```

        [-0.01205],
        [ 0.12915],
        [ 0.24355],
        [ 0.13305],
        [-0.1617 ],
        [-0.51625],
        [-0.841  ],
        [-1.0975 ],
        [-1.28045],
        [-1.3997  ]]]
    }

```

In the second example below, there is formation enthalpy data for multiple sublattice configurations. All of the keys and values are conceptually similar. Here, instead of describing how the output quantity changes with temperature or pressure, we are instead only comparing HM_FORM values for different sublattice configurations. The key differences from the previous example are that there are 9 different sublattice configurations described by `sublattice_configurations` and `sublattice_occupancies`. Note that the `sublattice_configurations` and `sublattice_occupancies` should have exactly the same shape. Sublattices without mixing should have single strings and occupancies of one. Sublattices that do have mixing should have a site ratio for each active component in that sublattice. If the sublattice of a phase is ["AL", "NI", "VA"], it should only have two occupancies if only ["AL", "NI"] are active in the sublattice configuration.

The last difference to note is the shape of the values array. Here there is one pressure, one temperature, and 9 sublattice configurations to give a shape of (1, 1, 9).

```

{
  "reference": "C. Jiang 2009 (constrained SQS)",
  "components": ["AL", "NI", "VA"],
  "phases": ["BCC_B2"],
  "solver": {
    "sublattice_occupancies": [
      [1, [0.5, 0.5], 1],
      [1, [0.75, 0.25], 1],
      [1, [0.75, 0.25], 1],
      [1, [0.5, 0.5], 1],
      [1, [0.5, 0.5], 1],
      [1, [0.25, 0.75], 1],
      [1, [0.75, 0.25], 1],
      [1, [0.5, 0.5], 1],
      [1, [0.5, 0.5], 1]
    ],
    "sublattice_site_ratios": [0.5, 0.5, 1],
    "sublattice_configurations": [
      ["AL", ["NI", "VA"], "VA"],
      ["AL", ["NI", "VA"], "VA"],
      ["NI", ["AL", "NI"], "VA"],
      ["NI", ["AL", "NI"], "VA"],
      ["AL", ["AL", "NI"], "VA"],
      ["AL", ["AL", "NI"], "VA"],
      ["NI", ["AL", "VA"], "VA"],
      ["NI", ["AL", "VA"], "VA"],
      ["VA", ["AL", "NI"], "VA"]
    ],
    "comment": "BCC_B2 sublattice configuration (2SL)"
  },
  "conditions": {

```

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```

        "P": 101325,
        "T": 300
    },
    "output": "HM_FORM",
    "values": [[[-40316.61077, -56361.58554,
                  -49636.39281, -32471.25149, -10890.09929,
                  -35190.49282, -38147.99217, -2463.55684,
                  -15183.13371]]]
}

```

7.1.5 Multi-phase Data

The difference between single- and multi-phase data is in the absence of the `solver` key, since we are no longer concerned with individual site configurations, and the `values` key where we need to represent phase equilibria rather than thermodynamic quantities. Notice that the type of data we are entering in the `output` key is `ZPF` (zero-phase fraction) rather than `CP_FORM` or `H_MIX`. Each entry in the `ZPF` list is a list of all phases in equilibrium, here `[["AL3NI2", ["NI"], [0.4083]], ["BCC_B2", ["NI"], [0.4340]]]` where each phase entry has the name of the phase, the composition element, and the composition of the tie line point. If there is no corresponding tie line point, such as on a liquidus line, then one of the compositions will be `null`: `[["LIQUID", ["NI"], [0.6992]], ["BCC_B2", ["NI"], [null]]]`. Three- or n-phase equilibria are described as expected: `[["LIQUID", ["NI"], [0.752]], ["BCC_B2", ["NI"], [0.71]], ["FCC_L12", ["NI"], [0.76]]]`.

Note that for higher-order systems the component names and compositions are lists and should be of length $c-1$, where c is the number of components.

```

{
  "components": ["AL", "NI"],
  "phases": ["AL3NI2", "BCC_B2"],
  "conditions": {
    "P": 101325,
    "T": [1348, 1176, 977]
  },
  "output": "ZPF",
  "values": [
    [
      ["AL3NI2", ["NI"], [0.4083]], ["BCC_B2", ["NI"], [0.4340]],
      ["AL3NI2", ["NI"], [0.4114]], ["BCC_B2", ["NI"], [0.4456]],
      ["AL3NI2", ["NI"], [0.4114]], ["BCC_B2", ["NI"], [0.4532]]
    ],
    "reference": "37ALE"
  ]
}

```

7.1.6 Activity Data

Activity data is very similar to thermochemical data, except we must enter a reference state. Another minor detail is that non-endmember compositions must be represented by composition conditions rather than as sublattice occupancies because it's the result of equilibrium calculations where we cannot know the sublattice occupancies. An example for Cu-Mg activities follows, with data digitized from S.P. Garg, Y.J. Bhatt, C. V. Sundaram, Thermodynamic study of liquid Cu-Mg alloys by vapor pressure measurements, Metall. Trans. 4 (1973) 283–289. doi:10.1007/BF02649628.

```

{
  "components": ["CU", "MG", "VA"],

```

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```

"phases": ["LIQUID"],
"solver": {
  "mode": "manual",
  "sublattice_site_ratios": [1],
  "sublattice_configurations": [["CU", "MG"]]
},
"reference_state": {
  "phases": ["LIQUID"],
  "conditions": {
    "P": 101325,
    "T": 1200,
    "X_CU": 0.0
  }
},
"conditions": {
  "P": 101325,
  "T": 1200,
  "X_CU": [0.9, 0.8, 0.7, 0.6, 0.5, 0.4, 0.3, 0.2, 0.1, 0.0]
},

"output": "ACR_MG",
"values": [[0.0057, 0.0264, 0.0825, 0.1812, 0.2645, 0.4374, 0.5852, 0.7296, 0.882, 1.
↪ 0]],
"reference": "garg1973thermodynamic",
"comment": "Digitized Figure 3 and converted from activity coefficients."
}

```

7.1.7 Common Mistakes

1. A single element sublattice is different in a phase model ([["A", "B"], ["A"]]) than a sublattice configuration ([["A", "B"], "A"]).
2. Make sure you use the right units (J/mole-atom, mole fractions, Kelvin, Pascal)
3. Mixing configurations should not have ideal mixing contributions.

Part III

Reference

YAML input files

8.1 ESPEI YAML input files

This page aims to completely describe the ESPEI input file in the YAML format. Possibly useful links are the [YAML refcard](#) and the (possibly less useful) [Full YAML specification](#). These are all key value pairs in the format

```
key: value
```

They are nested for purely organizational purposes.

```
top_level_key:
  key: value
```

As long as keys are nested under the correct heading, they have no required order. All of the possible keys are

```
system:
  phase_models
  datasets

output:
  verbosity
  output_db
  tracefile
  probfile

generate_parameters:
  excess_model
  ref_state
  ridge_alpha

mcmc:
  iterations
  save_interval
  cores
```

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```
scheduler
input_db
restart_trace
chains_per_parameter
chain_std_deviation
deterministic
```

The next sections describe each of the keys individually. If a setting has a default of `required` it must be set explicitly.

8.1.1 system

The `system` key is intended to describe the specific system you are fitting, including the components, phases, and the data to fit to.

phase_models

type string

default required

The JSON file describing the CALPHAD models for each phase. See [Phase Descriptions](#) for an example of how to write this file.

datasets

type string

default required

The path to a directory containing JSON files of input datasets. The file extension to each of the datasets must be named as `.json`, but they can otherwise be named freely.

For an examples of writing these input JSON files, see [Making ESPEI datasets](#).

8.1.2 output

verbosity

type int

default 0

Controls the logging level.

Value	Log Level
0	Warning
1	Info
2	Debug

output_db

type string

default out.tdb

The database to write out. Can be any file format that can be written by a pycalphad [Database](#).

tracefile

type string

default trace.npy

Name of the file that the MCMC trace is written to. The array has shape (number of chains, iterations, number of parameters).

The array is preallocated and padded with zeros, so if you selected to take 2000 MCMC iterations, but only got through 1500, the last 500 values would be all 0.

You must choose a unique file name. An error will be raised if file specified by `tracefile` already exists.

probfile

type string

default Inprob.npy

Name of the file that the MCMC ln probabilities are written to. The array has shape (number of chains, iterations).

The array is preallocated and padded with zeros, so if you selected to take 2000 MCMC iterations, but only got through 1500, the last 500 values would be all 0.

You must choose a unique file name. An error will be raised if file specified by `probfile` already exists.

8.1.3 generate_parameters

The options in `generate_parameters` are used to control parameter selection and fitting to single phase data. This should be used if you have input thermochemical data, such as heat capacities and mixing energies.

Generate parameters will use the [Akaike information criterion](#) to select model parameters and fit them, creating a database.

excess_model

type string

default required

options linear

Which type of model to use for excess mixing parameters. Currently only *linear* is supported.

The *exponential* model is planned, as well as support for custom models.

ref_state

type string

default required

options SGTE91 | SR2016

The reference state to use for the pure elements and lattice stabilities. Currently only *SGTE91* and *SR2016* (for certain elements) is supported.

There are plans to extend to support custom reference states.

ridge_alpha

type float

default 1.0e-100

Controls the ridge regression hyperparameter, \$ \alpha \$, as given in the following equation for the ridge regression problem

$$\min_w ||Xw - y||_2^2 + \alpha ||w||_2^2$$

ridge_alpha should be a positive floating point number which scales the relative contribution of parameter magnitudes to the residuals.

If an exponential form is used, the floating point value must have a decimal place before the e, that is 1e-4 is invalid while 1.e-4 is valid. More generally, the floating point must match the following regular expression per the [YAML 1.1 spec](#): `[-+] ? ([0 - 9] [0 - 9 _] *) ? \ . [0 - 9 .] * ([e E] [- +] [0 - 9] +) ? .`

8.1.4 mcmc

The options in `mcmc` control how Markov Chain Monte Carlo is performed using the `emcee` package.

In order to run an MCMC fitting, you need to specify one and only one source of parameters somewhere in the input file. The parameters can come from including a `generate_parameters` step, or by specifying the `mcmc.input_db` key with a file to load as `pycalphad` Database.

If you choose to use the parameters from a database, you can then further control settings based on whether it is the first MCMC run for a system (you are starting fresh) or whether you are continuing from a previous run (a 'restart').

iterations

type int

default required

Number of iterations to perform in `emcee`. Each iteration consists of accepting one step for each chain in the ensemble.

save_interval

type int

default 1

Controls the interval (in number of iterations) for saving the MCMC chain and probability files. By default, new files will be written out every iteration. For large files (many mcmc iterations and chains per parameter), these might become expensive to write out to disk.

cores

type int

min 1

How many cores from available cores to use during parallelization with dask or emcee. If the chosen number of cores is larger than available, then this value is ignored and espei defaults to using the number available.

Cores does not take affect for MPIPool scheduler option. MPIPool requires the number of processors be set directly with MPI.

scheduler

type string

default dask

options dask | None | JSON file

Which scheduler to use for parallelization. You can choose from either *dask*, *None*, or pass the path to a JSON scheduler file created by dask-distributed.

Choosing dask allows for the choice of cores used through the cores key.

Choosing None will result in no parallel scheduler being used. This is useful for debugging.

Passing the path to a JSON scheduler file will use the resources set up by the scheduler. JSON file schedulers are most useful because schedulers can be started on MPI clusters using `dask-mpi` command. See [Advanced Schedulers](#) for more information.

input_db

type string

default null

A file path that can be read as a pycalphad [Database](#). The parameters to fit will be taken from this database.

For a parameter to be fit, it must be a symbol where the name starts with VV, e.g. VV0001. For a TDB formatted database, this means that the free parameters must be functions of a single value that are used in your parameters. For example, the following is a valid symbol to fit:

```
FUNCTION VV0000 298.15 10000; 6000 N !
```

restart_trace

type string

default null

If you have run a previous MCMC calculation, then you will have a trace file that describes the position and history of all of the chains from the run. You can use these chains to start the emcee run and pick up from where you left off in the MCMC run by passing the trace file (e.g. `chain.npy`) to this key.

If you are restarting from a previous calculation, you must also specify the same database file (with `input_db`) as you used to run that calculation.

chains_per_parameter

type int

default 2

This controls the number of chains to run in the MCMC calculation as an integer multiple of the number of parameters.

This parameter can only be used when initializing the first MCMC run. If you are restarting a calculation, the number of chains per parameter is fixed by the number you chose previously.

Ensemble samplers require at least $2 \times p$ chains for p fitting parameters to be able to make proposals. If `chains_per_parameter = 2`, then the number of chains if there are 10 parameters to fit is 20.

The value of `chains_per_parameter` must be an **EVEN integer**.

chain_std_deviation

type float

default 0.1

The standard deviation to use when initializing chains in a Gaussian distribution from a set of parameters as a fraction of the parameter.

A value of 0.1 means that for parameters with values $(-1.5, 2000, 50000)$ the chains will be initialized using those values as the mean and $(0.15, 200, 5000)$ as standard deviations for each parameter, respectively.

This parameter can only be used when initializing the first MCMC run. If you are restarting a calculation, the standard deviation for your chains are fixed by the value you chose previously.

You may technically set this to any positive value, you would like. Be warned that too small of a standard deviation may cause convergence to a local minimum in parameter space and slow convergence, while a standard deviation that is too large may cause convergence to meaningless thermodynamic descriptions.

deterministic

type bool

default True

Toggles whether ESPEI runs are deterministic. If this is True, running ESPEI with the same Database and initial settings (either the same `chains_per_parameter` and `chain_std_deviation` or the same `restart_trace`) will result in exactly the same results.

Starting two runs with the same TDB or with parameter generation (which is deterministic) will result in the chains being at exactly the same position after 100 iterations. If these are both restarted after 100 iterations for another 50 iterations, then the final chain after 150 iterations will be the same.

It is important to note that this is only explicitly True when *starting* at the same point. If Run 1 and Run 2 are started with the same initial parameters and Run 1 proceeds 50 iterations while Run 2 proceeds 100 iterations, restarting Run 1 for 100 iterations and Run 2 for 50 iterations (so they are both at 150 total iterations) will **NOT** give the same result.

9.1 Theory

ESPEI has two types of fitting – parameter generation and MCMC optimization. The parameter generation step uses experimental and DFT data of the Gibbs free energy derivatives (C_P , H , S) for each phase and for the mixing energies within sublattices for each phase to generate and fit parameters of given CALPHAD models. The MCMC optimization step uses a Bayesian optimization procedure to fit parameters in a Database to experimental phase equilibria.

9.1.1 Parameter generation

A simple model with few parameters is better than a complex model that describes the same data marginally better. Parameter generation in ESPEI aims to achieve a balance of a simple parameterization and goodness of fit in the Redlich-Kister polynomial used in CALPHAD assessments. To achieve this, parameters are selected using the corrected [Akaike information criterion](#) (AICc) to choose an optimal set of parameters from candidate parameterizations.

The general Redlich Kister polynomial has the form $G = a + bT + cT \ln T + \sum_n d_n T^n$. Different parameterizations, e.g. only considering a , considering a and b , a and c , etc. are fit to all of the input formation or mixing data (depending on the parameter being selected) by a least squares pseudo-inverse optimization.

Each parameterization is compared in the AICc and the most suitable optimization balances the goodness of fit and the number of parameters. The key aspect of this is that ESPEI will avoid overfitting your data and will not add parameters you do not have data for.

This is important for phases that would have a temperature dependent contribution to the Gibbs energy, but the input data only gives 0K formation energies. ESPEI cannot add temperature dependence to the parameterized model. Because of this, an abundance of single-phase data is critical to provide enough degrees of freedom in later optimization.

9.1.2 MCMC optimization

Details of Markov Chain Monte Carlo as an algorithm are better covered elsewhere. A good example is MacKay's (free) book: [Information Theory, Inference, and Learning Algorithms](#).

Using MCMC for optimizing CALPHAD models might appear to have several drawbacks. The parameters in the models are correlated and due to the nature of single phase first-principles data the shape and size of the posterior distribution for each parameter is not known before fitting. Traditional Metropolis-Hastings MCMC algorithms require the a prior to be defined for each parameter, which is a challenge for parameters in CALPHAD models which vary over more than 6 orders of magnitude.

ESPEI solves these potential problems by using an Ensemble sampler, as introduced by Goodman and Weare¹, rather than the Metropolis-Hastings algorithm. Ensemble samplers have the property of affine invariance, which uses multiple ($\geq 2N$ for N parameters) parallel chains to scale new proposal parameters by linear transforms. These chains, together an ensemble, define a proposal distribution to sample parameters from that is scaled to the magnitude and sensitivity of each parameter. Thus, Ensemble samplers directly address the challenges we expect to encounter with traditional MCMC.

ESPEI uses an Ensemble sampler algorithm by using the `emcee` package that implements parallelizable ensemble samplers. To use `emcee`, ESPEI defines the initial ensemble of chains and a function that returns the error as a log-probability. ESPEI defines the error as the mean square error between experimental phase equilibria and the equilibria calculated by the CALPHAD database.

Here, again, it is critical to point out the importance of abundant phase equilibria data. Traditional CALPHAD modeling has involved the modeler participating in tight feedback loops between updates to parameters and the resulting phase diagram. ESPEI departs from this by optimizing just a single scalar error function based on phase equilibria. The implication of this is that if there are phase equilibria that are observed to exist, but they are not in the datasets that are considered by ESPEI, those equilibria cannot be optimized against and may deviate from ‘known’ equilibria. A possible approach to address this in ESPEI is to estimate the points for the equilibria.

9.1.3 References

¹ Goodman, J. & Weare, J. Ensemble samplers with affine invariance. *Commun. Appl. Math. Comput. Sci.* 5, 65–80 (2010). doi:10.2140/camcos.2010.5.65.

10.1 Recipes

Here you can find some useful snippets of code to make using ESPEI easier.

10.1.1 Optimal parameter TDBs

Creating TDBs of optimal parameters from a tracefile and probfile:

```
"""
This script updates an input TDB file with the optimal parameters from an ESPEI run.

Change the capitalized variables to your desired input and output filenames.
"""

INPUT_TDB_FILENAME = 'CU-MG_param_gen.tdb'
OUTPUT_TDB_FILENAME = 'CU-MG_opt_params.tdb'
TRACE_FILENAME = 'trace.npy'
LNPROB_FILENAME = 'lnprob.npy'

import numpy as np
from pycalphad import Database
from espei.analysis import truncate_arrays
from espei.utils import database_symbols_to_fit, optimal_parameters

trace = np.load(TRACE_FILENAME)
lnprob = np.load(LNPROB_FILENAME)
trace, lnprob = truncate_arrays(trace, lnprob)

dbf = Database(INPUT_TDB_FILENAME)
opt_params = dict(zip(database_symbols_to_fit(dbf), optimal_parameters(trace,
↪ lnprob)))
```

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```
dbf.symbols.update(opt_params)
dbf.to_file(OUTPUT_TDB_FILENAME)
```

11.1 Advanced Schedulers

ESPEI uses dask-distributed for parallelization and provides an easy way to deploy clusters locally via TCP with the `mcmc.scheduler: dask` setting.

Sometimes ESPEI's dask scheduling options are not sufficiently flexible for different environments.

As an alternative to setting the cores with the `mcmc.scheduler: dask` setting, you can provide ESPEI with a scheduler file from dask that has information about how to connect to a dask parallel scheduler.

This is generally a two step process of

1. Starting a scheduler with workers and writing a scheduler file
2. Running ESPEI and connecting to the existing scheduler

In order to let the system manage the memory and prevent dask from pausing or killing workers, the memory limit should be set to zero.

11.1.1 Starting a scheduler

MPI-based dask scheduler

Dask provides a `dask-mpi` command that sets this up for you and creates a scheduler file to pass to ESPEI. The scheduler information will be serialized as a JSON file that you set in your ESPEI input file.

To start the scheduler and workers in the background, you can run the `dask-mpi` command (use `dask-mpi --help` to check the arguments). The following command will start a scheduler on the main MPI task, then a worker for each remaining MPI task that `mpirun` sees.

```
mpirun dask-mpi --scheduler-file my_scheduler.json --nthreads 1 --memory-limit 0 &
```

Generic scheduler

If you need further customization of dask schedulers, you can start a distributed Client any way you like, then write out the scheduler file for ESPEI to use.

For example, if you name the following file `start_scheduler.py`, you can run this Python script in the background, which will contain the scheduler and workers, then ESPEI will connect to it.

```
# start_scheduler.py
from distributed import Client, LocalCluster
from tornado.ioloop import IOLoop

if __name__ == '__main__':
    loop = IOLoop()
    cluster = LocalCluster(n_workers=4, threads_per_worker=1, memory_limit=0)
    client = Client(cluster)
    client.write_scheduler_file('my-scheduler.json')
    loop.start() # keeps the scheduler running
    loop.close()
```

Running `start_scheduler.py &`, will run this process in the background with 4 processes.

11.1.2 ESPEI Input

After starting the scheduler on the cluster, you run ESPEI like normal.

For the most part, this ESPEI input file is the same as you use locally, except the `scheduler` parameter is set to the name of your scheduler file.

Here is an example for multiphase fitting starting from a generated TDB with a scheduler file named `my-scheduler.json`:

```
system:
  phase_models: my-phases.json
  datasets: my-input-data
mcmc:
  iterations: 1000
  input_db: my-tdb.tdb
  scheduler: my-scheduler.json
```

11.1.3 Example Queue Script - MPI

To run on through a queueing system, you'll often use queue scripts that start batch jobs.

This example will create an MPI scheduler using `dask-mpi` via `mpirun` (or other MPI executable). Since many MPI jobs are run through batch schedulers, an example script for a PBS job looks like:

```
#!/bin/bash

#PBS -l nodes=1:ppn=20
#PBS -l walltime=48:00:00
#PBS -A open
#PBS -N espei-mpi
#PBS -o espei-mpi.out
#PBS -e espei-mpi.error
```

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```
# starts the scheduler on MPI and creates the scheduler file called 'my_scheduler.json'
↪ '
# you can replace this line with any script that starts a scheduler
# e.g. a `start_scheduler.py` file
# make sure it ends with `&` to run the process in the background
mpirun dask-mpi --scheduler-file my_scheduler.json --nthreads 1 --memory-limit 0 &

# runs ESPEI as normal
espei --in espei-mpi-input.yaml
```

11.1.4 References

See <http://distributed.readthedocs.io/en/latest/setup.html?highlight=dask-mpi#using-mpi> for more details.

11.2 API Documentation

11.2.1 espei package

Subpackages

espei.error_functions package

Submodules

espei.error_functions.activity_error module

Calculate error due to measured activities.

```
espei.error_functions.activity_error.calculate_activity_error(dbf, comps,
                                                             phases, datasets,
                                                             param-
                                                             eters=None,
                                                             phase_models=None,
                                                             callables=None,
                                                             grad_callables=None,
                                                             hess_callables=None,
                                                             massfuncs=None,
                                                             massgrad-
                                                             funcs=None)
```

Return the sum of square error from activity data

Parameters

- **dbf** (*pycalphad.Database*) – Database to consider
- **comps** (*list*) – List of active component names
- **phases** (*list*) – List of phases to consider
- **datasets** (*espei.utils.PickleableTinyDB*) – Datasets that contain single phase data

- **parameters** (*dict*) – Dictionary of symbols that will be overridden in pycalphad.equilibrium
- **phase_models** (*dict*) – Phase models to pass to pycalphad calculations
- **callables** (*dict*) – Callables to pass to pycalphad
- **grad_callables** (*dict*) – Gradient callables to pass to pycalphad
- **hess_callables** (*dict*) – Hessian callables to pass to pycalphad
- **massfuncs** (*dict*) – Callables of mass derivatives to pass to pycalphad
- **massgradfuncs** (*dict*) – Gradient callables of mass derivatives to pass to pycalphad

Returns A single float of the sum of square errors

Return type float

Notes

General procedure: 1. Get the datasets 2. For each dataset

1. Calculate reference state equilibrium
2. Calculate current chemical potentials
3. Find the target chemical potentials
4. Calculate error due to chemical potentials

`espei.error_functions.activity_error.chempot_error` (*sample_chempots*, *target_chempots*)

Return the sum of square error from chemical potentials

sample_chempots [numpy.ndarray] Calculated chemical potentials

target_activity [numpy.ndarray] Chemical potentials to target

Returns Error due to chemical potentials

Return type float

`espei.error_functions.activity_error.target_chempots_from_activity` (*component*, *target_activity*, *temperatures*, *reference_result*)

Return an array of experimental chemical potentials for the component

Parameters

- **component** (*str*) – Name of the component
- **target_activity** (*numpy.ndarray*) – Array of experimental activities
- **temperatures** (*numpy.ndarray*) – Ravelled array of temperatures (of same size as *exp_activity*).
- **reference_result** (*xarray.Dataset*) – Dataset of the equilibrium reference state. Should contain a single point calculation.

Returns Array of experimental chemical potentials

Return type numpy.ndarray

espei.error_functions.thermochemical_error module

Calculate error due to thermochemical quantities: heat capacity, entropy, enthalpy.

`espei.error_functions.thermochemical_error.calculate_points_array` (*phase_constituents*,
configuration,
occupancies=None)

Calculate the points array to use in pycalphad calculate calls.

Converts the configuration data (and occupancies for mixing data) into the points array by looking up the indices in the active phase constituents.

Parameters

- **phase_constituents** (*list*) – List of active constituents in a phase
- **configuration** (*list*) – List of the sublattice configuration
- **occupancies** (*list*) – List of sublattice occupancies. Required for mixing sublattices, otherwise takes no effect.

Returns

Return type numpy.ndarray

Notes

Errors will be raised if components in the configuration are not in the corresponding phase constituents sublattice.

`espei.error_functions.thermochemical_error.calculate_thermochemical_error` (*dbf*,
comps,
phases,
datasets,
parameters=None,
phase_models=None,
callable=None)

Calculate the weighted single phase error in the Database

Parameters

- **dbf** (*pycalphad.Database*) – Database to consider
- **comps** (*list*) – List of active component names
- **phases** (*list*) – List of phases to consider
- **datasets** (*espei.utils.PickleableTinyDB*) – Datasets that contain single phase data

- **parameters** (*dict*) – Dictionary of symbols that will be overridden in `picalphad.calculate`
- **phase_models** (*dict*) – Phase models to pass to `picalphad` calculations. Ideal mixing contributions must be removed.
- **callables** (*dict*) – Dictionary of `{output_property: callables_dict}` where `callables_dict` is a dictionary of `{‘callables’: {phase_name: callables}, ‘massfuncs’: {phase_name: callables}}` to pass to `picalphad`. These must have ideal mixing portions removed.

Returns A single float of the residual sum of square errors

Return type float

Notes

There are different single phase values, HM_MIX, SM_FORM, CP_FORM, etc. Each of these have different units and the error cannot be compared directly. To normalize all of the errors, a normalization factor must be used. Equation 2.59 and 2.60 in Lukas, Fries, and Sundman “Computational Thermodynamics” shows how this can be considered. Each type of error will be weighted by the reciprocal of the estimated uncertainty in the measured value and conditions. The weighting factor is calculated by $\$p_i = (\Delta L_i)^{-1}\$$ where ΔL_i is the uncertainty in the measurement. We will neglect the uncertainty for quantities such as temperature, assuming they are small.

```
espei.error_functions.thermochemical_error.get_prop_data(comps, phase_name,  
                                                         prop, datasets)
```

Return datasets that match the components, phase and property

Parameters

- **comps** (*list*) – List of components to get data for
- **phase_name** (*str*) – Name of the phase to get data for
- **prop** (*str*) – Property to get data for
- **datasets** (*espei.utils.PickleableTinyDB*) – Datasets to search for data

Returns List of dictionary datasets that match the criteria

Return type list

```
espei.error_functions.thermochemical_error.get_prop_samples(dbf, comps,  
                                                           phase_name, desired_data)
```

Return data values and the conditions to calculate them by `picalphad` calculate from the datasets

Parameters

- **dbf** (*picalphad.Database*) – Database to consider
- **comps** (*list*) – List of active component names
- **phase_name** (*str*) – Name of the phase to consider from the Database
- **desired_data** (*list*) – List of dictionary datasets that contain the values to sample

Returns Dictionary of condition kwargs for `picalphad`’s `calculate` and the expected values

Return type dict

espei.error_functions.zpf_error module

Calculate error due to ZPF tielines.

The general approach is similar to the PanOptimizer rough search method.

1. With all phases active, calculate the chemical potentials of the tieline endpoints via `equilibrium` calls. Done in `estimate_hyperplane`.
2. Calculate the target chemical potentials, which are the average chemical potentials of all of the current chemical potentials at the tieline endpoints.
3. Calculate the current chemical potentials of the desired single phases
4. The error is the difference between these chemical potentials

There's some special handling for tieline endpoints where we do not know the composition conditions to calculate chemical potentials at.

```
espei.error_functions.zpf_error.calculate_zpf_error(dbf, comps, phases, datasets,
                                                    phase_models, parameters=None, scheduler=None,
                                                    massfuncs=None, massgradfuncs=None, callables=None,
                                                    grad_callables=None, hess_callables=None)
```

Calculate error due to phase equilibria data

Parameters

- **dbf** (*pycalphad.Database*) – Database to consider
- **comps** (*list*) – List of active component names
- **phases** (*list*) – List of phases to consider
- **datasets** (*espei.utils.PickleableTinyDB*) – Datasets that contain single phase data
- **phase_models** (*dict*) – Phase models to pass to pycalphad calculations
- **parameters** (*dict*) – Dictionary of symbols that will be overridden in pycalphad.equilibrium
- **scheduler** (*class*) – Scheduler implementing a `get_sync` method
- **massfuncs** (*dict*) – Callables of mass derivatives to pass to pycalphad
- **massgradfuncs** (*dict*) – Gradient callables of mass derivatives to pass to pycalphad
- **callables** (*dict*) – Callables to pass to pycalphad
- **grad_callables** (*dict*) – Gradient callables to pass to pycalphad
- **hess_callables** (*dict*) – Hessian callables to pass to pycalphad

Returns List of errors from phase equilibria data

Return type list

```
espei.error_functions.zpf_error.estimate_hyperplane(dbf, comps, phases, current_statevars, comp_dicts,  
                                                    phase_models, parameters,  
                                                    massfuncs=None, massgradfuncs=None, callables=None,  
                                                    grad_callables=None,  
                                                    hess_callables=None)
```

Calculate the chemical potentials for a hyperplane, one vertex at a time

Parameters

- **dbf** (*pycalphad.Database*) – Database to consider
- **comps** (*list*) – List of active component names
- **phases** (*list*) – List of phases to consider
- **current_statevars** (*dict*) – Dictionary of state variables, e.g. v.P and v.T, no compositions.
- **comp_dicts** (*list*) – List of tuples of composition dictionaries and phase flags. Composition dictionaries are pycalphad variable dicts and the flag is a string e.g. ({v.X('CU'): 0.5}, 'disordered')
- **phase_models** (*dict*) – Phase models to pass to pycalphad calculations
- **parameters** (*dict*) – Dictionary of symbols that will be overridden in pycalphad.equilibrium
- **massfuncs** (*dict*) – Callables of mass derivatives to pass to pycalphad
- **massgradfuncs** (*dict*) – Gradient callables of mass derivatives to pass to pycalphad
- **callables** (*dict*) – Callables to pass to pycalphad
- **grad_callables** (*dict*) – Gradient callables to pass to pycalphad
- **hess_callables** (*dict*) – Hessian callables to pass to pycalphad

Returns Array of chemical potentials.

Return type numpy.ndarray

Notes

This takes just *one* set of phase equilibria, e.g. a dataset point of [['FCC_A1', ['CU'], [0.1]], ['LAVES_C15', ['CU'], [0.3]]] and calculates the chemical potentials given all the phases possible at the given compositions. Then the average chemical potentials of each end point are taken as the target hyperplane for the given equilibria.

```
espei.error_functions.zpf_error.tieline_error(dbf, comps, current_phase,  
                                              cond_dict, region_chemical_potentials,  
                                              phase_flag, phase_models, parameters,  
                                              debug_mode=False, massfuncs=None,  
                                              massgradfuncs=None, callables=None,  
                                              grad_callables=None,  
                                              hess_callables=None)
```

Parameters

- **dbf** (*pycalphad.Database*) – Database to consider
- **comps** (*list*) – List of active component names

- **current_phase** (*list*) – List of phases to consider
- **current_statevars** (*dict*) – Dictionary of state variables, e.g. v.P and v.T, no compositions.
- **comp_dicts** (*list*) – List of tuples of composition dictionaries and phase flags. Composition dictionaries are pycalphad variable dicts and the flag is a string e.g. ({v.X('CU'): 0.5}, 'disordered')
- **phase_models** (*dict*) – Phase models to pass to pycalphad calculations
- **parameters** (*dict*) – Dictionary of symbols that will be overridden in pycalphad.equilibrium
- **massfuncs** (*dict*) – Callables of mass derivatives to pass to pycalphad
- **massgradfuncs** (*dict*) – Gradient callables of mass derivatives to pass to pycalphad
- **callables** (*dict*) – Callables to pass to pycalphad
- **grad_callables** (*dict*) – Gradient callables to pass to pycalphad
- **hess_callables** (*dict*) – Hessian callables to pass to pycalphad
- **cond_dict** –
- **region_chemical_potentials** (*numpy.ndarray*) – Array of chemical potentials for target equilibrium hyperplane.
- **phase_flag** (*str*) – String of phase flag, e.g. 'disordered'.
- **phase_models** – Phase models to pass to pycalphad calculations
- **parameters** – Dictionary of symbols that will be overridden in pycalphad.equilibrium
- **debug_mode** (*bool*) – If True, will write out scripts when pycalphad fails to find a stable equilibrium. These scripts can be used to debug pycalphad.
- **massfuncs** – Callables of mass derivatives to pass to pycalphad
- **massgradfuncs** – Gradient callables of mass derivatives to pass to pycalphad
- **callables** – Callables to pass to pycalphad
- **grad_callables** – Gradient callables to pass to pycalphad
- **hess_callables** – Hessian callables to pass to pycalphad

Returns Single value for the total error between the current hyperplane and target hyperplane.

Return type float

Module contents

Functions for calculating error.

espei.parameter_selection package

Submodules

espei.parameter_selection.model_building module

Building candidate models

`espei.parameter_selection.model_building.build_candidate_models` (*configuration*,
features)

Return a dictionary of features and candidate models

Parameters

- **configuration** (*tuple*) – Configuration tuple, e.g. (('A', 'B', 'C'), 'A')
- **features** (*dict*) – Dictionary of {str: list} of generic features for a model, not considering the configuration. For example: {'CPM_FORM': [sympy.S.One, v.T, v.T**2, v.T**3]}

Returns Dictionary of {feature: [candidate_models]}

Return type dict

Notes

Currently only works for binary and ternary interactions.

Candidate models match the following spec: 1. Candidates with multiple features specified will have 2. orders of parameters (L0, L0 and L1, ...) have the same number of temperatures

Note that high orders of parameters with multiple temperatures are not required to contain all the temperatures of the low order parameters. For example, the following parameters can be generated L0: A L1: A + BT

`espei.parameter_selection.model_building.build_feature_sets` (*temperature_features*,
interaction_features)

Return a list of broadcasted features

Parameters

- **temperature_features** (*list*) – List of temperature features that will become a successive_list, such as [TlogT, T-1, T2]
- **interaction_features** (*list*) – List of interaction features that will become a successive_list, such as [YS, YS*Z, YS*Z**2]

Returns

Return type list

Notes

This allows two sets of features, e.g. [TlogT, T-1, T2] and [YS, YS*Z, YS*Z**2] and generates a list of feature sets where the temperatures and interactions are broadcasted successively.

Generates candidate feature sets like: L0: A + BT, L1: A L0: A , L1: A + BT

but **not** lists that are not successive: L0: A + BT, L1: Nothing, L2: A L0: Nothing, L1: A + BT

There's still some debate whether it makes sense from an information theory perspective to add a L1 B term without an L0 B term. However this might be more representative of how people usually model thermodynamics.

Does not distribute multiplication/sums or make assumptions about the elements of the feature lists. They can be strings, ints, objects, tuples, etc..

The number of features (related to the complexity) is a geometric series. For N temperature features and M interaction features, the total number of feature sets should be $N*(1-N**M)/(1-N)$. If $N=1$, then there are M total feature sets.

```
espei.parameter_selection.model_building.generate_interactions(endmembers,
                                                              order, symmetry)
```

Returns a list of sorted interactions of a certain order

Parameters

- **endmembers** (*list*) – List of tuples/strings of all endmembers (including symmetrically equivalent)
- **order** (*int*) – Highest expected interaction order, e.g. ternary interactions should be 3
- **symmetry** (*list of lists*) – List of lists containing symmetrically equivalent sublattice indices, e.g. `[[0, 1], [2, 3]]` means that sublattices 0 and 1 are equivalent and sublattices 2 and 3 are also equivalent.

Returns List of interaction tuples, e.g. `[('A', ('A', 'B'))]`

Return type list

```
espei.parameter_selection.model_building.generate_symmetric_group(configuration,
                                                                symmetry)
```

For a particular configuration and list of sublattices with symmetry, generate all the symmetrically equivalent configurations.

Parameters

- **configuration** (*tuple*) – Tuple of a sublattice configuration.
- **symmetry** (*list of lists*) – List of lists containing symmetrically equivalent sublattice indices, e.g. `[[0, 1], [2, 3]]` means that sublattices 0 and 1 are equivalent and sublattices 2 and 3 are also equivalent.

Returns Tuple of configuration tuples that are all symmetrically equivalent.

Return type tuple

```
espei.parameter_selection.model_building.make_successive(xs)
```

Return a list of successive combinations

Parameters **xs** (*list*) – List of elements, e.g. `[X, Y, Z]`

Returns List of combinations where each combination include all the preceding elements

Return type list

Examples

```
>>> make_successive(['W', 'X', 'Y', 'Z'])
[['W'], ['W', 'X'], ['W', 'X', 'Y'], ['W', 'X', 'Y', 'Z']]
```

`espei.parameter_selection.model_building.sorted_interactions` (*interactions*,
max_interaction_order,
symmetry)

Return interactions sorted by interaction order

Parameters

- **interactions** (*list*) – List of tuples/strings of potential interactions
- **max_interaction_order** (*int*) – Highest expected interaction order, e.g. ternary interactions should be 3
- **symmetry** (*list of lists*) – List of lists containing symmetrically equivalent sublattice indices, e.g. `[[0, 1], [2, 3]]` means that sublattices 0 and 1 are equivalent and sublattices 2 and 3 are also equivalent.

Returns Sorted list of interactions

Return type list

Notes

Sort by number of full interactions, e.g. (A:A,B) is before (A,B:A,B) The goal is to return a sort key that can sort through multiple interaction orders, e.g. (A:A,B,C), which should be before (A,B:A,B,C), which should be before (A,B,C:A,B,C).

espei.parameter_selection.selection module

Fit, score and select models

`espei.parameter_selection.selection.fit_model` (*feature_matrix*, *data_quantities*,
ridge_alpha)

Return model coefficients fit by scikit-learn's LinearRegression

Parameters

- **feature_matrix** (*ndarray*) – (M*N) regressor matrix. The transformed model inputs (*y_i*, *T*, *P*, etc.)
- **data_quantities** (*ndarray*) – (M,) response vector. Target values of the output (e.g. HM_MIX) to reproduce.
- **ridge_alpha** (*float*) – Value of the α hyperparameter used in ridge regression. Defaults to 1.0e-100, which should be degenerate with ordinary least squares regression. For now, the parameter is applied to all features.

Returns List of model coefficients of shape (N,)

Return type list

Notes

Solve $Ax = b$. *x* are the desired model coefficients. *A* is the 'feature_matrix'. *b* corresponds to 'data_quantities'.

`espei.parameter_selection.selection.score_model` (*feature_matrix*, *data_quantities*,
model_coefficients, *feature_list*,
rss_numerical_limit=1e-16)

Use the AICc to score a model that has been fit.

Parameters

- **feature_matrix** (*ndarray*) – (M*N) regressor matrix. The transformed model inputs (y_i, T, P, etc.)
- **data_quantities** (*ndarray*) – (M,) response vector. Target values of the output (e.g. HM_MIX) to reproduce.
- **model_coefficients** (*list*) – List of fitted model coefficients to be scored. Has shape (N,).
- **feature_list** (*list*) – Polynomial coefficients corresponding to each column of ‘feature_matrix’. Has shape (N,). Purely a logging aid.
- **rss_numerical_limit** (*float*) – Anything with an absolute value smaller than this is set to zero.

Returns A model score

Return type float

Notes

Solve $Ax = b$, where ‘feature_matrix’ is A and ‘data_quantities’ is b.

The likelihood function is a simple least squares with no regularization. The form of the AIC is valid under assumption all sample variances are random and Gaussian, model is univariate. It is assumed the model here is univariate with T.

`espei.parameter_selection.selection.select_model(candidate_models, ridge_alpha)`

Select a model from a series of candidates by fitting and scoring them

Parameters

- **candidate_models** (*list*) – List of tuples of (features, feature_matrix, data_quantities)
- **ridge_alpha** (*float*) – Value of the α hyperparameter used in ridge regression. Defaults to 1.0e-100, which should be degenerate with ordinary least squares regression. For now, the parameter is applied to all features.

Returns Tuple of (feature_list, model_coefficients) for the highest scoring model

Return type tuple

espei.parameter_selection.ternary_parameters module

Build fittable models for ternary parameter selection

`espei.parameter_selection.ternary_parameters.build_ternary_feature_matrix(prop, candidate_models, desired_data)`

Return an MxN matrix of M data sample and N features.

Parameters

- **prop** (*str*) – String name of the property, e.g. ‘HM_MIX’

- **candidate_models** (*list*) – List of SymPy parameters that can be fit for this property.
- **desired_data** (*dict*) – Full dataset dictionary containing values, conditions, etc.

Returns An MxN matrix of M samples (from desired data) and N features.

Return type `numpy.ndarray`

`espei.parameter_selection.ternary_parameters.get_muggianu_samples(desired_data)`

Return the data values from `desired_data`, transformed to interaction products. Specifically works for Muggianu extrapolation.

Parameters **desired_data** (*list*) – List of matched desired data, e.g. for a single property

Returns List of sample values that are properly transformed.

Return type `list`

Notes

Transforms data to interaction products, e.g. $YS*\{ \}^{\{xs\}}G=YS*XS*DXS^{\{n\}} \{ \}^{\{n\}}L$ Each tuple in the list is a tuple of (temperature, (site_fraction_product, interaction_product)) for each data sample Interaction product itself is a list that corresponds to the Muggianu corrected interactions products for components [I, J, K]

espei.parameter_selection.utils module

Tools used across parameter selection modules

`espei.parameter_selection.utils.interaction_test(configuration, order=None)`

Returns True if the configuration has an interaction

Parameters **order** (*int, optional*) – Specific order to check for. E.g. a value of 3 checks for ternary interactions

Returns True if there is an interaction.

Return type `bool`

Examples

```
>>> configuration = [['A'], ['A', 'B']]
>>> interaction_test(configuration)
True # has an interaction
>>> interaction_test(configuration, order=2)
True # has a binary interaction
>>> interaction_test(configuration, order=3)
False # has no ternary interaction
```

`espei.parameter_selection.utils.shift_reference_state(desired_data, feature_transform, fixed_model)`

Shift data to a new common reference state.

Module contents

`espei.tests` package

Submodules

`espei.tests.fixtures` module

Fixtures for use in tests

`espei.tests.test_core_utils` module

`espei.tests.test_core_utils.test_get_data_for_a_minimal_example()`
Given a dataset and the configuration pertaining to that dataset, we should find the values.

`espei.tests.test_core_utils.test_recursive_map()`
Test that recursive map function works

`espei.tests.test_datasets` module

`espei.tests.test_datasets.test_check_datasets_raises_on_misaligned_data()`
Passed datasets that have misaligned data and conditions should raise `DatasetError`.

`espei.tests.test_datasets.test_check_datasets_raises_with_incorrect_components()`
Passed datasets that have incorrect components entered vs. used should raise.

`espei.tests.test_datasets.test_check_datasets_raises_with_incorrect_zpf_phases()`
Passed datasets that have incorrect phases entered than used should raise.

`espei.tests.test_datasets.test_check_datasets_raises_with_malformed_sublattice_configuration()`
Passed datasets that have malformed ZPF values should raise.

`espei.tests.test_datasets.test_check_datasets_raises_with_malformed_zpf()`
Passed datasets that have malformed ZPF values should raise.

`espei.tests.test_datasets.test_check_datasets_raises_with_unsorted_interactions()`
Passed datasets that have sublattice interactions not in sorted order should raise.

`espei.tests.test_datasets.test_check_datasets_raises_with_zpf_fractions_greater_than_one()`
Passed datasets that have mole fractions greater than one should raise.

`espei.tests.test_datasets.test_check_datasets_run_on_good_data()`
Passed valid datasets that should raise `DatasetError`.

`espei.tests.test_datasets.test_check_datasets_works_on_activity_data()`
Passed activity datasets should work correctly.

`espei.tests.test_datasets.test_datasets_convert_thermochemical_string_values_producing_correct_value()`
Strings where floats are expected should give correct answers for thermochemical datasets

`espei.tests.test_datasets.test_datasets_convert_zpf_string_values_producing_correct_value()`
Strings where floats are expected should give correct answers for ZPF datasets

espei.tests.test_error_functions module

Test different error functions as isolated units.

`espei.tests.test_error_functions.test_activity_error(datasets_db)`

Test that activity error returns a correct result

`espei.tests.test_error_functions.test_thermochemical_error_for_mixing_entropy_error_is_excess_only(datasets_db)`

Tests that error in mixing entropy data is excess only (the ideal part is removed).

`espei.tests.test_error_functions.test_thermochemical_error_for_of_enthalpy_mixing(datasets_db)`

Tests that error in mixing entropy data is excess only (the ideal part is removed).

`espei.tests.test_error_functions.test_thermochemical_error_with_multiple_T_X_points(datasets_db)`

Multiple temperature and composition datapoints in a dataset for a mixing phase should be successful.

`espei.tests.test_error_functions.test_thermochemical_error_with_multiple_T_points(datasets_db)`

Multiple temperature datapoints in a dataset for a stoichiometric compound should be successful.

`espei.tests.test_error_functions.test_thermochemical_error_with_multiple_X_points(datasets_db)`

Multiple composition datapoints in a dataset for a mixing phase should be successful.

`espei.tests.test_error_functions.test_zpf_error_zero(datasets_db)`

Test that sum of square ZPF errors returns 0 for an exactly correct result

espei.tests.test_mcmc module

`espei.tests.test_mcmc.test_lnprob_calculates_multi_phase_probability_for_success(datasets_db)`

lnprob() successfully calculates the probability for equilibrium

`espei.tests.test_mcmc.test_lnprob_calculates_single_phase_probability_for_success(datasets_db)`

lnprob() successfully calculates the probability from single phase data

`espei.tests.test_mcmc.test_parameter_initialization()`

Deterministically generated parameters should match.

espei.tests.test_model_building module

Tests for building models for parameter selection

`espei.tests.test_model_building.test_binary_candidate_models_are_constructed_correctly()`

Candidate models should be generated for all valid combinations of possible models in the binary case

`espei.tests.test_model_building.test_build_feature_sets_generates_desired_binary_features_1()`

Binary feature sets can be correctly generated for heat capacity-like features

`espei.tests.test_model_building.test_build_feature_sets_generates_desired_binary_features_2()`

Binary feature sets can be correctly generated for enthalpy-like models

`espei.tests.test_model_building.test_build_feature_sets_generates_desired_ternary_features_1()`

Ternary feature sets can be correctly generated

`espei.tests.test_model_building.test_interaction_sorting_is_correct()`

High order (order >= 3) interactions should sort correctly

`espei.tests.test_model_building.test_symmetric_group_can_be_generated_for_2_sl_endmembers_1()`

A phase with symmetric sublattices should find a symmetric endmember

`espei.tests.test_model_building.test_symmetric_group_can_be_generated_for_2_sl_mixing_with_1()`

A phase with two sublattices that are mixing should generate a cross interaction

`espei.tests.test_model_building.test_ternary_candidate_models_are_constructed_correctly()`
 Candidate models should be generated for all valid combinations of possible models in the ternary case

espei.tests.test_parameter_generation module

The `test_parameter_generation` module tests that parameter selection is correct

`espei.tests.test_parameter_generation.test_asymmetric_ternary_parameters_can_be_generated()`
 3 asymmetric ternary parameters should be generated correctly.

`espei.tests.test_parameter_generation.test_asymmetric_ternary_parameters_can_be_generated_1()`
 3 asymmetric ternary parameters should be generated correctly in a 2 sublattice model.

`espei.tests.test_parameter_generation.test_formation_energies_are_fit(datasets_db)`
 Tests that given formation energy data, the parameter is fit.

`espei.tests.test_parameter_generation.test_mixing_data_is_excess_only(datasets_db)`
 Tests that given an entropy of mixing datapoint of 0, no excess parameters are fit (meaning datasets do not include ideal mixing).

`espei.tests.test_parameter_generation.test_mixing_energies_are_fit(datasets_db)`
 Tests that given mixing energy data, the excess parameter is fit.

`espei.tests.test_parameter_generation.test_mixing_energies_are_fit_with_higher_order_data(datasets_db)`
 Tests that given mixing energy data with high order terms, the excess parameter is fit.

`espei.tests.test_parameter_generation.test_mixing_energies_are_reduced_with_ridge_alpha(datasets_db)`
 Tests that given mixing energy data, the excess parameter is fit.

`espei.tests.test_parameter_generation.test_multi_sublattice_mixing_energies_are_fit(datasets_db)`
 Tests the correct excess parameter is fit for phases with multiple sublattices with vacancies.

`espei.tests.test_parameter_generation.test_sgte_reference_state_naming_is_correct_for_characters(datasets_db)`
 Elements with single character names should get the correct GHSER reference state name (V => GHSERVV)

`espei.tests.test_parameter_generation.test_symmetric_ternary_parameter_can_be_generated(datasets_db)`
 A symmetric ternary parameter should be generated correctly.

`espei.tests.test_parameter_generation.test_symmetric_ternary_parameter_can_be_generated_in_2_sublattice_model(datasets_db)`
 A symmetric ternary parameter should be generated correctly when low order binary data is also fit.

espei.tests.test_parameter_generation_utils module

Test the utilities for parameter generation

`espei.tests.test_parameter_generation_utils.test_interaction_detection()`
`interaction_test` should correctly calculate interactions for different candidate configurations

espei.tests.test_plotting module

Uses matplotlib functionality to test graphical outputs

espei.tests.test_schema module

Tests for input file validation

```
espei.tests.test_schema.test_SR2016_refdata()
```

`espei.tests.test_schema.test_chains_per_parameter_read_correctly()`
The chains per parameter option should take effect when passed.

```
espei.tests.test_schema.test_correct_defaults_are_applied_from_minimal_specification()
```

A minimal run should generate several default settings for i/o and optional settings.

```
espei.tests.test_schema.test_input_yaml_invalid_for_mcmc_when_input_is_overspecified()
```

An MCMC run must get input from only generate_parameters or an input tdb (w/ or w/o a restart).

```
espei.tests.test_schema.test_input_yaml_invalid_for_mcmc_when_input_not_defined()
```

An MCMC run must get input from generate_parameters, an input tdb, or a restart and input tdb.

```
espei.tests.test_schema.test_input_yaml_valid_for_full_run()
```

A minimal full run input file should validate

```
espei.tests.test_schema.test_input_yaml_valid_for_generate_parameters_only()
```

A minimal generate parameters only input file should validate

```
espei.tests.test_schema.test_input_yaml_valid_for_mcmc_from_restart()
```

A minimal mcmc run from a restart should validate

```
espei.tests.test_schema.test_input_yaml_valid_for_mcmc_from_tdb()
```

A minimal mcmc run from tdb input file should validate

espei.tests.test_utils module

Test espei.utils classes and functions.

```
espei.tests.test_utils.test_adding_bibtex_entries_to_bibliography_db(datasets_db)
```

Adding a BibTeX entries to a database works and the database can be searched.

```
espei.tests.test_utils.test_bib_marker_map()
```

bib_marker_map should return a proper dict

```
espei.tests.test_utils.test_flexible_open_string_file_like(tmp_file)
```

File-like objects support read methods should have their content returned by flexible_open_string.

```
espei.tests.test_utils.test_flexible_open_string_path_like(tmp_file)
```

Path-like strings should be opened, read and returned

```
espei.tests.test_utils.test_flexible_open_string_raw_string()
```

Raw multiline strings should be directly returned by flexible_open_string.

```
espei.tests.test_utils.test_immediate_client_returns_map_results_directly()
```

Calls ImmediateClient.map should return the results, instead of Futures.

```
espei.tests.test_utils.test_pickleable_tinydb_can_be_pickled_and_unpickled()
```

PickleableTinyDB should be able to be pickled and unpickled.

```
espei.tests.test_utils.test_sympy_build_functions_can_be_cloudpickled()
```

Wrapped, compiled code from build_functions should be pickleable by cloudpickle

espei.tests.testing_data module

Databases and datasets used in common tests

Module contents

Submodules

espei.analysis module

Tools for analyzing ESPEI runs

`espei.analysis.truncate_arrays` (*trace_array*, *prob_array=None*)

Return slides of ESPEI output arrays with any empty remaining iterations (zeros) removed.

Parameters

- **trace_array** (*np.ndarray*) – Array of the trace from an ESPEI run. Should have shape (chains, iterations, parameters)
- **prob_array** (*np.ndarray*) – Array of the Inprob output from an ESPEI run. Should have shape (chains, iterations)

Returns A slide of the zeros-removed trace array is returned if only the trace is passed. Otherwise a tuple of both the trace and Inprob are returned.

Return type *np.ndarray* or (*np.ndarray*, *np.ndarray*)

espei.core_utils module

Internal utilities for developer use. May not be useful to users.

`espei.core_utils.canonical_sort_key` (*x*)

Wrap strings in tuples so they'll sort.

Parameters *x* (*list*) – List of strings to sort

Returns tuple of strings that can be sorted

Return type tuple

`espei.core_utils.canonicalize` (*configuration*, *equivalent_sublattices*)

Sort a sequence with symmetry. This routine gives the sequence a deterministic ordering while respecting symmetry.

Parameters

- **configuration** (*[str]*) – Sublattice configuration to sort.
- **equivalent_sublattices** (*{{int}}*) – Indices of 'configuration' which should be equivalent by symmetry, i.e., *[[0, 4], [1, 2, 3]]* means permuting elements 0 and 4, or 1, 2 and 3, respectively, has no effect on the equivalence of the sequence.

Returns sorted tuple that has been canonicalized.

Return type *str*

`espei.core_utils.get_data` (*comps*, *phase_name*, *configuration*, *symmetry*, *datasets*, *prop*)

Return list of cleaned single phase datasets matching the passed arguments.

Parameters

- **comps** (*list*) – List of string component names
- **phase_name** (*str*) – Name of phase

- **configuration** (*tuple*) – Sublattice configuration as a tuple, e.g. (“CU”, (“CU”, “MG”))
- **symmetry** (*list of lists*) – List of sublattice indices with symmetry
- **datasets** (*espei.utils.PickleableTinyDB*) – Database of datasets to search for data
- **prop** (*list*) – String name of the property of interest.

Returns List of datasets matching the arguments.

Return type list

`espei.core_utils.get_samples(desired_data)`

Return the data values from `desired_data`, transformed to interaction products.

Parameters **desired_data** (*list*) – List of matched desired data, e.g. for a single property

Returns List of sample values that are properly transformed.

Return type list

Notes

Transforms data to interaction products, e.g. $YS*\{ \}^{\{xs\}}G=YS*XS*DXS^{\{n\}}\{ \}^{\{n\}}L$

`espei.core_utils.list_to_tuple(x)`

Convert a nested list to a tuple

`espei.core_utils.ravel_conditions(values, *conditions, **kwargs)`

Broadcast and flatten conditions to the shape dictated by the values.

Special handling for ZPF data that does not have nice array values.

Parameters

- **values** (*list*) – Multidimensional lists of values
- **conditions** (*list*) – List of conditions to broadcast. Must be the same length as the number of dimensions of the values array. In code, the following must be True: $\text{all}([s == \text{len}(\text{cond}) \text{ for } s, \text{cond} \text{ in } \text{zip}(\text{values.shape}, \text{conditions})])$
- **zpf** (*bool, optional*) – Whether to consider values as a special case of ZPF data (not an even grid of conditions) Default is False

Returns Tuple of ravelled conditions

Return type tuple

Notes

The current implementation of ZPF data only has the shape for one condition and this assumption is hardcoded in various places.

Here we try to be as general as possible by explicitly calculating the shape of the ZPF values.

A complication of this is that the user of this function must pass the correct conditions because usually T and P are specified in ZPF (but, again, only one can actually be a condition given the current shape).

`espei.core_utils.ravel_zpf_values(desired_data, independent_comps, conditions=None)`

Unpack the phases and compositions from ZPF data. Dependent components are converted to independent components.

Parameters

- **desired_data** (*espei.utils.PickleableTinyDB*) – The selected data
- **independent_comps** (*list*) – List of independent components. Used for mass balance component conversion
- **conditions** (*dict*) – Conditions to filter for. Right now only considers fixed temperatures

Returns A dictionary of list of lists of tuples. Each dictionary key is the number of phases in equilibrium, e.g. a key “2” might have values [[(PHASE_NAME_1, {'C1': X1, 'C2': X2}, refkey), (PHASE_NAME_2, {'C1': X1, 'C2': X2}, refkey)], ...] Three would have three inner tuples and so on.

Return type dict

`espei.core_utils.recursive_map(f, x)`

map, but over nested lists

Parameters

- **f** (*callable*) – Function to apply to x
- **x** (*list or value*) – Value passed to v

Returns

Return type list or value

`espei.core_utils.symmetry_filter(x, config, symmetry)`

Return True if the candidate sublattice configuration has any symmetry which matches the phase model symmetry.

Parameters

- **x** (*the candidate dataset 'solver' dict. Must contain the "sublattice_configurations" key*) –
- **config** (*the configuration of interest: e.g. ['AL', ['AL', 'NI'], 'VA']*) –
- **symmetry** (*tuple of tuples where each inner tuple is a group of equivalent*) – sublattices. A value of ((0, 1), (2, 3, 4)) means that sublattices at indices 0 and 1 are symmetrically equivalent to each other and sublattices at indices 2, 3, and 4 are symmetrically equivalent to each other.

Returns

Return type bool

espei.datasets module

exception `espei.datasets.DatasetError`

Bases: `Exception`

Exception raised when datasets are invalid.

`espei.datasets.check_dataset(dataset)`

Ensure that the dataset is valid and consistent.

Currently supports the following validation checks: * data shape is valid * phases and components used match phases and components entered * individual shapes of keys, such as ZPF, sublattice configs and site ratios

Planned validation checks: * all required keys are present

Note that this follows some of the implicit assumptions in ESPEI at the time of writing, such that conditions are only P, T, configs for single phase and essentially only T for ZPF data.

Parameters `dataset` (*dict*) – Dictionary of the standard ESPEI dataset.

Returns

Return type None

Raises `DatasetError` – If an error is found in the dataset

`espei.datasets.clean_dataset(dataset)`

Clean an ESPEI dataset dictionary.

Parameters `dataset` (*dict*) – Dictionary of the standard ESPEI dataset. `dataset` : dic

Returns Modified dataset that has been cleaned

Return type dict

Notes

Assumes a valid, checked dataset. Currently handles * Converting expected numeric values to floats

`espei.datasets.load_datasets(dataset_filenames)`

Create a PickleableTinyDB with the data from a list of filenames.

Parameters `dataset_filenames` (*[str]*) – List of filenames to load as datasets

Returns

Return type PickleableTinyDB

`espei.datasets.recursive_glob(start, pattern)`

Recursively glob for the given pattern from the start directory.

Parameters

- **start** (*str*) – Path of the directory to walk while for file globbing
- **pattern** (*str*) – Filename pattern to match in the glob

Returns List of matched filenames

Return type [str]

espei.espei_script module

Automated fitting script.

A minimal run must specify an input.json and a datasets folder containing input files.

`espei.espei_script.get_run_settings(input_dict)`

Validate settings from a dict of possible input.

Performs the following actions: 1. Normalize (apply defaults) 2. Validate against the schema

Parameters `input_dict` (*dict*) – Dictionary of input settings

Returns Validated run settings

Return type `dict`

Raises `ValueError`

`espei.espei_script.main()`

Handle starting ESPEI from the command line. Parse command line arguments and input file.

`espei.espei_script.run_espei(run_settings)`

Wrapper around the ESPEI fitting procedure, taking only a settings dictionary.

Parameters `run_settings` (*dict*) – Dictionary of input settings

Returns

Return type Either a Database (for generate parameters only) or a tuple of (Database, sampler)

espei.mcmc module

Module for running MCMC in ESPEI

MCMC uses an EnsembleSampler based on Goodman and Weare, Ensemble Samplers with Affine Invariance. Commun. Appl. Math. Comput. Sci. 5, 65-80 (2010).

`espei.mcmc.generate_parameter_distribution(parameters, num_samples, std_deviation, deterministic=True)`

Return an array of num_samples from a Gaussian distribution about each parameter.

Parameters

- **parameters** (*ndarray*) – 1D array of initial parameters that will be the mean of the distribution.
- **num_samples** (*int*) – Number of chains to initialize.
- **std_deviation** (*float*) – Fractional standard deviation of the parameters to use for initialization.
- **deterministic** (*bool*) – True if the parameters should be generated deterministically.

Returns

Return type `ndarray`

`espei.mcmc.lnprob(params, comps=None, dbf=None, phases=None, datasets=None, symbols_to_fit=None, phase_models=None, scheduler=None, massfuncs=None, massgradfuncs=None, callables=None, grad_callables=None, hess_callables=None, thermochemical_callables=None)`

Returns the error from multiphase fitting as a log probability.

`espei.mcmc.mcmc_fit(dbf, datasets, iterations=1000, save_interval=100, chains_per_parameter=2, chain_std_deviation=0.1, scheduler=None, tracefile=None, probfile=None, restart_trace=None, deterministic=True)`

Run Markov Chain Monte Carlo on the Database given datasets

Parameters

- **dbf** (*Database*) – A pycalphad Database to fit with symbols to fit prefixed with VV followed by a number, e.g. `VV0001`
- **datasets** (*PickleableTinyDB*) – A database of single- and multi-phase to fit

- **iterations** (*int*) – Number of trace iterations to calculate in MCMC. Default is 1000 iterations.
- **save_interval** (*int*) – interval of iterations to save the tracefile and profile
- **chains_per_parameter** (*int*) – number of chains for each parameter. Must be an even integer greater or equal to 2. Defaults to 2.
- **chain_std_deviation** (*float*) – standard deviation of normal for parameter initialization as a fraction of each parameter. Must be greater than 0. Default is 0.1, which is 10%.
- **scheduler** (*callable*) – Scheduler to use with emcee. Must implement a map method.
- **tracefile** (*str*) – filename to store the trace with NumPy.save. Array has shape (chains, iterations, parameters)
- **probfile** (*str*) – filename to store the log probability with NumPy.save. Has shape (chains, iterations)
- **restart_trace** (*np.ndarray*) – ndarray of the previous trace. Should have shape (chains, iterations, parameters)
- **deterministic** (*bool*) – If True, the emcee sampler will be seeded to give deterministic sampling draws. This will ensure that the runs with the exact same database, chains_per_parameter, and chain_std_deviation (or restart_trace) will produce exactly the same results.

Returns

- **dbf** (*Database*) – Resulting pycalphad database of optimized parameters
- **sampler** (*EnsembleSampler, ndarray*) – emcee sampler for further data wrangling

espei.paramselect module

The paramselect module handles automated parameter selection for linear models.

Automated Parameter Selection End-members

Note: All magnetic parameters from literature for now. Note: No fitting below 298 K (so neglect third law issues for now).

For each step, add one parameter at a time and compute AICc with max likelihood.

Cp - TlnT, T**2, T**-1, T**3 - 4 candidate models (S and H only have one required parameter each. Will fit in full MCMC procedure)

Choose parameter set with best AICc score.

`espei.paramselect.fit_formation_energy` (*dbf, comps, phase_name, configuration, symmetry, datasets, ridge_alpha=1e-100, features=None*)

Find suitable linear model parameters for the given phase. We do this by successively fitting heat capacities, entropies and enthalpies of formation, and selecting against criteria to prevent overfitting. The “best” set of parameters minimizes the error without overfitting.

Parameters

- **dbf** (*Database*) – pycalphad Database. Partially complete, so we know what degrees of freedom to fix.
- **comps** (*[str]*) – Names of the relevant components.
- **phase_name** (*str*) – Name of the desired phase for which the parameters will be found.

- **configuration** (*ndarray*) – Configuration of the sublattices for the fitting procedure.
- **symmetry** (*[[int]]*) – Symmetry of the sublattice configuration.
- **datasets** (*PickleableTinyDB*) – All the datasets desired to fit to.
- **ridge_alpha** (*float*) – Value of the α hyperparameter used in ridge regression. Defaults to 1.0e-100, which should be degenerate with ordinary least squares regression. For now, the parameter is applied to all features.
- **features** (*dict*) – Maps “property” to a list of features for the linear model. These will be transformed from “GM” coefficients e.g., {“CPM_FORM”: (v.T*sympy.log(v.T), v.T**2, v.T**-1, v.T**3)} (Default value = None)

Returns {feature: estimated_value}

Return type dict

```
espei.paramselect.fit_ternary_interactions(dbf, phase_name, symmetry, endmembers,
                                         datasets, ridge_alpha=0.0)
```

Fit ternary interactions for a database in place

Parameters

- **dbf** (*Database*) – pycalphad Database to add parameters to
- **phase_name** (*str*) – Name of the phase to fit
- **symmetry** (*list*) – List of symmetric sublattices, e.g. [[0, 1, 2], [3, 4]]
- **endmembers** (*list*) – List of endmember tuples, e.g. [(‘CU’, ‘MG’)]
- **datasets** (*PickleableTinyDB*) – TinyDB database of datasets
- **ridge_alpha** (*float*) – Value of the α hyperparameter used in ridge regression. Defaults to 1.0e-100, which should be degenerate with ordinary least squares regression. For now, the parameter is applied to all features.

Returns Modified the Database in place

Return type None

```
espei.paramselect.generate_parameters(phase_models, datasets, ref_state, excess_model,
                                     ridge_alpha=1e-100)
```

Generate parameters from given phase models and datasets

Parameters

- **phase_models** (*dict*) – Dictionary of components and phases to fit.
- **datasets** (*PickleableTinyDB*) – database of single- and multi-phase to fit.
- **ref_state** (*str*) – String of the reference data to use, e.g. ‘SGTE91’ or ‘SR2016’
- **excess_model** (*str*) – String of the type of excess model to fit to, e.g. ‘linear’
- **ridge_alpha** (*float*) – Value of the α hyperparameter used in ridge regression. Defaults to 1.0e-100, which should be degenerate with ordinary least squares regression. For now, the parameter is applied to all features.

Returns

Return type pycalphad.Database

```
espei.paramselect.get_next_symbol(dbf)
```

Return a string name of the next free symbol to set

Parameters **dbf** (*Database*) – pycalphad Database. Must have the `varcounter` attribute set to an integer.

Returns

Return type `str`

`espei.paramsselect.phase_fit` (*dbf, phase_name, symmetry, subl_model, site_ratios, datasets, refdata, ridge_alpha, aliases=None*)

Generate an initial CALPHAD model for a given phase and sublattice model.

Parameters

- **dbf** (*Database*) – pycalphad Database to add parameters to.
- **phase_name** (*str*) – Name of the phase.
- **symmetry** (*[[int]]*) – Sublattice model symmetry.
- **subl_model** (*[[str]]*) – Sublattice model for the phase of interest.
- **site_ratios** (*[float]*) – Number of sites in each sublattice, normalized to one atom.
- **datasets** (*PickleableTinyDB*) – All datasets to consider for the calculation.
- **refdata** (*dict*) – Maps tuple(element, phase_name) -> SymPy object defining energy relative to SER
- **ridge_alpha** (*float*) – Value of the α hyperparameter used in ridge regression. Defaults to 1.0e-100, which should be degenerate with ordinary least squares regression. For now, the parameter is applied to all features.
- **aliases** (*[str]*) – Alternative phase names. Useful for matching against reference data or other datasets. (Default value = None)

Returns Modifies the dbf.

Return type `None`

espei.plot module

Plotting of input data and calculated database quantities

`espei.plot.dataplot` (*comps, phases, conds, datasets, ax=None, plot_kwargs=None, tieline_plot_kwargs=None*)

Plot datapoints corresponding to the components, phases, and conditions.

Parameters

- **comps** (*list*) – Names of components to consider in the calculation.
- **phases** (*[]*) – Names of phases to consider in the calculation.
- **conds** (*dict*) – Maps StateVariables to values and/or iterables of values.
- **datasets** (*PickleableTinyDB*) –
- **ax** (*matplotlib.Axes*) – Default axes used if not specified.
- **plot_kwargs** (*dict*) – Additional keyword arguments to pass to the matplotlib plot function for points
- **tieline_plot_kwargs** (*dict*) – Additional keyword arguments to pass to the matplotlib plot function for tielines

Returns A plot of phase equilibria points as a figure

Return type matplotlib.Axes

Examples

```
>>> from espei.datasets import load_datasets, recursive_glob
>>> from espei.plot import dataplot
>>> datasets = load_datasets(recursive_glob('.', '*.json'))
>>> my_phases = ['BCC_A2', 'CUMG2', 'FCC_A1', 'LAVES_C15', 'LIQUID']
>>> my_components = ['CU', 'MG', 'VA']
>>> conditions = {v.P: 101325, v.T: (500, 1000, 10), v.X('MG'): (0, 1, 0.01)}
>>> dataplot(my_components, my_phases, conditions, datasets)
```

`espei.plot.eqdataplot` (*eq*, *datasets*, *ax=None*, *plot_kwargs=None*)

Plot datapoints corresponding to the components and phases in the eq Dataset. A convenience function for `dataplot`.

Parameters

- **eq** (*xarray.Dataset*) – Result of equilibrium calculation.
- **datasets** (*PickleableTinyDB*) – Database of phase equilibria datasets
- **ax** (*matplotlib.Axes*) – Default axes used if not specified.
- **plot_kwargs** (*dict*) – Keyword arguments to pass to `dataplot`

Returns

Return type A plot of phase equilibria points as a figure

Examples

```
>>> from pycalphad import equilibrium, Database, variables as v
>>> from pycalphad.plot.eqplot import eqplot
>>> from espei.datasets import load_datasets, recursive_glob
>>> datasets = load_datasets(recursive_glob('.', '*.json'))
>>> dbf = Database('my_databases.tdb')
>>> my_phases = list(dbf.phases.keys())
>>> eq = equilibrium(dbf, ['CU', 'MG', 'VA'], my_phases, {v.P: 101325, v.T: (500,
↪1000, 10), v.X('MG'): (0, 1, 0.01)})
>>> ax = eqplot(eq)
>>> ax = eqdataplot(eq, datasets, ax=ax)
```

`espei.plot.multiplot` (*dbf*, *comps*, *phases*, *conds*, *datasets*, *eq_kwargs=None*, *plot_kwargs=None*, *data_kwargs=None*)

Plot a phase diagram with datapoints described by datasets. This is a wrapper around `pycalphad.equilibrium`, `pycalphad`'s `eqplot`, and `dataplot`.

Parameters

- **dbf** (*Database*) – `pycalphad` thermodynamic database containing the relevant parameters.
- **comps** (*list*) – Names of components to consider in the calculation.
- **phases** (*list*) – Names of phases to consider in the calculation.
- **conds** (*dict*) – Maps StateVariables to values and/or iterables of values.

- **datasets** (*PickleableTinyDB*) – Database of phase equilibria datasets
- **eq_kwargs** (*dict*) – Keyword arguments passed to pycalphad equilibrium()
- **plot_kwargs** (*dict*) – Keyword arguments passed to pycalphad eqplot()
- **data_kwargs** (*dict*) – Keyword arguments passed to dataplot()

Returns

Return type A phase diagram with phase equilibria data as a figure

Examples

```
>>> from pycalphad import Database, variables as v
>>> from pycalphad.plot.eqplot import eqplot
>>> from espei.datasets import load_datasets, recursive_glob
>>> datasets = load_datasets(recursive_glob('.', '*.json'))
>>> dbf = Database('my_databases.tdb')
>>> my_phases = list(dbf.phases.keys())
>>> multiplot(dbf, ['CU', 'MG', 'VA'], my_phases, {v.P: 101325, v.T: 1000, v.X('MG
↪'): (0, 1, 0.01)}, datasets)
```

`espei.plot.plot_parameters` (*dbf*, *comps*, *phase_name*, *configuration*, *symmetry*, *datasets=None*,
fig=None, *require_data=True*)

Plot parameters of interest compared with data in subplots of a single figure

Parameters

- **dbf** (*Database*) – pycalphad thermodynamic database containing the relevant parameters.
- **comps** (*list*) – Names of components to consider in the calculation.
- **phase_name** (*str*) – Name of the considered phase phase
- **configuration** (*tuple*) – Sublattice configuration to plot, such as ('CU', 'CU') or (('CU', 'MG'), 'CU')
- **symmetry** (*list*) – List of lists containing indices of symmetric sublattices e.g. [[0, 1], [2, 3]]
- **datasets** (*PickleableTinyDB*) – ESPEI datasets to compare against. If None, nothing is plotted.
- **fig** (*matplotlib.Figure*) – Figure to create with axes as subplots.
- **require_data** (*bool*) – If True, plot parameters that have data corresponding data. Defaults to True. Will raise an error for non-interaction configurations.

Returns

Return type None

Examples

```
# plot the LAVES_C15 (Cu)(Mg) endmember >>> plot_parameters(dbf, ['CU', 'MG'], 'LAVES_C15',
('CU', 'MG'), symmetry=None, datasets=datasets) # plot the mixing interaction in the first sublattice
>>> plot_parameters(dbf, ['CU', 'MG'], 'LAVES_C15', (('CU', 'MG'), 'MG'), symmetry=None,
datasets=datasets)
```

espei.refdata module

Create a new *Mock* object. *Mock* takes several optional arguments that specify the behaviour of the Mock object:

- *spec*: This can be either a list of strings or an existing object (a class or instance) that acts as the specification for the mock object. If you pass in an object then a list of strings is formed by calling `dir` on the object (excluding unsupported magic attributes and methods). Accessing any attribute not in this list will raise an *AttributeError*.

If *spec* is an object (rather than a list of strings) then `mock.__class__` returns the class of the spec object. This allows mocks to pass *isinstance* tests.

- *spec_set*: A stricter variant of *spec*. If used, attempting to *set* or get an attribute on the mock that isn't on the object passed as *spec_set* will raise an *AttributeError*.
- *side_effect*: A function to be called whenever the Mock is called. See the *side_effect* attribute. Useful for raising exceptions or dynamically changing return values. The function is called with the same arguments as the mock, and unless it returns *DEFAULT*, the return value of this function is used as the return value.

If *side_effect* is an iterable then each call to the mock will return the next value from the iterable. If any of the members of the iterable are exceptions they will be raised instead of returned.

- *return_value*: The value returned when the mock is called. By default this is a new Mock (created on first access). See the *return_value* attribute.
- *wraps*: Item for the mock object to wrap. If *wraps* is not None then calling the Mock will pass the call through to the wrapped object (returning the real result). Attribute access on the mock will return a Mock object that wraps the corresponding attribute of the wrapped object (so attempting to access an attribute that doesn't exist will raise an *AttributeError*).

If the mock has an explicit *return_value* set then calls are not passed to the wrapped object and the *return_value* is returned instead.

- *name*: If the mock has a name then it will be used in the repr of the mock. This can be useful for debugging. The name is propagated to child mocks.

Mocks can also be called with arbitrary keyword arguments. These will be used to set attributes on the mock after it is created.

espei.rstate module

espei.utils module

Utilities for ESPEI

Classes and functions defined here should have some reuse potential.

`espei.utils.add_bibtex_to_bib_database(bibtex, bib_db=None)`

Add entries from a BibTeX file to the bibliography database

Parameters

- **bibtex** (*str*) – Either a multiline string, a path, or a file-like object of a BibTeX file
- **bib_db** (*PickleableTinyDB*) – Database to put the BibTeX entries. Defaults to a module-level default database

Returns

Return type The modified bibliographic database

`espei.utils.bib_marker_map(bib_keys, markers=None)`

Return a dict with reference keys and marker dicts

Parameters

- **bib_keys** –
- **markers** (*list*) – List of 2-tuples of ('fillstyle', 'marker') e.g. [('top', 'o'), ('full', 's')]. Defaults to cycling through the filled markers, the different fill styles.

Returns Dictionary with bib_keys as keys, dict values of formatted strings and marker dicts

Return type dict

Examples

```
>>> bib_marker_map(['otis2016', 'bocklund2018'])
{
  'bocklund2018': {
    'formatted': 'bocklund2018',
    'markers': {'fillstyle': 'full', 'marker': 'o'}
  },
  'otis2016': {
    'formatted': 'otis2016',
    'markers': {'fillstyle': 'full', 'marker': 'v'}
  }
}
```

`espei.utils.build_sitefractions` (*phase_name*, *sublattice_configurations*, *sublattice_occupancies*)

Convert nested lists of sublattice configurations and occupancies to a list of dictionaries. The dictionaries map SiteFraction symbols to occupancy values. Note that zero occupancy site fractions will need to be added separately since the total degrees of freedom aren't known in this function.

Parameters

- **phase_name** (*str*) – Name of the phase
- **sublattice_configurations** (*[[str]]*) – sublattice configuration
- **sublattice_occupancies** (*[[float]]*) – occupancy of each sublattice

Returns a list of site fractions over sublattices

Return type `[[float]]`

`espei.utils.database_symbols_to_fit` (*dbf*, *symbol_regex*='`^V[V]?([0-9]+)$`')

Return names of the symbols to fit that match the regular expression

Parameters

- **dbf** (*Database*) – pycalphad Database
- **symbol_regex** (*str*) – Regular expression of the fitting symbols. Defaults to V or VV followed by one or more numbers.

Returns

Return type list

`espei.utils.endmembers_from_interaction` (*configuration*)

For a given configuration with possible interactions, return all the endmembers

`espei.utils.eq_callables_dict` (*dbf*, *comps*, *phases*, *model*=None, *param_symbols*=None, *output*='GM', *build_gradients*=True)

Create a dictionary of callable dictionaries for phases in equilibrium

Parameters

- **dbf** (*pycalphad.Database*) – A pycalphad Database object
- **comps** (*list*) – List of component names
- **phases** (*list*) – List of phase names
- **model** (*dict or type*) – Dictionary of {phase_name: Model subclass} or a type corresponding to a Model subclass. Defaults to `Model`.
- **param_symbols** (*list*) – SymPy Symbol objects that will be preserved in the callable functions.
- **output** (*str*) – Output property of the particular Model to sample
- **build_gradients** (*bool*) – Whether or not to build gradient functions. Defaults to `True`.

Returns Dictionary of keyword argument callables to pass to equilibrium.

Return type dict

Notes

Based on the pycalphad equilibrium method for building phases as of commit 37ff75ce.

Examples

```
>>> dbf = Database('AL-NI.tdb')
>>> comps = ['AL', 'NI', 'VA']
>>> phases = ['FCC_L12', 'BCC_B2', 'LIQUID', 'AL3NI5', 'AL3NI2', 'AL3NI']
>>> eq_callables = eq_callables_dict(dbf, comps, phases)
>>> equilibrium(dbf, comps, phases, conditions, **eq_callables)
```

`espei.utils.flexible_open_string(obj)`

Return the string of an object that is either file-like, a file path, or the raw string.

Parameters **obj** (*string-like or file-like*) – Either a multiline string, a path, or a file-like object

Returns

Return type str

`espei.utils.formatted_constituent_array(constituent_array)`

Given a constituent array of Species, return the classic CALPHAD-style interaction.

Parameters **constituent_array** (*list*) – List of sublattices, which are lists of Species in that sublattice

Returns String of the constituent array formatted in the classic CALPHAD style

Return type str

Examples

```
>>> from pycalphad import variables as v
>>> const_array = [[v.Species('CU'), v.Species('MG')], [v.Species('MG')]]
>>> formatted_constituent_array(const_array)
'CU,MG:MG'
```

`espei.utils.formatted_parameter` (*dbf, symbol, unique=True*)

Get the deconstructed pretty parts of the parameter/term a symbol belongs to in a Database.

Parameters

- **dbf** (*pycalphad.Database*) –
- **symbol** (*string or sympy.Symbol*) – Symbol in the Database to get the parameter for.
- **unique** (*bool*) – If True, will raise if more than one parameter containing the symbol is found.

Returns A named tuple with the following attributes: *phase_name*, *interaction*, *symbol*, *term*, *parameter_type* or *term_symbol* (which is just the Symbol * temperature term)

Return type FormattedParameter

`espei.utils.get_pure_elements` (*dbf, comps*)

Return a list of pure elements in the system

Parameters

- **dbf** (*pycalphad.Database*) – A Database object
- **comps** (*list*) – A list of component names (species and pure elements)

Returns A list of pure elements in the Database

Return type list

`espei.utils.optimal_parameters` (*trace_array, lnprob_array, kth=0*)

Return the optimal parameters in the trace based on the highest likelihood. If *kth* is specified, return the *kth* set of *unique* optimal parameters.

Parameters

- **trace_array** (*ndarray*) – Array of shape (number of chains, iterations, number of parameters)
- **lnprob_array** (*ndarray*) – Array of shape (number of chains, iterations)
- **kth** (*int*) – Zero-indexed optimum. 0 (the default) is the most optimal solution. 1 is the second most optimal, etc.. Only *unique* solutions will be returned.

Returns

Return type Array of optimal parameters

Notes

It is ok if the calculation did not finish and the arrays are padded with zeros. The number of chains and iterations in the trace and lnprob arrays must match.

`espei.utils.parameter_term` (*expression, symbol*)

Determine the term, e.g. $T \cdot \log(T)$ that belongs to the symbol in expression

Parameters

- **expression** –

- **symbol** –

`espei.utils.sigfigs(x, n)`

Round x to n significant digits

Module contents

ESPEI

Part IV

Developer

12.1 Contributing to ESPEI

This is the place to start as a new ESPEI contributor.

The next sections lay out the basics of getting an ESPEI development set up and the development standards. Then the *Software design* sections walk through the key parts of the codebase.

12.1.1 Installing in develop mode

It is suggested to use ESPEI in development mode if you will be contributing features to the source code. As usual, you should install ESPEI into a virtual environment.

All of the dependencies can be installed either by conda or pip.

Then clone the source and install ESPEI in development mode with pip:

```
git clone https://github.com/PhasesResearchLab/espei.git
pip install --editable espei
```

Even if you use Anaconda, it is recommended that you use either `pip` or `python setup.py develop` to install ESPEI in development mode. This is because the `conda-build` tool, which would typically be used for this, is not well maintained at the time of writing.

Develop mode on Windows

Because of compiler issues, ESPEI's dependencies are challenging to install on Windows. As mentioned above, ideally the `conda-build` tool could be used, but it is not able to be used. Therefore the recommended way to install ESPEI is to

1. Install ESPEI into a virtual environment from Anaconda, pulling all of the packages with it
2. Remove ESPEI without removing the other packages

3. Install ESPEI in develop mode with pip or setuptools from the source repository

The steps to do this on the command line are as follows

```
conda create -n espe_i_dev espe_i
activate espe_i_dev
conda remove --force espe_i
git clone https://github.com/PhasesResearchLab/espe_i.git
pip install --editable espe_i
```

12.1.2 Tests

Even though much of ESPEI is devoted to being a multi-core, stochastic user tool, we strive to test all logic and functionality. We are continuously maintaining tests and writing tests for previously untested code.

As a general rule, any time you write a new function or modify an existing function you should write or maintain a test for that function.

ESPEI uses `pytest` as a test runner.

Some tips for testing:

- Ideally you would practicing test driven development by writing tests of your intended results before you write the function.
- If possible, keep the tests small and fast. If you do have a long running tests (longer than ~15 second run time) mark the test with the `@pytest.mark.slow` decorator.
- See the [NumPy/SciPy testing guidelines](#) for more tips

12.1.3 Style

Code style

For most naming and style, follow [PEP8](#). One exception to PEP8 is regarding the line length, which we suggest a 120 character maximum, but may be longer within reason.

Code documentation

ESPEI uses the [NumPy documentation](#) style. All functions and classes should be documented with at least a description, parameters, and return values, if applicable.

Using `Examples` in the documentation is especially encouraged for utilities that are likely to be run by users. See `espe_i.plot.multiplot()` for an example.

If you add any new external (non-ESPEI) imports in any code, they must be added to the `MOCK_MODULES` list in `docs/conf.py`.

Web documentation

Documentation on ESPEI is split into user tutorials, reference and developer documentation.

- Tutorials are resources for users new to ESPEI or new to certain features of ESPEI to be *guided* through typical actions.

- Reference pages should be concise articles that explain how to complete specific goals for users who know what they want to accomplish.
- Developer documentation should describe what should be considered when contributing source code back to ESPEI.

You can check changes you make to the documentation by going to the documentation folder in the root repository `cd docs/`. Running the command `make html && cd build/html && python3 -m http.server && cd ../.. && make clean` from that folder will build the docs and run them on a local HTTP server. You can see the documentation when the server is running by visiting the URL at the end of the output, usually `localhost port 8000 <http://0.0.0.0:8000>`_`. When you are finished, type `Ctrl-C` to stop the server and the command will clean up the build for you.

Make sure to fix any warnings that come up if you are adding documentation.

12.1.4 Logging

Since ESPEI is intended to be run by users, we must provide useful feedback on how their runs are progressing. ESPEI uses the logging module to allow control over verbosity of the output.

There are 5 different logging levels provided by Python. They should be used as follows:

Critical or Error (`logging.critical` or `logging.error`) Never use these. These log levels would only be used when there is an unrecoverable error that requires the run to be stopped. In that case, it is better to `raise` an appropriate error instead.

Warning (`logging.warning`) Warnings are best used when we are able to recover from something bad that has happened. The warning should inform the user about potentially incorrect results or let them know about something they have the potential to fix. Again, anything unrecoverable should not be logged and should instead be raised with a good error message.

Info (`logging.info`) Info logging should report on the progress of the program. Usually info should give feedback on milestones of a run or on actions that were taken as a result of a user setting. An example of a milestone is starting and finishing parameter generation. An example of an action taken as a result of a user setting is the logging of the number of chains in an mcmc run.

Debug (`logging.debug`) Debugging is the lowest level of logging we provide in ESPEI. Debug messages should consist of possibly useful information that is beyond the user's direct control. Examples are the values of initial parameters, progress of checking datasets and building phase models, and the acceptance ratios of MCMC iterations.

13.1 Software design

The following sections elaborate on the design principles on the software side. The goal is to make it clear how different modules in ESPEI fit together and where to find specific functionality to override or improve.

ESPEI provides tools to

1. Parameterize CALPHAD models by optimizing the compromise between model accuracy and complexity. We typically call this parameter generation or model selection.
2. Fit parameterized CALPHAD models to multi-phase or other custom data with uncertainty quantification via Markov chain Monte Carlo

13.1.1 API

ESPEI has two levels of API that users should expect to interact with:

1. Input from YAML files on the command line (via `espei --input <input_file>` or by Python via the `espei.espei_script.run_espei` function)
2. Work directly with the Python functions for parameter selection `espei.paramselect.generate_parameters` and MCMC `espei.mcmc.mcmc_fit`

YAML files are the recommended way to use ESPEI and should have a way to express most if not all of the options that the Python functions support. The schema for YAML files is located in the root of the ESPEI directory as `input-schema.yaml` and is validated in the `espei_script.py` module by the [Cerberus](#) package.

13.1.2 Module Hierarchy

- `espei_script.py` is the main entry point for the YAML input API.
- `paramselect.py` is where parameter generation happens.
- `mcmc.py` creates the likelihood function and runs MCMC.

- `error_functions` is a package with modules for each type of likelihood function.
- `parameter_selection` is a package with core pieces of parameter selection.
- `utils.py` are utilities with reuse potential across several parts of ESPEI.
- `plot.py` holds plotting functions.
- `datasets.py` manages validating and loading datasets into a TinyDB in memory database.
- `core_utils.py` are legacy utility functions that should be refactored out to be closer to individual modules and packages where they are used.

13.1.3 Parameter selection

Parameter selection goes through the `generate_parameters` function in the `espei.paramsselect` module. The goal of parameter selection is go through each phase (one at a time) and fit a CALPHAD model to the data.

For each phase, the endmembers are fit first, followed by binary and ternary interactions. For each individual endmember or interaction to fit, a series of candidate models are generated that have increasing complexity in both temperature and interaction order (an L0 excess parameter, L0 and L1, ...).

Each model is then fit by `espei.parameter_selection.selection.fit_model`, which currently uses a simple pseudo-inverse linear model from scikit-learn. Then the tradeoff between the goodness of fit and the model complexity is scored by the AICc (see [Theory](#)) in `espei.parameter_selection.selection.score_model`. The optimal scoring model is accepted as the model with the fit model parameters set as degrees of freedom for the MCMC step.

The main principle is that ESPEI transforms the data and candidate models to vectors and matrices that fit a typical machine learning type problem of $Ax = b$. Extending ESPEI to use different or custom models in the current scheme basically comes down to formulating candidate models in terms of this type of problem. The main ways to improve on the fitting or scoring methods used in parameter selection is to override the fit and score functions.

Currently the capabilities for providing custom models or contributions (e.g. magnetic data) in the form of generic pycalphad Model objects are limited. This is also true for custom types of data that one would use in fitting a custom model.

13.1.4 MCMC optimization and uncertainty quantification

Most of the Markov chain Monte Carlo optimization and uncertainty quantification happen in the `espei.mcmc` module through the `espei.mcmc.mcmc_fit` function.

The main reason ESPEI's parameter selection and MCMC routines are split up is that custom Models or existing TDB files can be provided and fit. In other words, if you are using a model that doesn't need parameter selection or is for a property that is not Gibbs energy, MCMC can fit it with uncertainty quantification.

The general process is

1. Take a database with degrees of freedom as database symbols named `VV####`, where `####` is a number, e.g. `0001`. The symbols correspond to `FUNCTION` in the TDB files.
2. Initialize those degrees of freedom to a starting distribution for ensemble MCMC (see [Theory](#)). The starting distribution is controlled by the `espei.mcmc.generate_parameter_distribution` function, which currently supports initializing the parameters to a Gaussian ball.
3. Use the `emcee` package to run ensemble MCMC

ESPEI's MCMC is quite flexible for customization. To fit a custom model, it just needs to be read by pycalphad and have correctly named degrees of freedom (`VV####`).

To fit an existing or custom model to new types of data, just write a function that takes in datasets and the parameters that are required to calculate the values (e.g. pycalphad Database, components, phases, ...) and returns the error. Then override the `espei.mcmc.lnprob` function to include your custom error contribution. There are examples of these functions `espei.error_functions` that ESPEI uses by default.

In addition, custom starting distributions can be obtained by overriding `espei.mcmc.generate_parameter_distribution`.

Part V

Appendix

14.1 Getting Help

For help on installing and using ESPEI, please join the [PhasesResearchLab/ESPEI Gitter room](#).

Bugs and software issues should be reported on [GitHub](#).

14.2 License

ESPEI is MIT licensed.

The MIT License (MIT)

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14.3 Citing ESPEI

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e

`espei.utils`, 79

`espei`, 83
`espei.analysis`, 69
`espei.core_utils`, 69
`espei.datasets`, 71
`espei.error_functions`, 59
`espei.error_functions.activity_error`, 53
`espei.error_functions.thermochemical_error`, 55
`espei.error_functions.zpf_error`, 57
`espei.espei_script`, 72
`espei.mcmc`, 73
`espei.parameter_selection`, 65
`espei.parameter_selection.model_building`, 60
`espei.parameter_selection.selection`, 62
`espei.parameter_selection.ternary_parameters`, 63
`espei.parameter_selection.utils`, 64
`espei.paramselect`, 74
`espei.plot`, 76
`espei.refdata`, 79
`espei.rstate`, 79
`espei.tests`, 69
`espei.tests.fixtures`, 65
`espei.tests.test_core_utils`, 65
`espei.tests.test_datasets`, 65
`espei.tests.test_error_functions`, 66
`espei.tests.test_mcmc`, 66
`espei.tests.test_model_building`, 66
`espei.tests.test_parameter_generation`, 67
`espei.tests.test_parameter_generation_utils`, 67
`espei.tests.test_plotting`, 67
`espei.tests.test_schema`, 67
`espei.tests.test_utils`, 68
`espei.tests.testing_data`, 68

A

`add_bibtex_to_bib_database()` (in module `espei.utils`), 79

B

`bib_marker_map()` (in module `espei.utils`), 79

`build_candidate_models()` (in module `espei.parameter_selection.model_building`), 60

`build_feature_sets()` (in module `espei.parameter_selection.model_building`), 60

`build_sitefractions()` (in module `espei.utils`), 80

`build_ternary_feature_matrix()` (in module `espei.parameter_selection.ternary_parameters`), 63

C

`calculate_activity_error()` (in module `espei.error_functions.activity_error`), 53

`calculate_points_array()` (in module `espei.error_functions.thermochemical_error`), 55

`calculate_thermochemical_error()` (in module `espei.error_functions.thermochemical_error`), 55

`calculate_zpf_error()` (in module `espei.error_functions.zpf_error`), 57

`canonical_sort_key()` (in module `espei.core_utils`), 69

`canonicalize()` (in module `espei.core_utils`), 69

`check_dataset()` (in module `espei.datasets`), 71

`chempot_error()` (in module `espei.error_functions.activity_error`), 54

`clean_dataset()` (in module `espei.datasets`), 72

D

`database_symbols_to_fit()` (in module `espei.utils`), 80

`dataplot()` (in module `espei.plot`), 76

`DatasetError`, 71

E

`endmembers_from_interaction()` (in module `espei.utils`), 80

`eq_callable_dict()` (in module `espei.utils`), 80

`eqdataplot()` (in module `espei.plot`), 77

`espei` (module), 83

`espei.analysis` (module), 69

`espei.core_utils` (module), 69

`espei.datasets` (module), 71

`espei.error_functions` (module), 59

`espei.error_functions.activity_error` (module), 53

`espei.error_functions.thermochemical_error` (module), 55

`espei.error_functions.zpf_error` (module), 57

`espei.espei_script` (module), 72

`espei.mcmc` (module), 73

`espei.parameter_selection` (module), 65

`espei.parameter_selection.model_building` (module), 60

`espei.parameter_selection.selection` (module), 62

`espei.parameter_selection.ternary_parameters` (module), 63

`espei.parameter_selection.utils` (module), 64

`espei.paramselect` (module), 74

`espei.plot` (module), 76

`espei.refdata` (module), 79

`espei.rstate` (module), 79

`espei.tests` (module), 69

`espei.tests.fixtures` (module), 65

`espei.tests.test_core_utils` (module), 65

`espei.tests.test_datasets` (module), 65

`espei.tests.test_error_functions` (module), 66

`espei.tests.test_mcmc` (module), 66

`espei.tests.test_model_building` (module), 66

`espei.tests.test_parameter_generation` (module), 67

`espei.tests.test_parameter_generation_utils` (module), 67

`espei.tests.test_plotting` (module), 67

`espei.tests.test_schema` (module), 67

`espei.tests.test_utils` (module), 68

`espei.tests.testing_data` (module), 68

`espei.utils` (module), 79

`estimate_hyperplane()` (in module `pei.error_functions.zpf_error`), 57

F

`fit_formation_energy()` (in module `espei.paramselect`), 74

`fit_model()` (in module `pei.parameter_selection.selection`), 62

`fit_ternary_interactions()` (in module `espei.paramselect`), 75

`flexible_open_string()` (in module `espei.utils`), 81

`formatted_constituent_array()` (in module `espei.utils`), 81

`formatted_parameter()` (in module `espei.utils`), 82

G

`generate_interactions()` (in module `pei.parameter_selection.model_building`), 61

`generate_parameter_distribution()` (in module `pei.mcmc`), 73

`generate_parameters()` (in module `espei.paramselect`), 75

`generate_symmetric_group()` (in module `pei.parameter_selection.model_building`), 61

`get_data()` (in module `espei.core_utils`), 69

`get_muggianu_samples()` (in module `pei.parameter_selection.ternary_parameters`), 64

`get_next_symbol()` (in module `espei.paramselect`), 75

`get_prop_data()` (in module `pei.error_functions.thermochemical_error`), 56

`get_prop_samples()` (in module `pei.error_functions.thermochemical_error`), 56

`get_pure_elements()` (in module `espei.utils`), 82

`get_run_settings()` (in module `espei.espei_script`), 72

`get_samples()` (in module `espei.core_utils`), 70

I

`interaction_test()` (in module `pei.parameter_selection.utils`), 64

L

`list_to_tuple()` (in module `espei.core_utils`), 70

`lnprob()` (in module `espei.mcmc`), 73

`load_datasets()` (in module `espei.datasets`), 72

M

`main()` (in module `espei.espei_script`), 73

`make_successive()` (in module `pei.parameter_selection.model_building`), 61

`mcmc_fit()` (in module `espei.mcmc`), 73

`multiplot()` (in module `espei.plot`), 77

O

`optimal_parameters()` (in module `espei.utils`), 82

P

`parameter_term()` (in module `espei.utils`), 82

`phase_fit()` (in module `espei.paramselect`), 76

`plot_parameters()` (in module `espei.plot`), 78

R

`ravel_conditions()` (in module `espei.core_utils`), 70

`ravel_zpf_values()` (in module `espei.core_utils`), 70

`recursive_glob()` (in module `espei.datasets`), 72

`recursive_map()` (in module `espei.core_utils`), 71

`run_espei()` (in module `espei.espei_script`), 73

S

`score_model()` (in module `pei.parameter_selection.selection`), 62

`select_model()` (in module `pei.parameter_selection.selection`), 63

`shift_reference_state()` (in module `pei.parameter_selection.utils`), 64

`sigfigs()` (in module `espei.utils`), 83

`sorted_interactions()` (in module `pei.parameter_selection.model_building`), 61

`symmetry_filter()` (in module `espei.core_utils`), 71

T

`target_chempots_from_activity()` (in module `pei.error_functions.activity_error`), 54

`test_activity_error()` (in module `pei.tests.test_error_functions`), 66

`test_adding_bibtex_entries_to_bibliography_db()` (in module `espei.tests.test_utils`), 68

`test_asymmetric_ternary_parameters_can_be_generated()` (in module `pei.tests.test_parameter_generation`), 67

`test_asymmetric_ternary_parameters_can_be_generated_for_2_sublattice()` (in module `pei.tests.test_parameter_generation`), 67

`test_bib_marker_map()` (in module `espei.tests.test_utils`), 68

`test_binary_candidate_models_are_constructed_correctly()` (in module `espei.tests.test_model_building`), 66

`test_build_feature_sets_generates_desired_binary_features_for_cp_like()` (in module `espei.tests.test_model_building`), 66

`test_build_feature_sets_generates_desired_binary_features_for_h_like()` (in module `espei.tests.test_model_building`), 66

`test_build_feature_sets_generates_desired_ternary_features()` (in module `espei.tests.test_model_building`), 66

test_chains_per_parameter_read_correctly() (in module espei.tests.test_schema), 68

test_check_datasets_raises_on_misaligned_data() (in module espei.tests.test_datasets), 65

test_check_datasets_raises_with_incorrect_components() (in module espei.tests.test_datasets), 65

test_check_datasets_raises_with_incorrect_zpf_phases() (in module espei.tests.test_datasets), 65

test_check_datasets_raises_with_malformed_sublattice_configuration() (in module espei.tests.test_datasets), 65

test_check_datasets_raises_with_malformed_zpf() (in module espei.tests.test_datasets), 65

test_check_datasets_raises_with_unsorted_interactions() (in module espei.tests.test_datasets), 65

test_check_datasets_raises_with_zpf_fractions_greater_than_one() (in module espei.tests.test_datasets), 65

test_check_datasets_run_on_good_data() (in module espei.tests.test_datasets), 65

test_check_datasets_works_on_activity_data() (in module espei.tests.test_datasets), 65

test_correct_defaults_are_applied_from_minimal_specification() (in module espei.tests.test_schema), 68

test_datasets_convert_thermochemical_string_values_producing_correct_value() (in module espei.tests.test_datasets), 65

test_datasets_convert_zpf_string_values_producing_correct_value() (in module espei.tests.test_datasets), 65

test_flexible_open_string_file_like() (in module espei.tests.test_utils), 68

test_flexible_open_string_path_like() (in module espei.tests.test_utils), 68

test_flexible_open_string_raw_string() (in module espei.tests.test_utils), 68

test_formation_energies_are_fit() (in module espei.tests.test_parameter_generation), 67

test_get_data_for_a_minimal_example() (in module espei.tests.test_core_utils), 65

test_immediate_client_returns_map_results_directly() (in module espei.tests.test_utils), 68

test_input_yaml_invalid_for_mcmc_when_input_is_overspecified() (in module espei.tests.test_schema), 68

test_input_yaml_invalid_for_mcmc_when_input_not_defined() (in module espei.tests.test_schema), 68

test_input_yaml_valid_for_full_run() (in module espei.tests.test_schema), 68

test_input_yaml_valid_for_generate_parameters_only() (in module espei.tests.test_schema), 68

test_input_yaml_valid_for_mcmc_from_restart() (in module espei.tests.test_schema), 68

test_input_yaml_valid_for_mcmc_from_tdb() (in module espei.tests.test_schema), 68

test_interaction_detection() (in module espei.tests.test_parameter_generation_utils), 67

test_interaction_sorting_is_correct() (in module espei.tests.test_model_building), 66

test_lnprob_calculates_multi_phase_probability_for_success() (in module espei.tests.test_mcmc), 66

test_lnprob_calculates_single_phase_probability_for_success() (in module espei.tests.test_mcmc), 66

test_mixing_data_is_excess_only() (in module espei.tests.test_parameter_generation), 67

test_mixing_energies_are_fit() (in module espei.tests.test_parameter_generation), 67

test_mixing_energies_are_fit_with_higher_order_data() (in module espei.tests.test_parameter_generation), 67

test_mixing_energies_are_reduced_with_ridge_alpha() (in module espei.tests.test_parameter_generation), 67

test_multi_sublattice_mixing_energies_are_fit() (in module espei.tests.test_parameter_generation), 67

test_parameter_initialization() (in module espei.tests.test_mcmc), 66

test_pickleable_tinydb_can_be_pickled_and_unpickled() (in module espei.tests.test_utils), 68

test_recursive_map() (in module espei.tests.test_core_utils), 65

test_sgte_reference_state_naming_is_correct_for_character_element() (in module espei.tests.test_parameter_generation), 67

test_SR2016_refdata() (in module espei.tests.test_schema), 67

test_symmetric_group_can_be_generated_for_2_sl_endmembers_with_symmetry() (in module espei.tests.test_model_building), 66

test_symmetric_group_can_be_generated_for_2_sl_mixing_with_symmetry() (in module espei.tests.test_model_building), 66

test_symmetric_ternary_parameter_can_be_generated() (in module espei.tests.test_parameter_generation), 67

test_symmetric_ternary_parameter_can_be_generated_in_presence_of_binaries() (in module espei.tests.test_parameter_generation), 67

test_test_copy_build_functions_can_be_cloudpickled() (in module espei.tests.test_utils), 68

test_ternary_candidate_models_are_constructed_correctly() (in module espei.tests.test_model_building), 67

test_thermochemical_error_for_mixing_entropy_error_is_excess_only() (in module espei.tests.test_error_functions), 66

test_thermochemical_error_for_of_enthalpy_mixing() (in module espei.tests.test_error_functions), 66

test_thermochemical_error_with_multiple_T_points() (in module espei.tests.test_error_functions), 66

test_thermochemical_error_with_multiple_T_X_points() (in module espei.tests.test_error_functions), 66

test_thermochemical_error_with_multiple_X_points() (in module espei.tests.test_error_functions), 66

test_zpf_error_zero() (in module espei.tests.test_error_functions), 66

`tieline_error()` (in module `espei.error_functions`, [58](#))
`truncate_arrays()` (in module `espei.analysis`), [69](#)