BAYESIAN METHODS FOR MATERIALS MODELING

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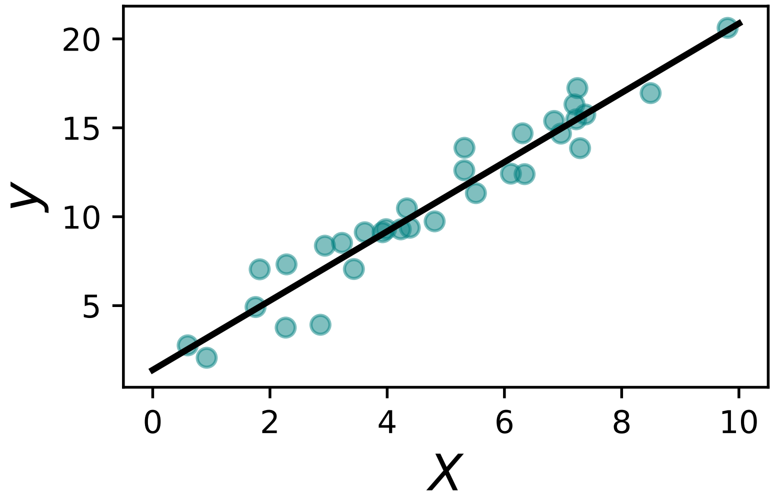
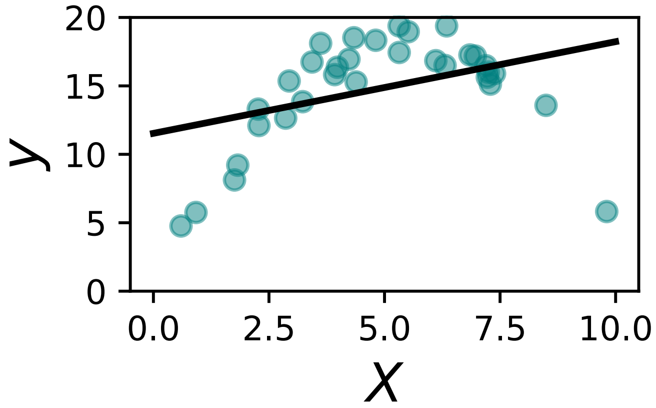
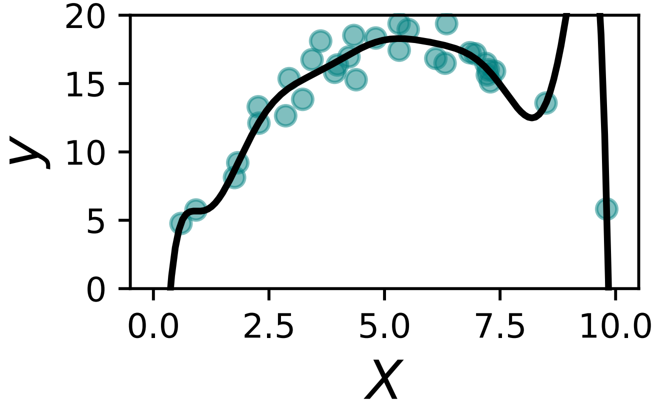
Why do we need Bayesian modeling?

Which model should I choose?

How certain should I be in my parameters?





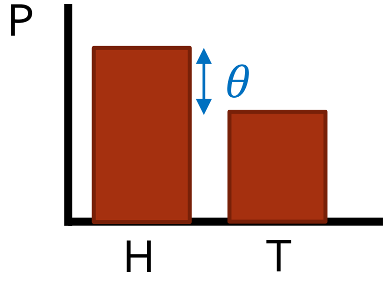


Bayes Rule: Infer parameters using evidence

"Posterior": Probability of parameters (θ) given observations (D) and model (M)

"Likelihood": Probability of observations given parameters and model

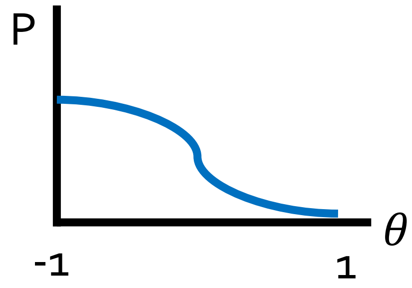
Model



$$P(\theta|D,M) = \frac{P(D|\theta,M)P(\theta|M)}{\mathrm{P}(D|M)}$$

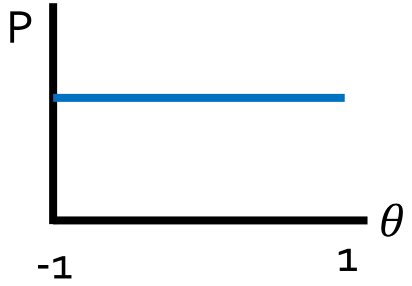
"Prior": Initial assumption of parameters given model

Posterior Distribution



"Evidence": Likelihood of observations given model

Prior Distribution



Using Bayes' rule: Integrals over the posterior

You can use integration to solve for probabilistic measures of the integral

Math: $E(h(\theta)|D) = \int h(\theta)p(\theta|D)d\theta$

English: Expected value of $h(\theta)$ by average over all possible θ weighted by the probability of θ

Solving that integral analytically is often impossible. Can always solve numerically:

Math: $\int h(\theta)p(\theta|D)d\theta \approx \frac{1}{S}\sum_{s=1}^{S} h(\theta_s)$

English: Compute the average of $h(\theta)$ for many samples of θ taken from the posterior distribution

Problem: How do you generate samples from the posterior!?

Markov-Chain Monte Carlo: Sampling S with balance

Algorithm:

1. Select initial point, θ_0, from prior distributions
2. Generate new point: $\theta_i = \mathcal{N}(\theta_{i-1}, \sigma)$ ← Pick a new point from Normal Distribution
3. Compute posterior probability for θ_i and θ_{i-1}

$$P(\theta_n|D,M) = P(D|\theta_n,M)P(\theta_n|M)$$

← See practical exercises

4. Compute "acceptance probability"

$$P(\text{accept}) = \min\left(1, \frac{P(\theta_i|D,M)}{P(\theta_{i-1}|D,M)}\right)$$

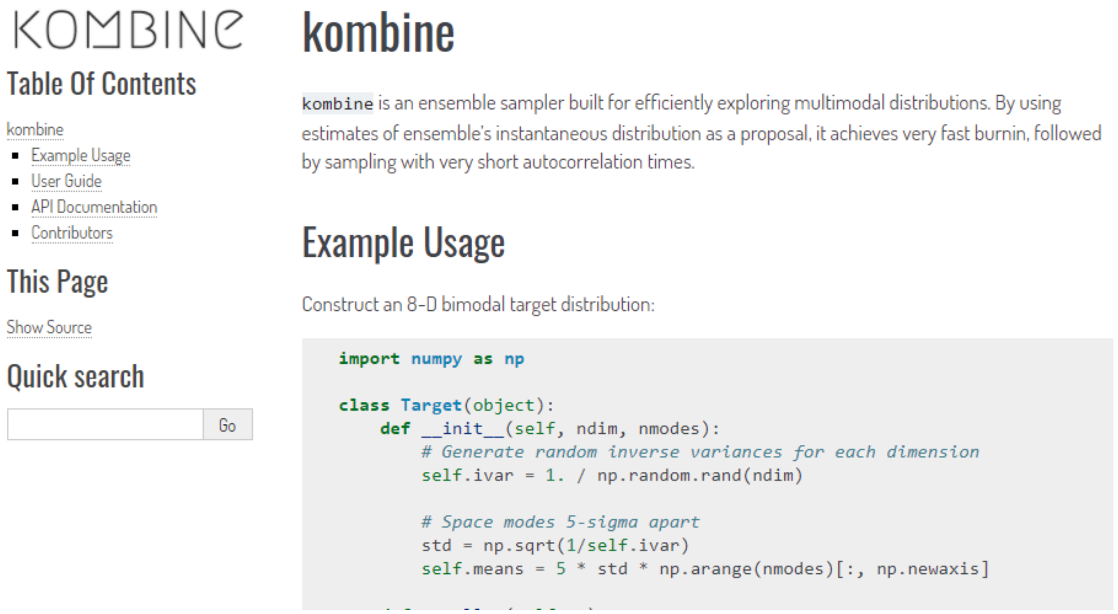
← This assures samples will follow posterior distribution "detailed balance"

5. With probability $P(\text{accept})$, keep θ_i as the current point
6. Repeat from 2

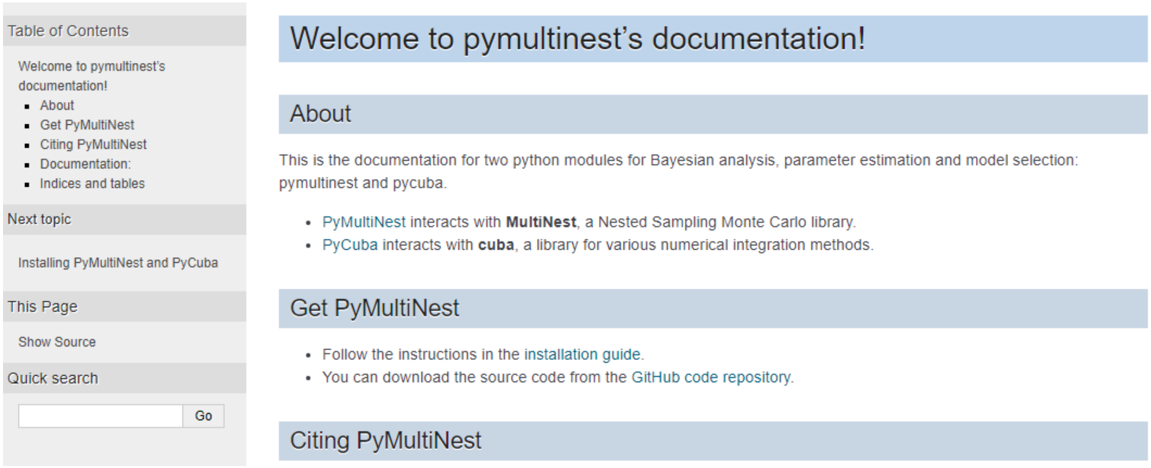
Run many iterations of "MCMC" and you will get samples that follow posterior

There are better methods for doing this

Kombine (Farr and Farr, 2015)



MultiNest (Feroz et al., 2013)

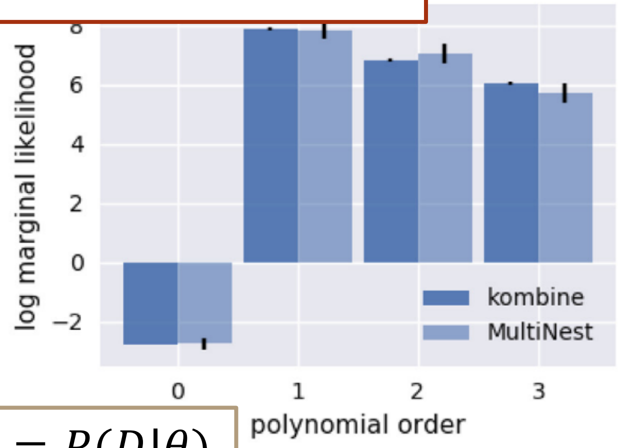


Many great things once you can compute integrals

Sample a many points from the posterior, then you can…

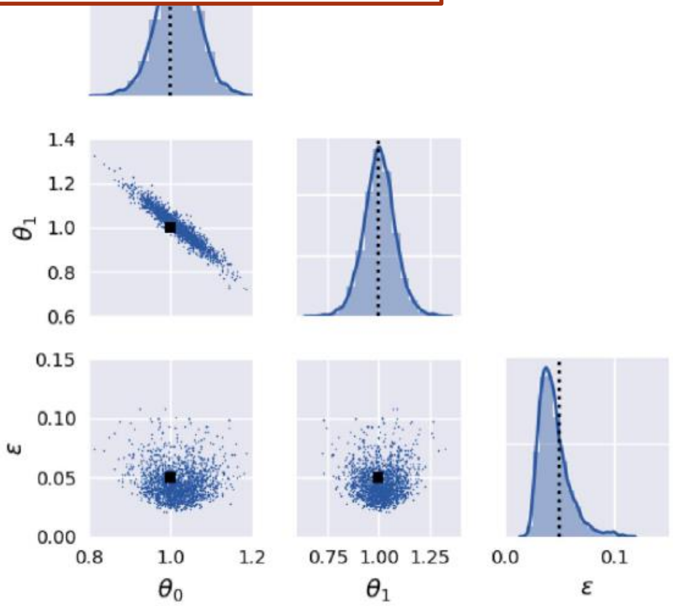
$$E(h(\theta)|D) = \int h(\theta)p(\theta|D)d\theta$$

Compare different models



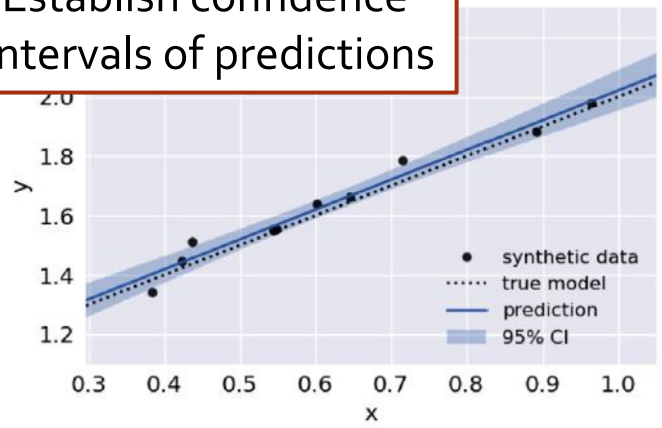
$h(\theta) = P(D|\theta)$

Establish confidence intervals of <u>parameters</u>



$h(\theta) = \theta_0$

Establish confidence intervals of predictions



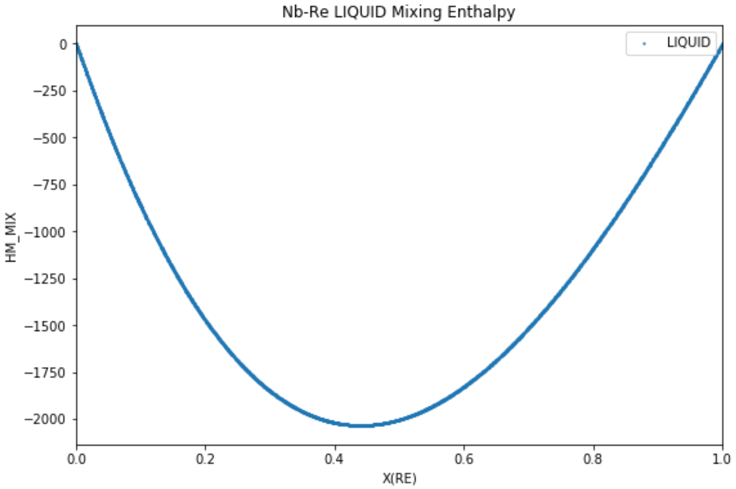
$h(\theta) = \theta_0 + \theta_1 x$

Figures: [Paulson, Jennings, Stan. IJES. (2019)]

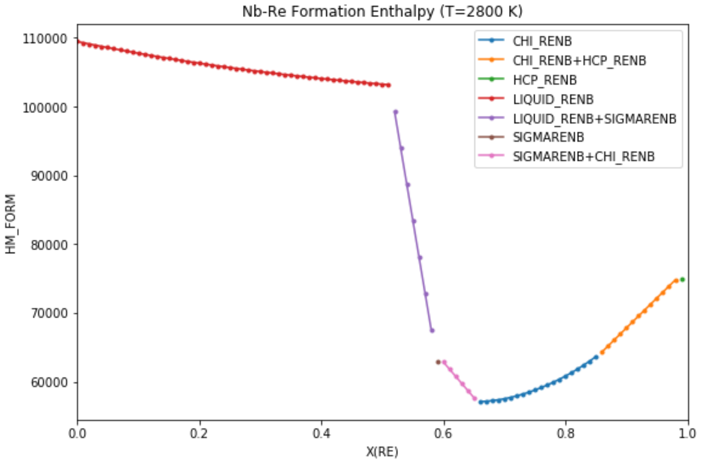
MATERIALS ENGINEERING EXAMPLE

Courtesy of Paulson et al.

Thermodynamic modeling: CALPHAD



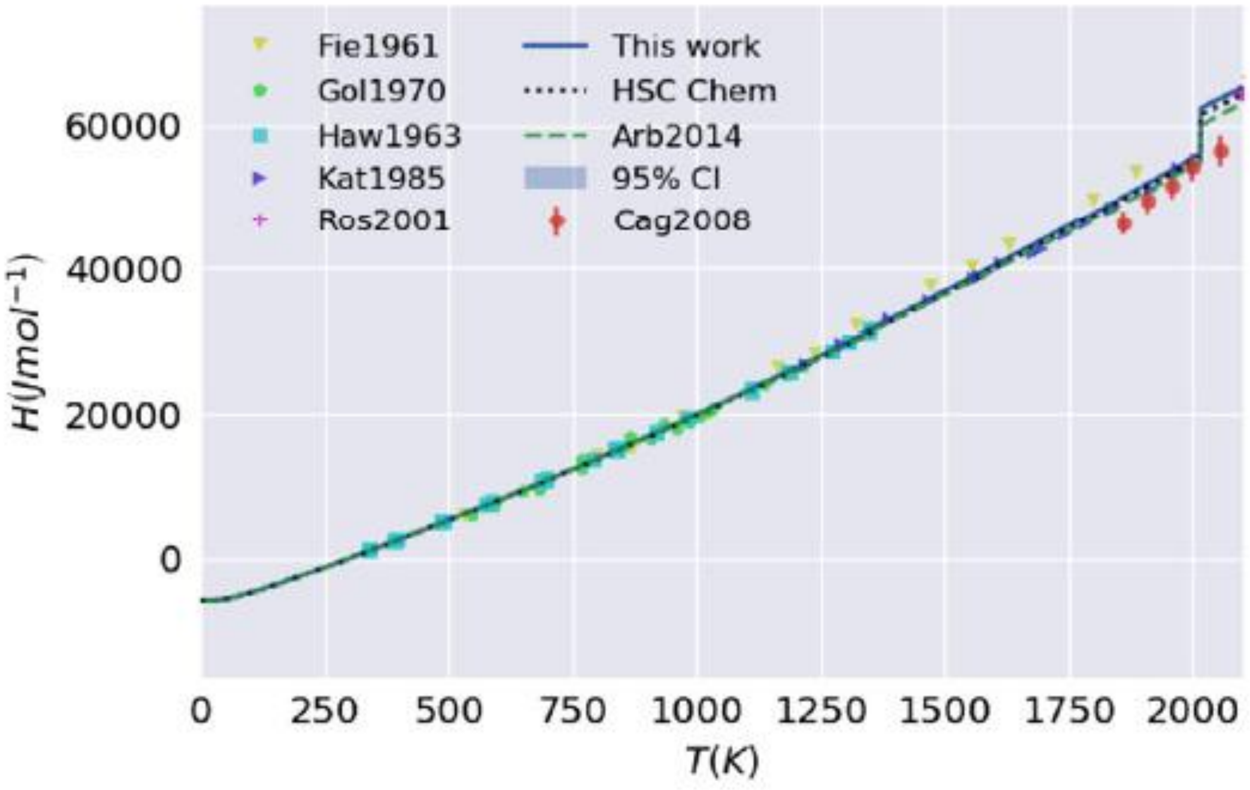
Step 1: Fit thermodynamic models of materials



Step 2: Use them to compute relative stability

Figure: PyCalphad

Key issue: Fitting thermodynamic models



Many problems:

1. Uncertainty in model form
2. Noise in data collection
3. Disagreement between sources

Solution: **Bayesian methods!**

Figures: Paulson, Jennings, Stan. IJES. (2019)

Fitting Thermodynamic Models

Innovation 1: Choosing different thermodynamic models

$$H(T) - H(298.15K) = \frac{3R\theta}{e^{\frac{\theta}{T}}-1} + a\frac{T^2}{2} + \frac{bT^3}{2} \qquad C_p(T) = \frac{d}{dT}H(T)$$

Innovation 2: Learning which data sources are more reliable

Larger α_i means more weight

$$P(D|\theta,\alpha,M) = \prod_i \prod_j \mathcal{N}\left(y_j^i | M\left(x_j^i,\theta\right), \frac{1}{\alpha^i}\right)$$

Include a “dataset uncertainty” (α)

Loop over datasets (i) and points within dataset (j)

Innovation 3: Fitting to more than one property at a time

$$P(D|\theta,M) = \prod_i \mathcal{N}\left(D_{H,i} | H(T_i,\theta), \epsilon_i\right) \prod_j \mathcal{N}\left(D_{C_p,j} | C_p\left(T_j,\theta\right), \epsilon_j\right)$$

Different terms for each type of data

Same parameters (θ) in both types

Result: Can fit models, parameters, datasets

Can rule out certain models

Parameters and errors for models

Table 1
Potential models, their log Marginal-Likelihoods and Bayes' Factor with respect to the selected model (marked with an asterisk) are presented for each phase.

Model α-phase	Number of model parameters	Log marginal likelihood	Bayes' factor
Einstein	1	−1744.2	∼0
Debye	1	−1262.9	∼0
Debye + Linear	2	−1072.6	∼0
Debye + Quadratic	3	−813.2	∼0
Debye + Cubic	4	−640.2	∼0
Debye + Quartic*	5	−623.1	1
Debye + Quintic	6	−627.4	1.4×10^{-2}
Debye + SR	5	−629.7	1.4×10^{-3}
β-phase			
Constant	2	−534.2	∼0
Linear	3	−511.1	3.0×10^{-3}
Quadratic*	4	−505.3	1
Cubic	5	−518.5	1.9×10^{-6}
Liquid-phase			
Constant	2	−491.4	∼0
Linear*	3	−471.0	1
Quadratic	4	−476.0	6.7×10^{-3}

Table 2
The mean, standard deviation, 2.5th percentile bound and 97.5th percentile bound are presented for each parameter for the best model for each phase.

Parameter α-phase	Mean	Std. dev.	2.5% CI	97.5% CI
θ_D	206.45	0.28	205.93	207.02
a_2	1.41×10^{-3}	7.58×10^{-5}	1.26×10^{-3}	1.56×10^{-3}
a_3	9.71×10^{-6}	2.29×10^{-7}	9.26×10^{-6}	1.02×10^{-5}
a_4	-5.61×10^{-9}	2.44×10^{-10}	-6.07×10^{-9}	-5.12×10^{-9}
a_5	1.10×10^{-12}	7.63×10^{-14}	9.41×10^{-13}	1.24×10^{-12}
$\alpha_{Ade1952}$ Adenstedt (1952)	1.111	0.532	0.348	2.402
$\alpha_{Aru1972}$ Arutyunov, Banchila, and Filippov (1972)	0.569	0.138	0.340	0.876
$\alpha_{Bur1958}$ Burk, Estermann, and Friedberg (1958)	0.188	0.023	0.147	0.237
$\alpha_{Cag2008}$ Cagran, Hüpf, Wilthan, and Pottlacher (2008)	0.533	0.217	0.210	1.046
$\alpha_{Cez1974}$ Cezairliyan and McClure (1975)	4.137	0.959	2.613	6.343
$\alpha_{Col1971}$ Collings and Ho (1971)	0.209	0.040	0.140	0.295
$\alpha_{Fie1961}$ Fieldhouse and Lang (1961)	0.444	0.118	0.250	0.709
$\alpha_{Fil1971}$ Filippov and Yurchak (1971)	0.640	0.163	0.367	1.002

Relative importance of data (α)

Take away points

Bayesian method lets you combine:

1. Initial guesses about parameters “priors”
2. Experimental evidence

to generate a new distribution of parameters **“posterior”**

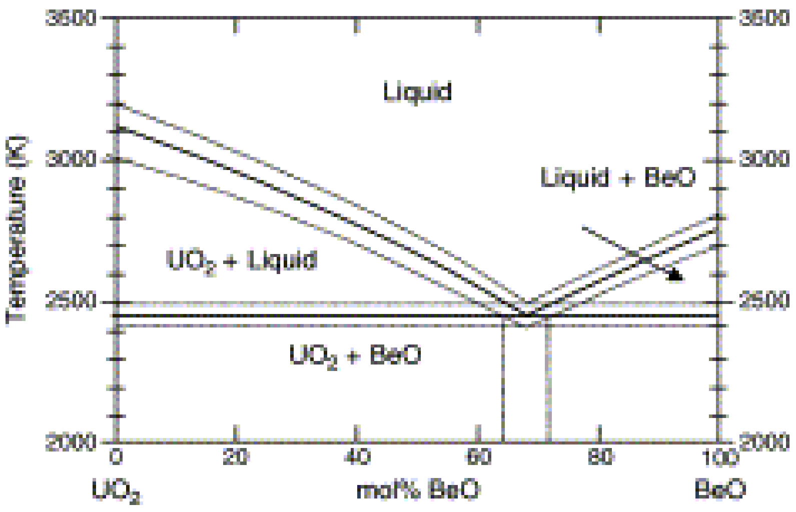


Figure: Stan, Reardon. Calphad (2003)

Compute properties by **“sampling posterior”**

Use Bayesian to get better **confidence intervals** on physics models