Semi-automated CALPHAD Modeling of Alloy Systems

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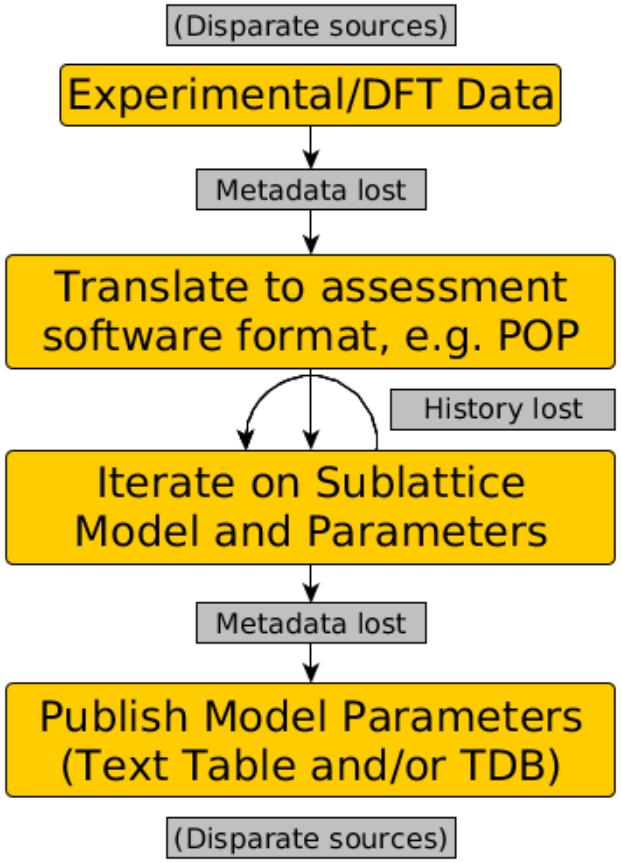
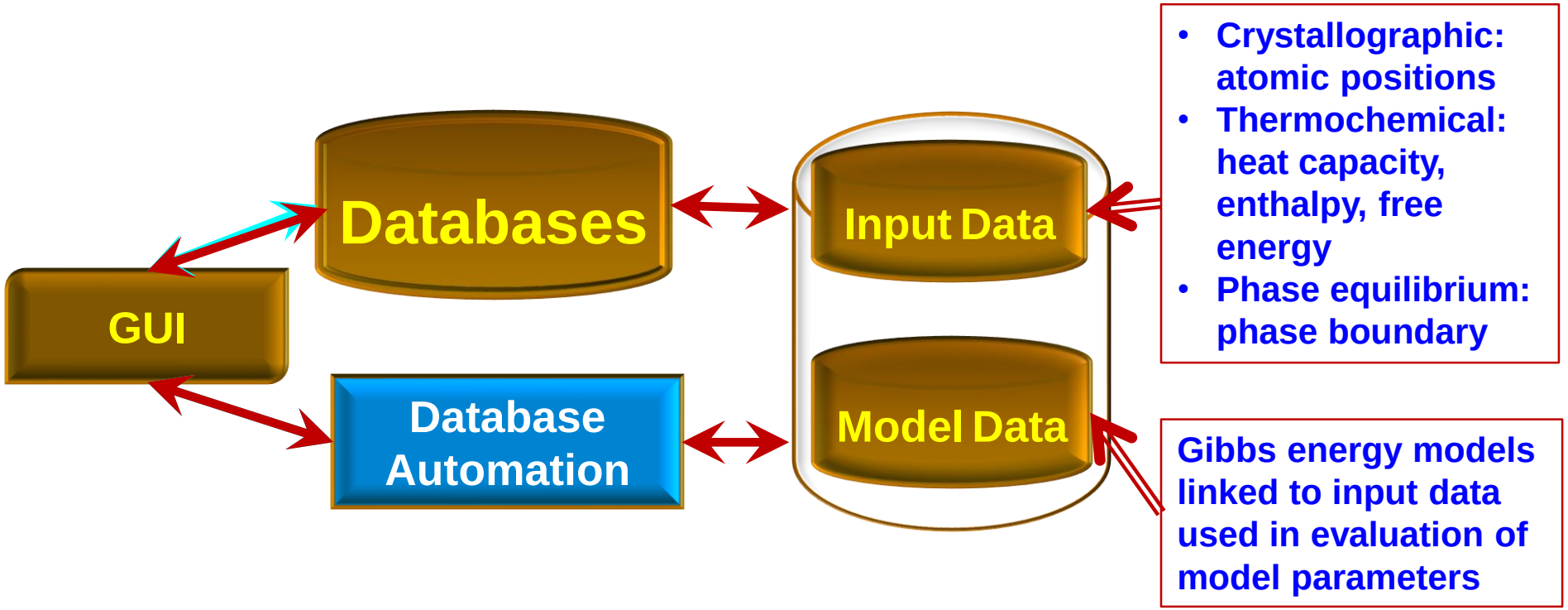
CALPHAD Data Challenges

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



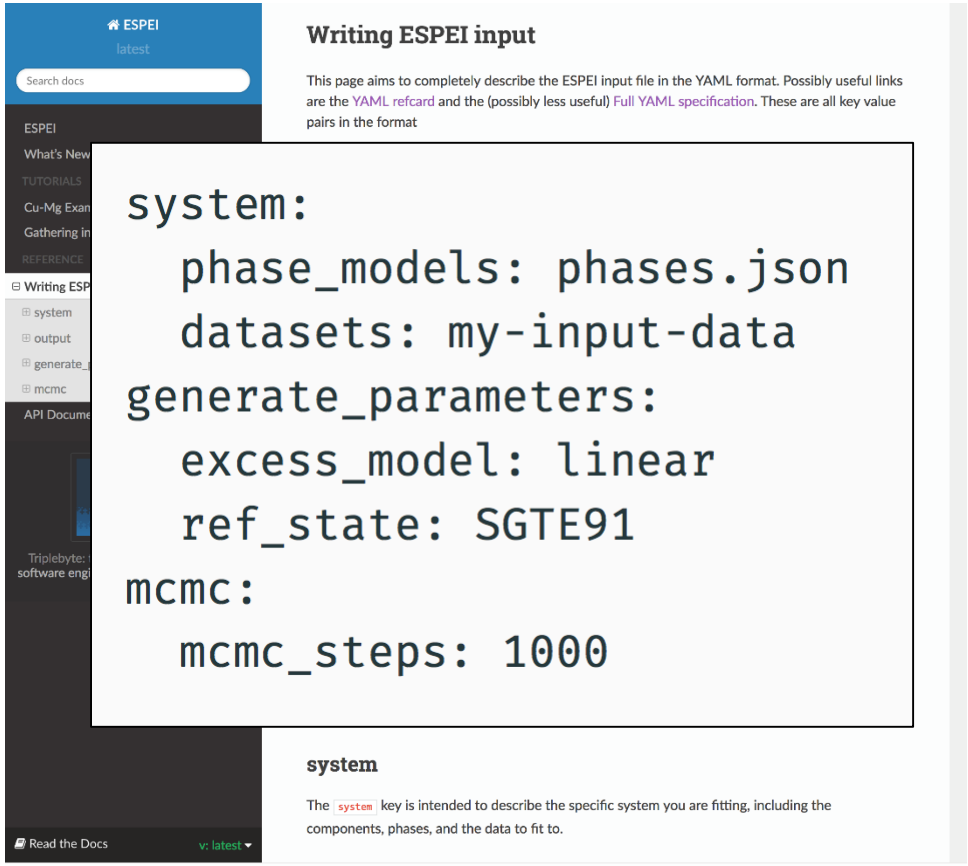
ESPEI: Extensible, Self-optimizing Phase Equilibrium Infrastructure



Shang, Wang, Liu, Magnesium Technology 2010, p. 617

Tutorials and Installation: ESPEI.org

- **Minimal input for a full run (*shown right*)**
- **Can do automated parameter generation, Monte Carlo, or both**
- **Restart from previous run**
- **Supports MPI on HPC clusters**
- **Many customization options**



IP[y]: Notebook BinaryExamples Last Checkpoint: Jan 08 23:25 (autosaved)

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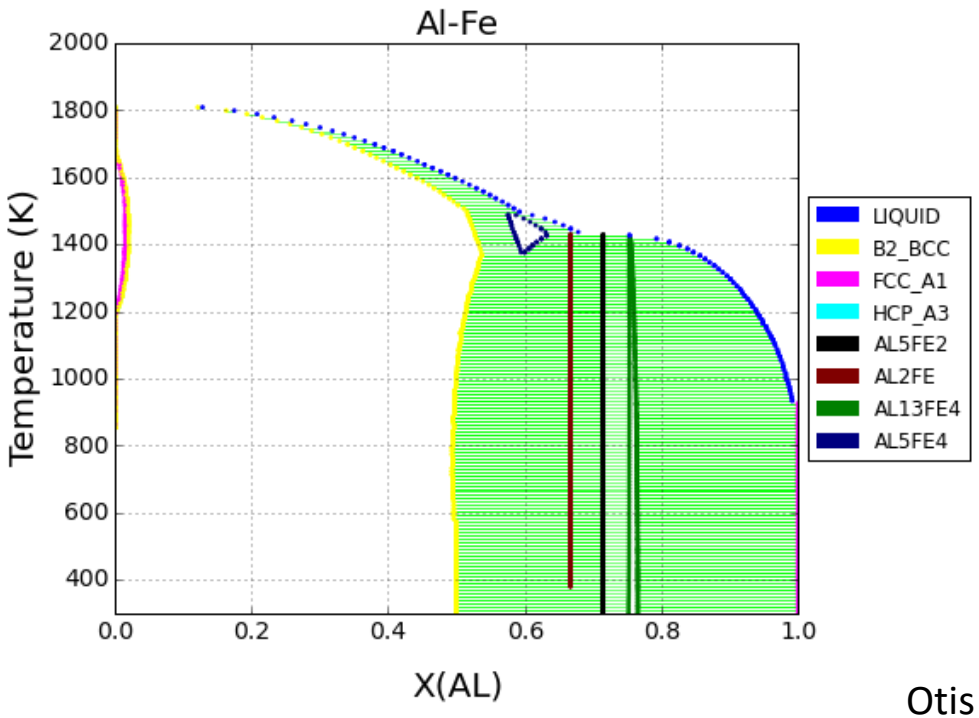
Al-Fe (M.Seiersten et al., 1991)

In [3]:
```
db_alfe = Database('alfe_sei.TDB')
my_phases_alfe = ['LIQUID', 'B2_BCC', 'FCC_A1', 'HCP_A3', 'AL5FE2', 'AL2FE', 'AL13FE4', 'AL5FE4']

fig = plt.figure(figsize=(9,6))
pdens = [{'B2_BCC': 20000}, 2000]
%time ax = binplot(db_alfe, ['AL', 'FE', 'VA'] , my_phases_alfe, 'X(AL)', 300, 2000, pdens=pdens, ax=fig.gca())
plt.show()
```

```
CPU times: user 27.5 s, sys: 639 ms, total: 28.1 s
Wall time: 17.1 s
```



pycalphad.org

- Open source CALPHAD tool

- Supports user-supplied phase models

Otis & Liu, *J. Open Res. Softw.* **5,** 1 (2017).

Ensemble MCMC

- Run many “random walk” parameter chains at once
- Fewer tunable parameters versus standard MCMC
- Better handling for parameter correlations

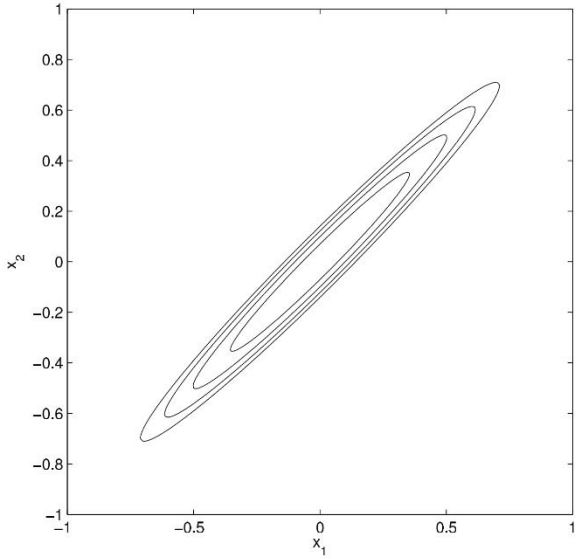
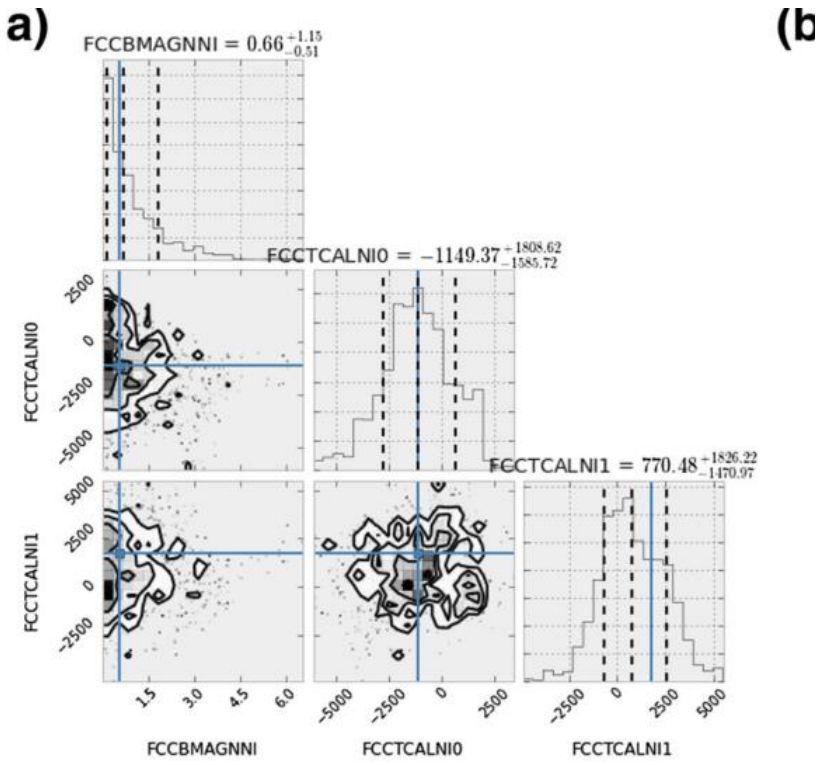


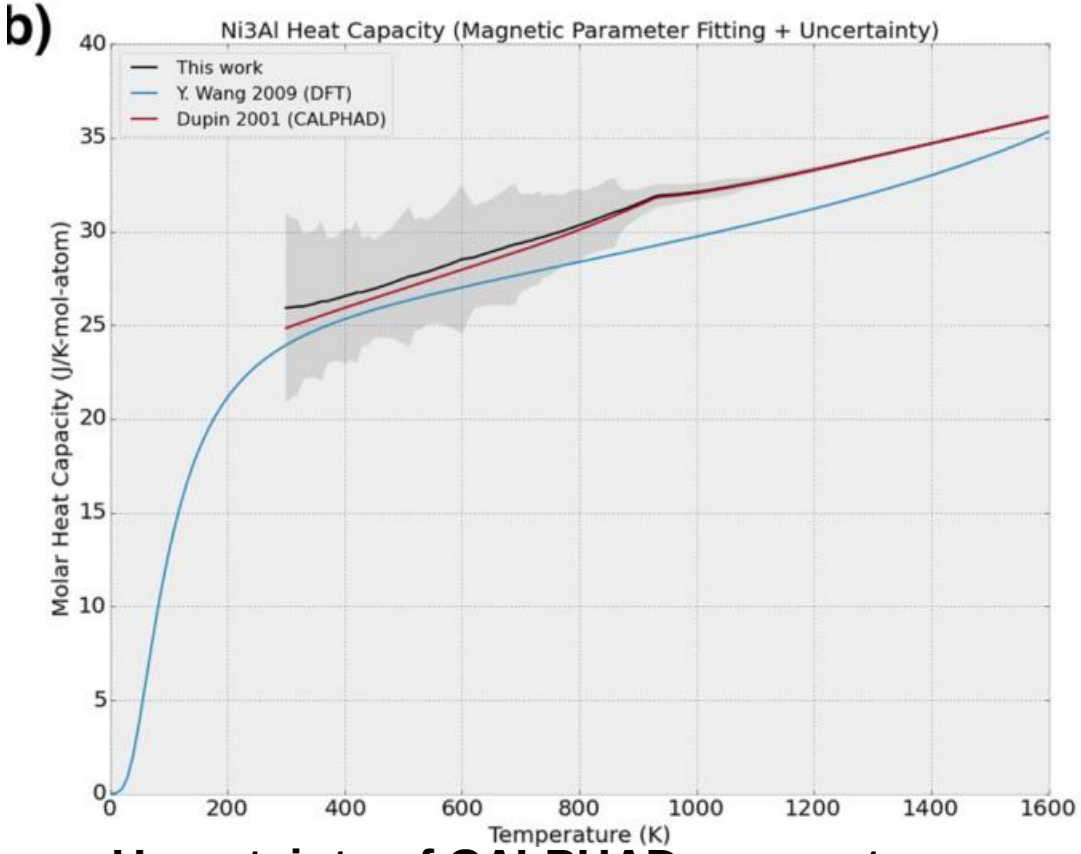
Figure 1. Contours of the Gaussian density defined in expression (3).

J. Goodman and J. Weare, 2010. doi: 10.2140/camcos.2010.5.65

Uncertainty in CALPHAD Modeling



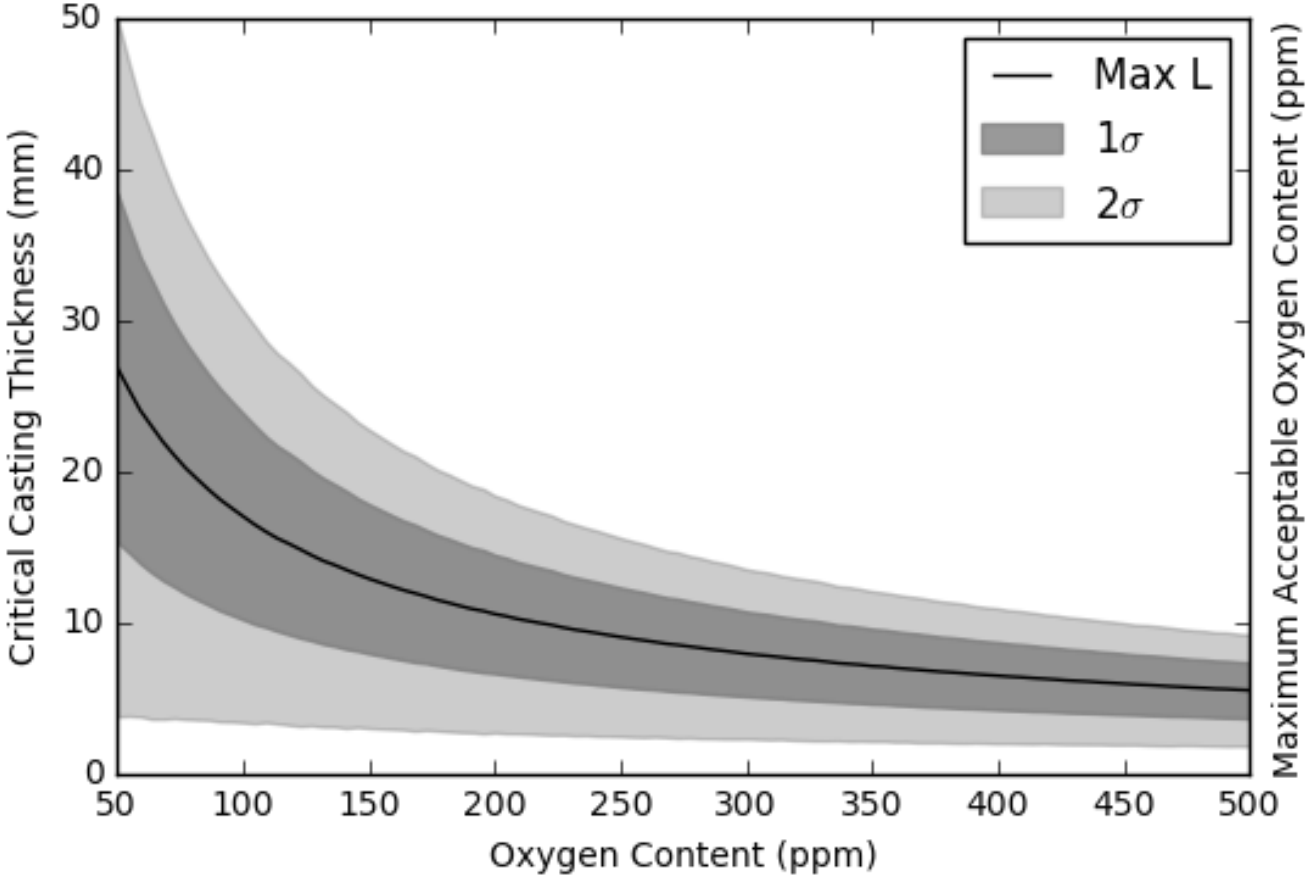
Probability distribution for magnetic parameters for Al-Ni

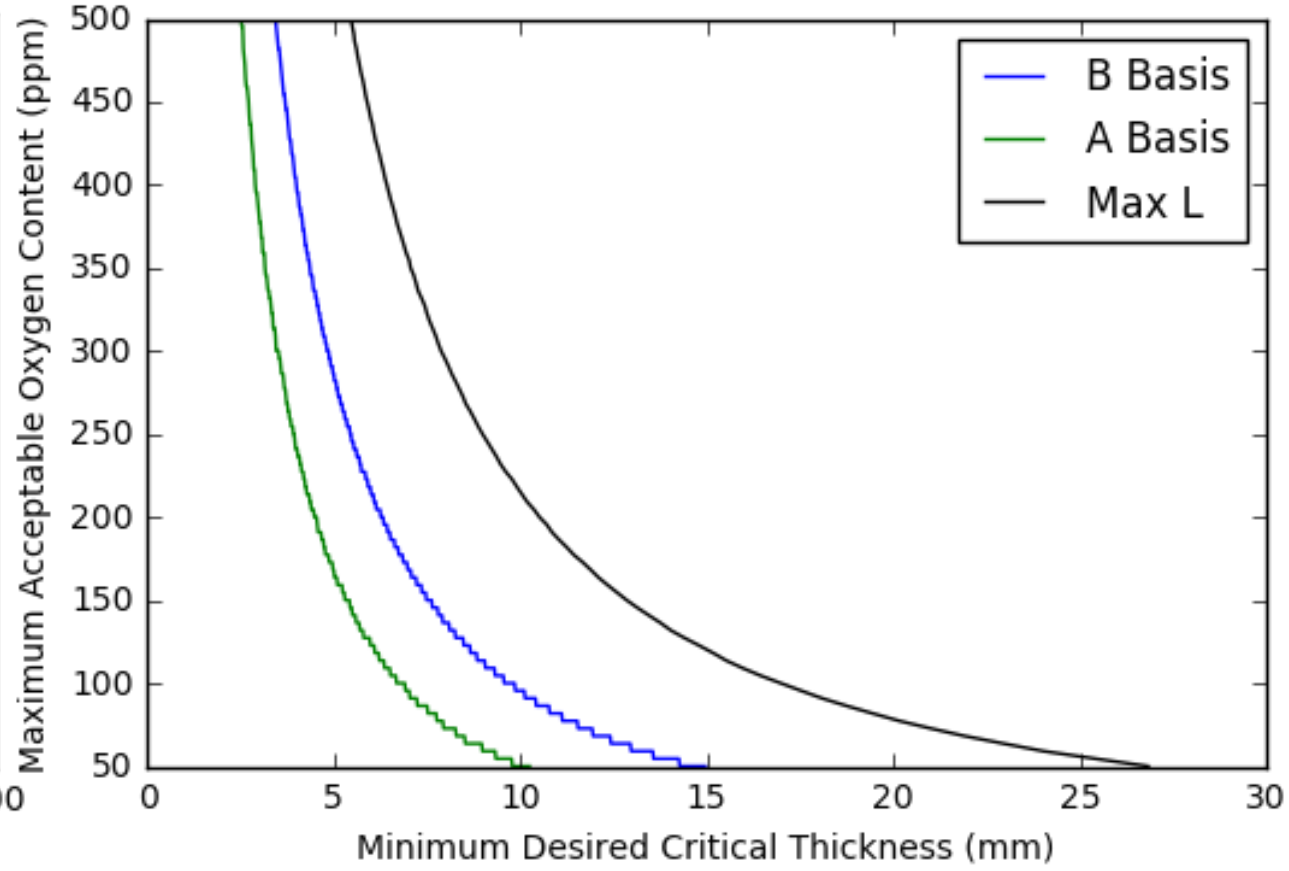


Uncertainty of CALPHAD parameters propagated to heat capacity of Ni3Al

Otis & Liu, *JOM* 69, 886–892 (2017).

CALPHAD Uncertainty for Process Modeling





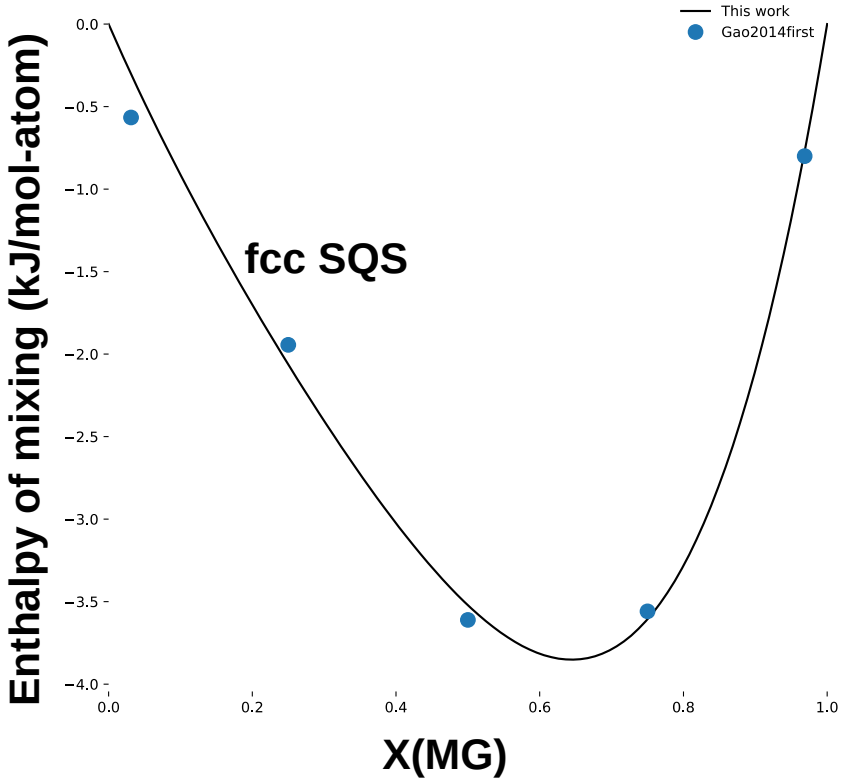
ESPEI Software Stack

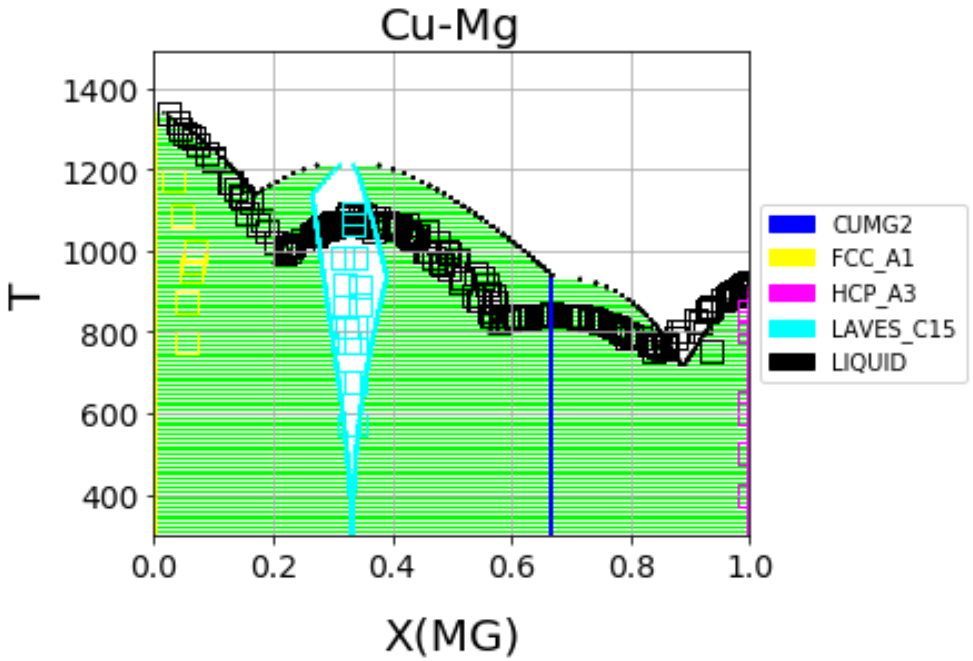
Led at Penn State	ESPEI	High-throughput modeling Data management
Led at JPL	pycalphad	CALPHAD modeling Phase diagrams
Externally developed	NumPy	Numeric computation
	SymPy	Symbolic computation

Otis & Liu, *JOM* 69, 886–892 (2017).

ESPEI Cu-Mg Case Study

Input first-principles data → **Automated parameter selection**
1 minute wall time

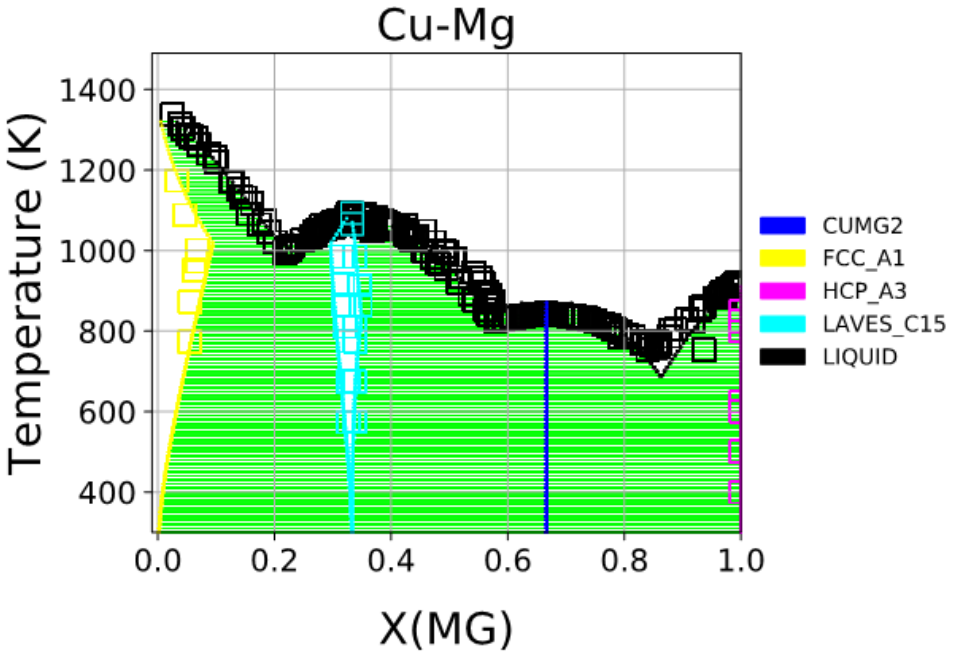




Available as tutorial: https://espei.org

ESPEI Cu-Mg Case Study

After Monte Carlo calculation
8 hours wall time on 4 cores



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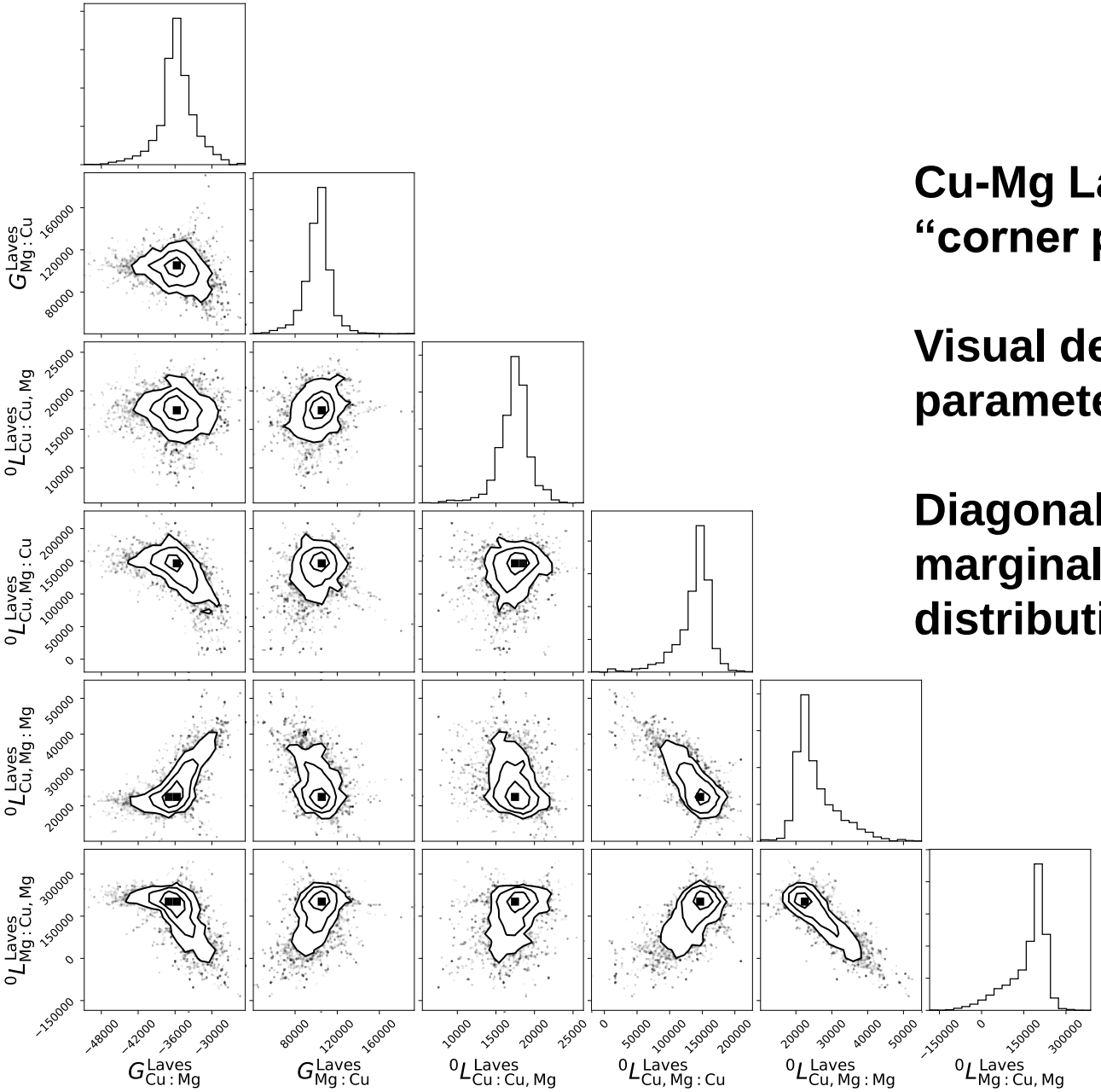

Cu-Mg Laves C15 "corner plot"

Visual depiction of parameter covariance

Diagonals show marginalized distributions

Thank You

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- https://pycalphad.org
  - Chat: gitter.im/pycalphad/pycalphad
- https://espei.org
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