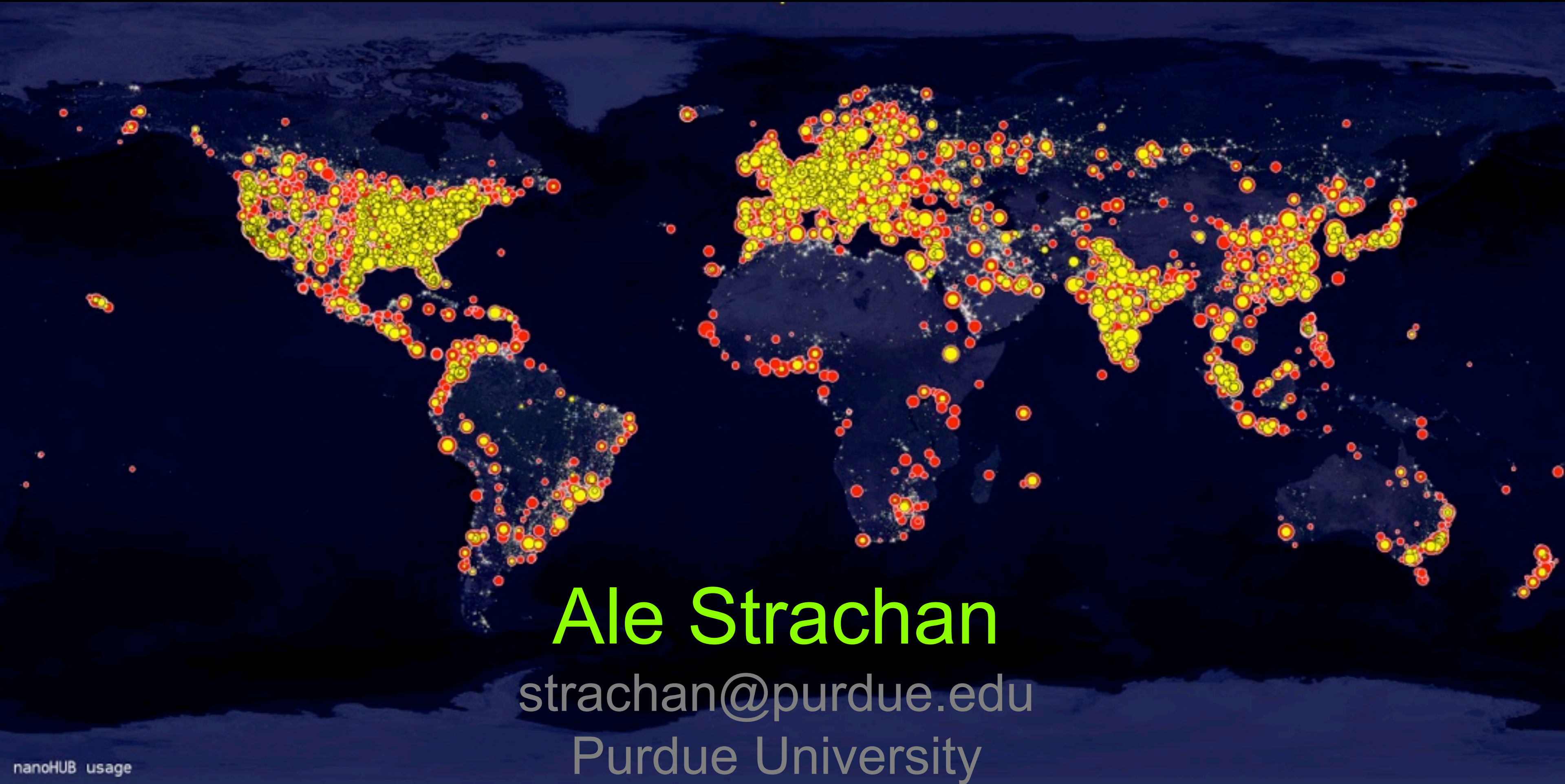
Uncertainty quantification tools in nanoHUB

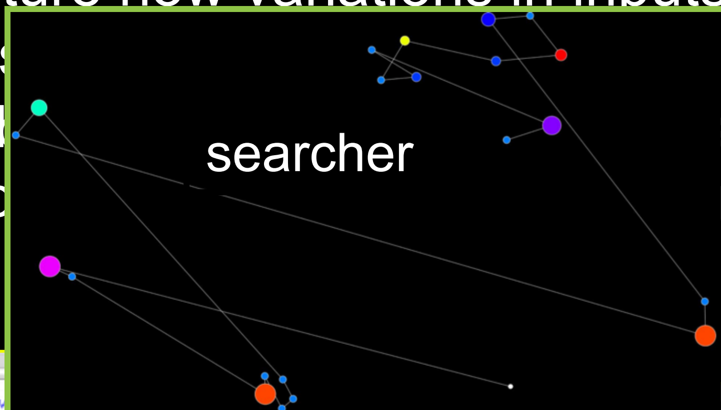
Towards predictions with quantified confidence

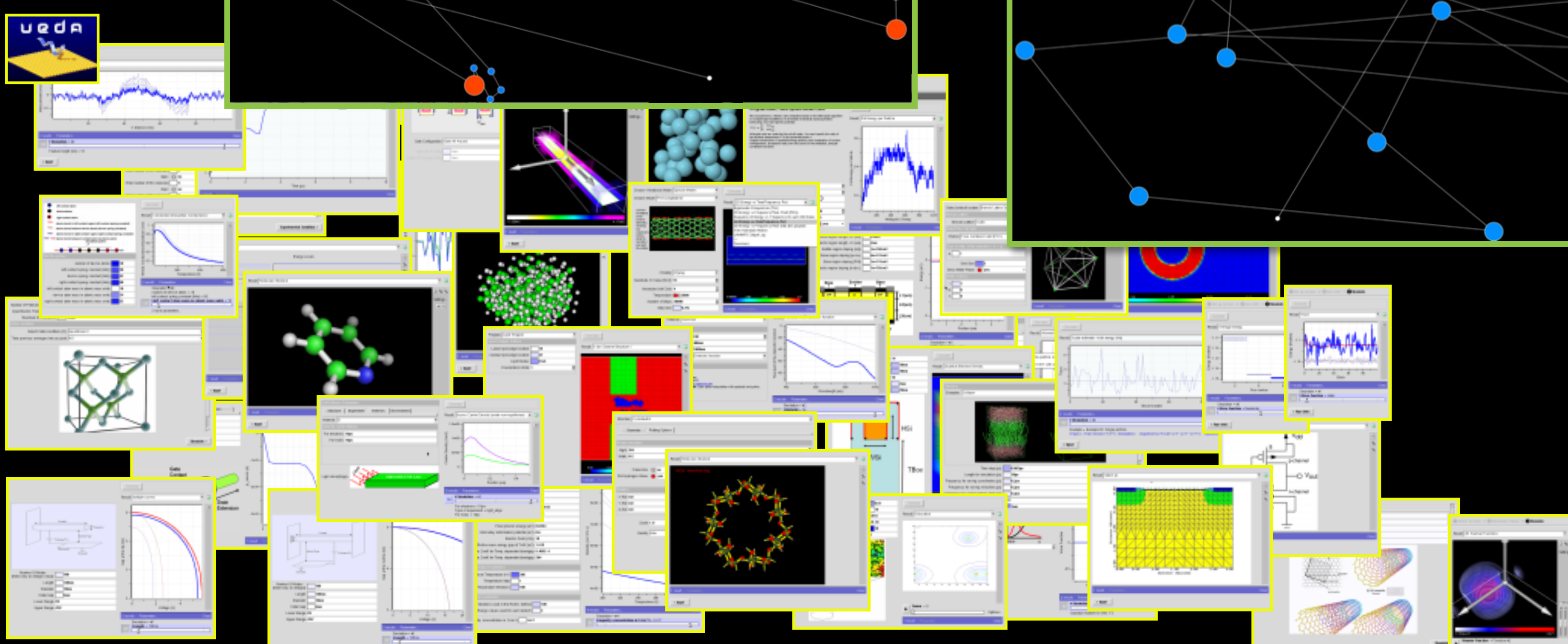


Ale Strachan
strachan@purdue.edu
Purdue University

Enhancing nanoHUB simulations

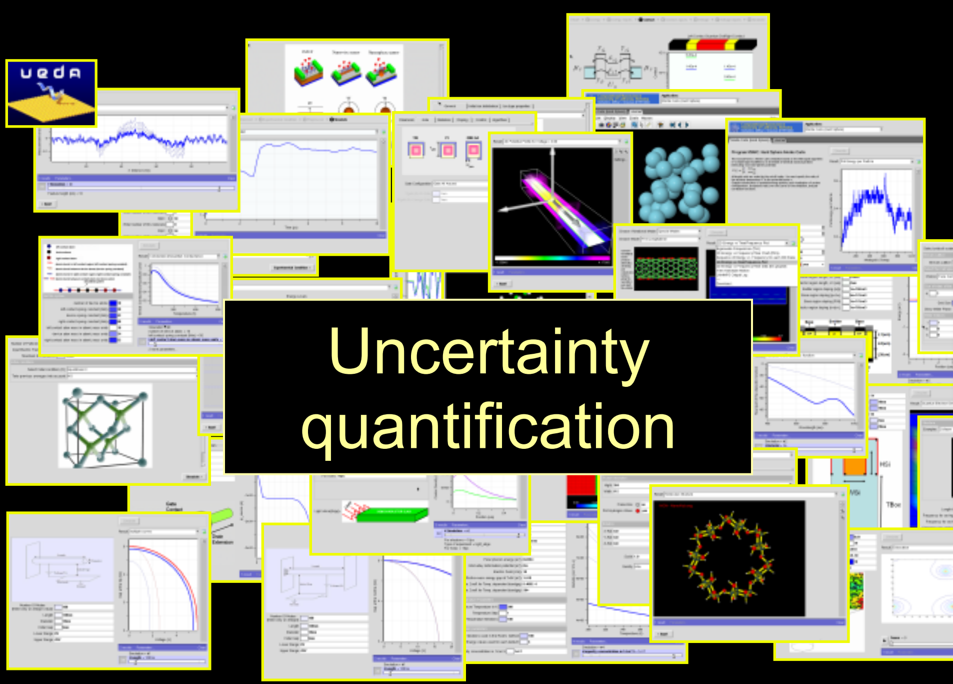
- Explore parameter space to obtain trends or optimal designs
- Capture how variations in inputs affect predictions
- Sens… allocation
- Calib… using experimental data
- Rigo… exp…



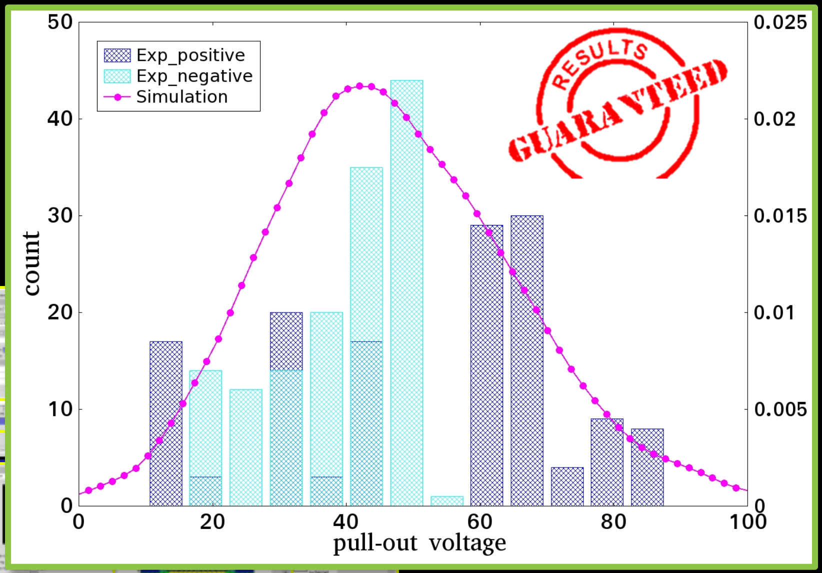


Enhancing nanoHUB simulations

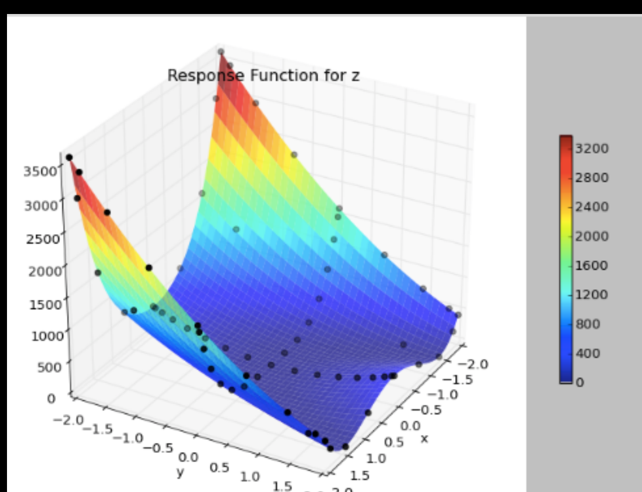
- Explore parameter space to obtain trends or optimal designs
- Capture how uncertainties in inputs affect predictions
- Sensitivity analysis for resource allocation
- Calibration of model parameters using experimental data
- Rigorous model validation using experimental data

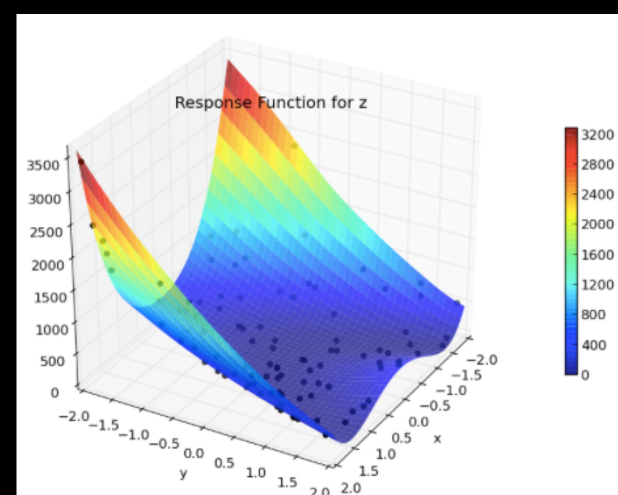


Uncertainty quantification



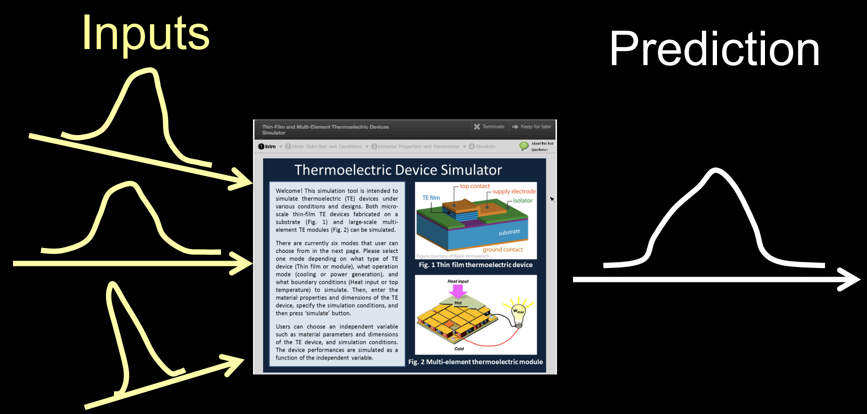
- NNSA PSAAP Center PRISM
  - 2008-2014
  - $17M investment by NNSA, $20 M total
- Open source – MIT license
  - http://c-primed.github.io/puq/



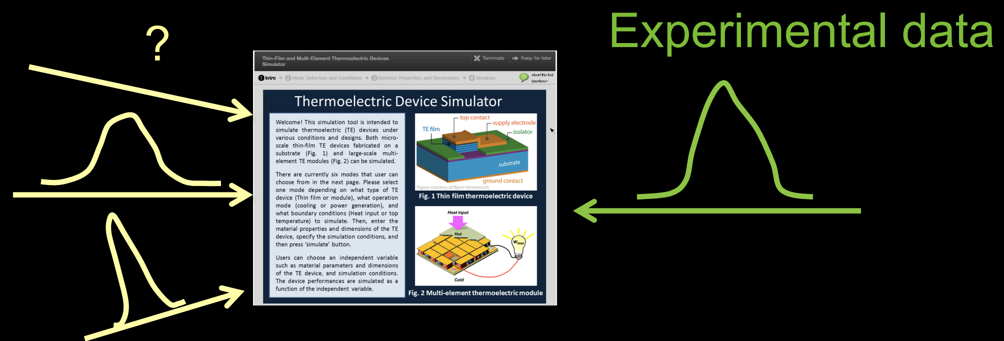


UQ in nanoHUB

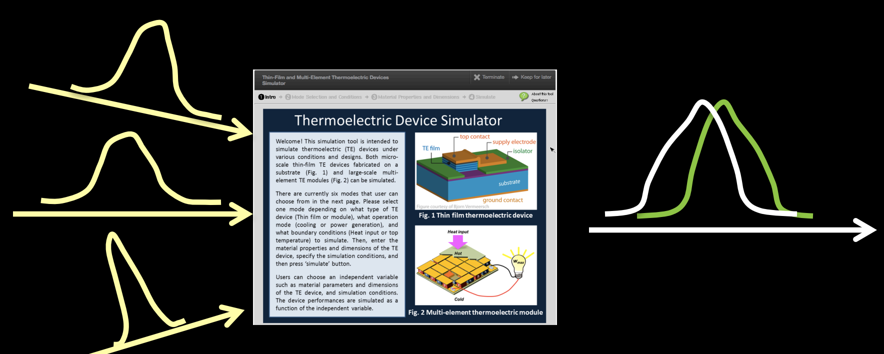
Uncertainty propagation



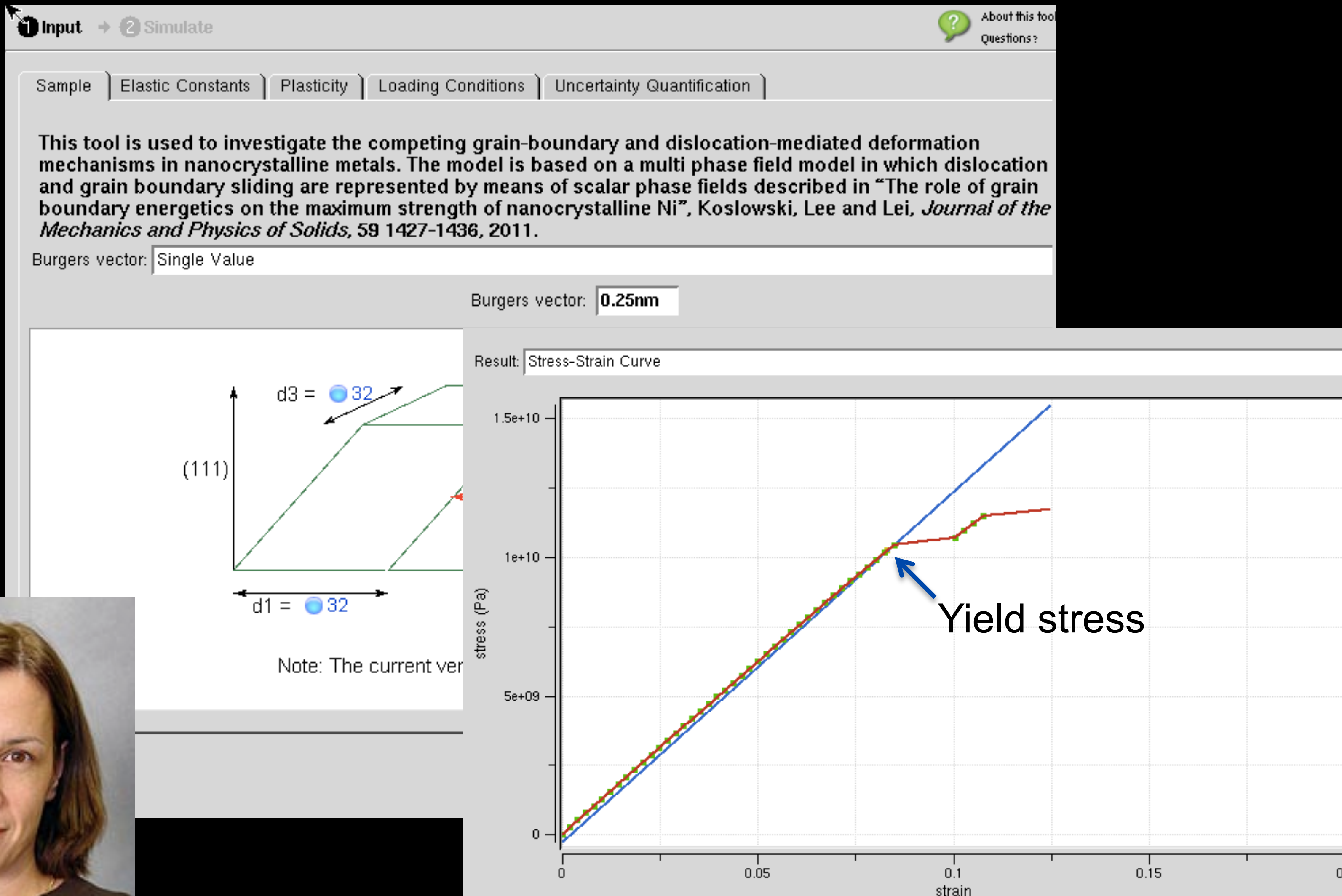
Parameter calibration



Model validation

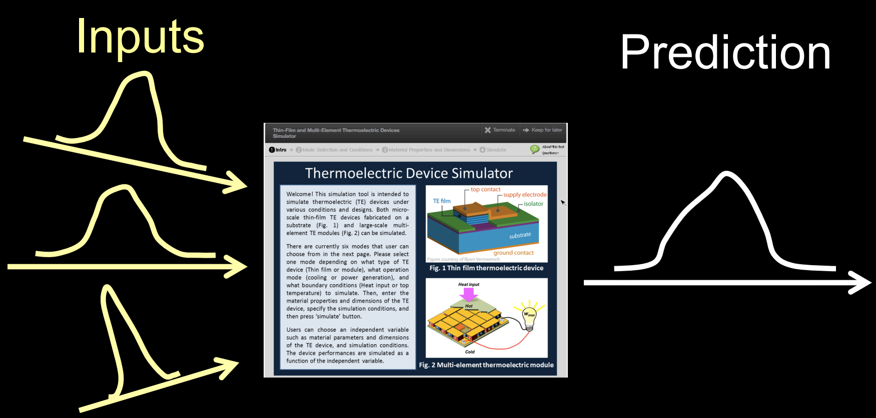


nanoPLASTICITY tool



Marisol Koslowski, Mechanical Engineering @ Purdue

Uncertainty propagation



Uncertainty propagation

Requirements

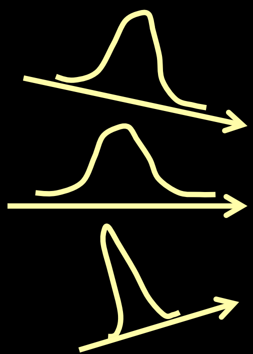
- Non-intrusive methods – no need to modify deterministic code
- Efficient for computationally intensive codes

Our solutions

- Monte Carlo sampling
- Surrogate models (response functions)
  - Generalized polynomial chaos
  - Latin hypercube + radial basis sets
  - Gaussian process regression

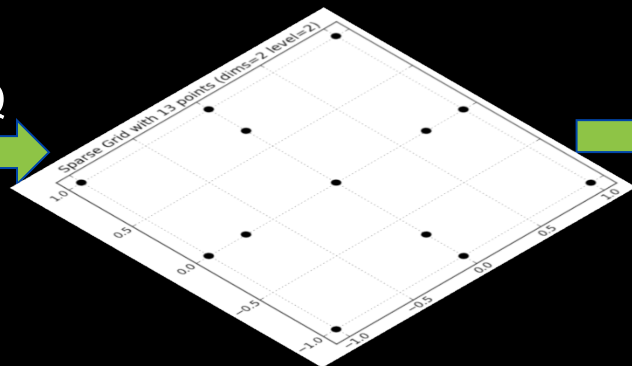
Uncertainty propagation

Inputs



PUQ

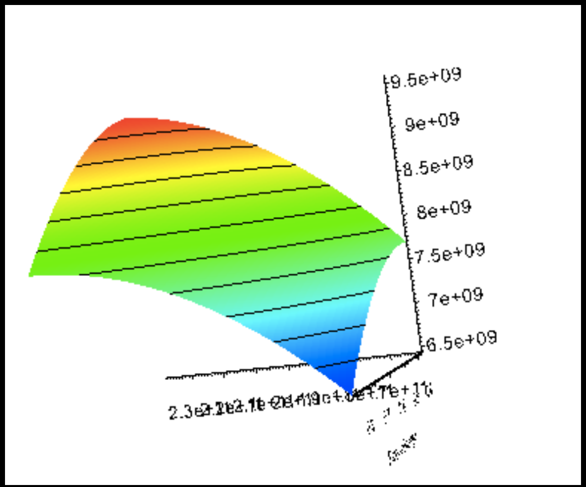
Sparse Smolyak grid



PUQ
+
submit

PUQ

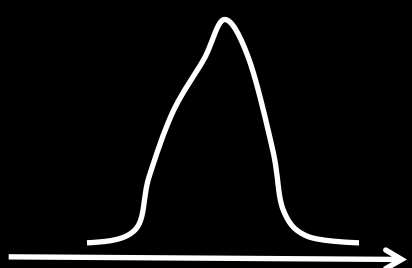
Orthogonal polynomials



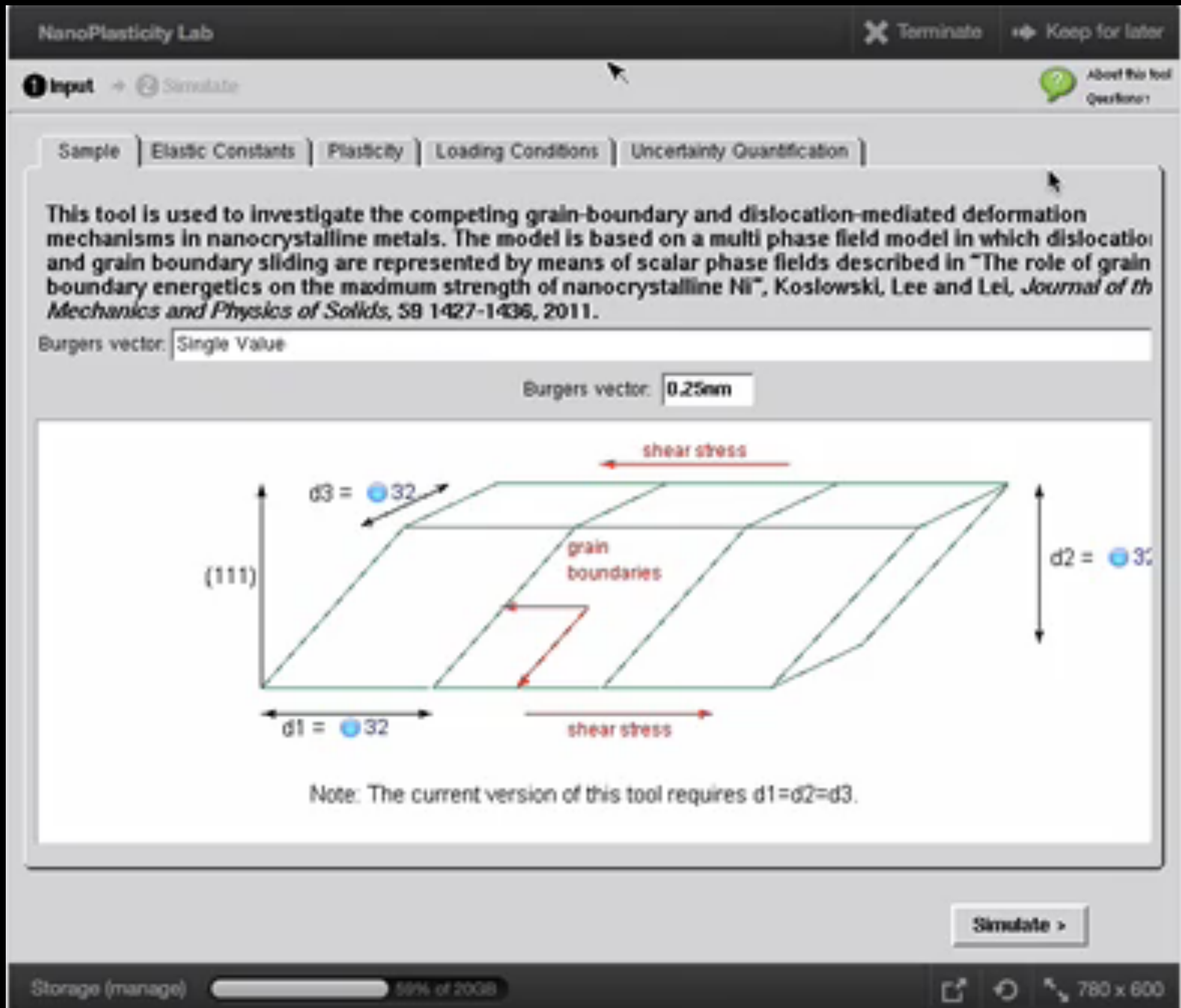
PUQ

Monte Carlo Sampling

Prediction

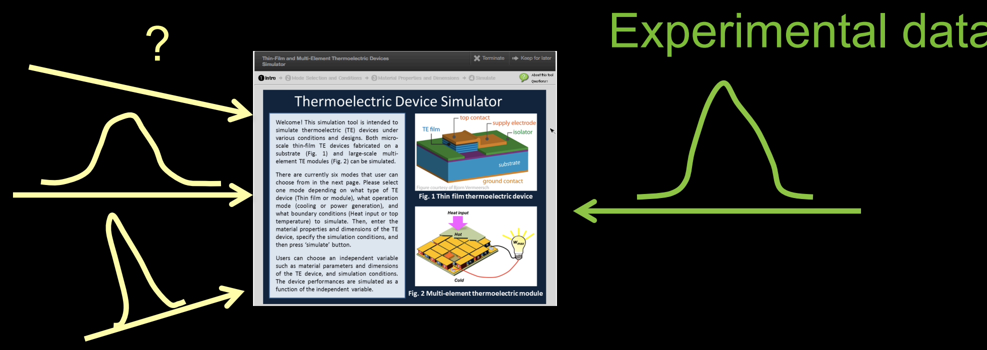


nanoPLASTICITY tool



Calibration

Parameter calibration



Bayesian theorem & calibration

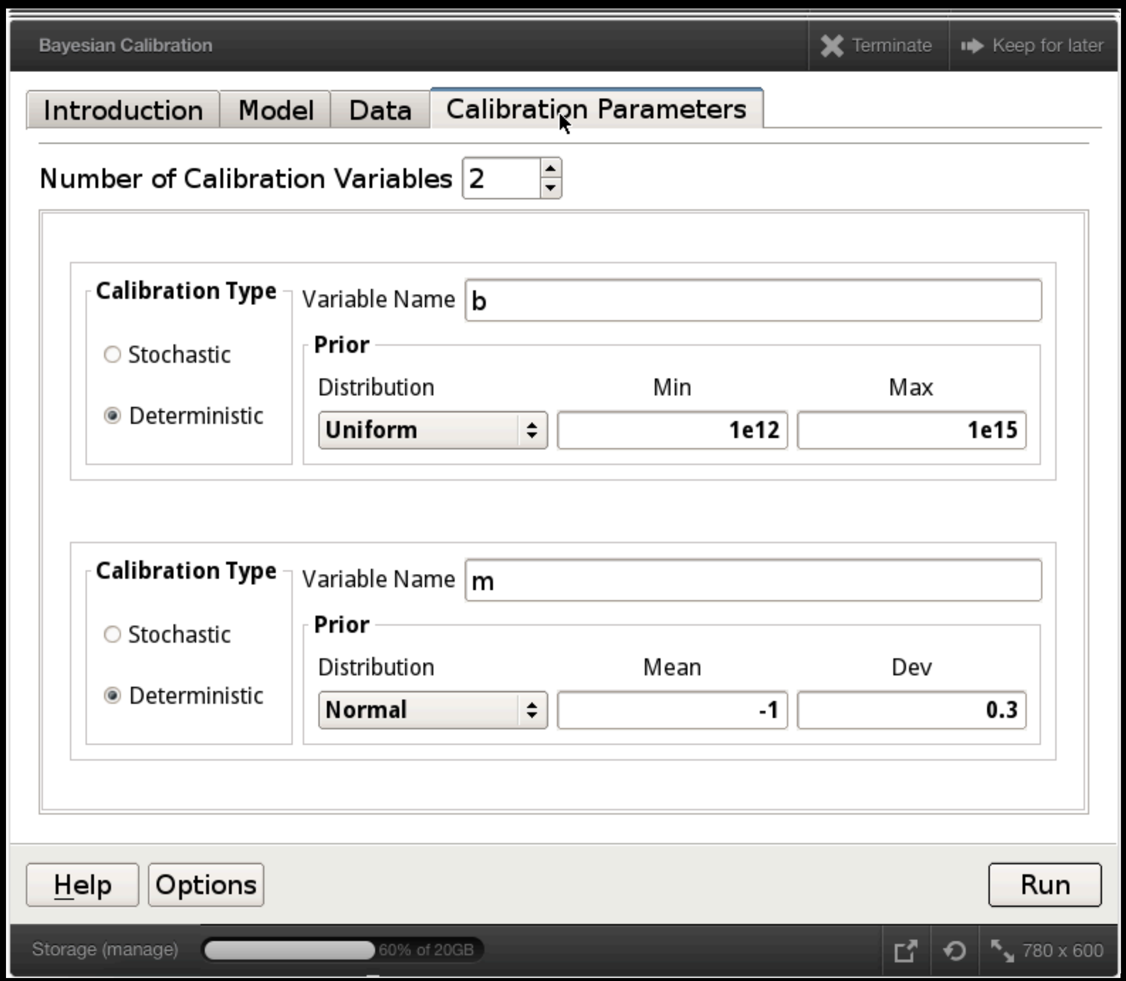
$$P(\text{Cold AND January}) = \begin{cases} P(\text{Cold})\, P(\text{January} \mid \text{Cold}) \\ P(\text{January})\, P(\text{Cold} \mid \text{January}) \end{cases}$$

$$P(A \mid B) = P(A)\,P(B \mid A) / P(B)$$

$$P(Param \mid Data) \propto P(Param)\,P(Data \mid Param)$$

Bayesian calibration tool

1. Specify model



2. Upload data

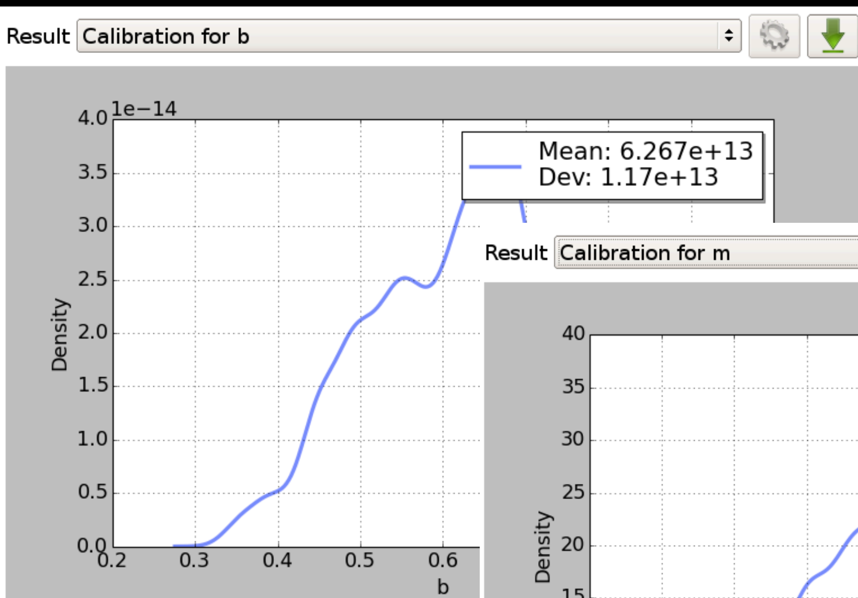
3. Setup prior information

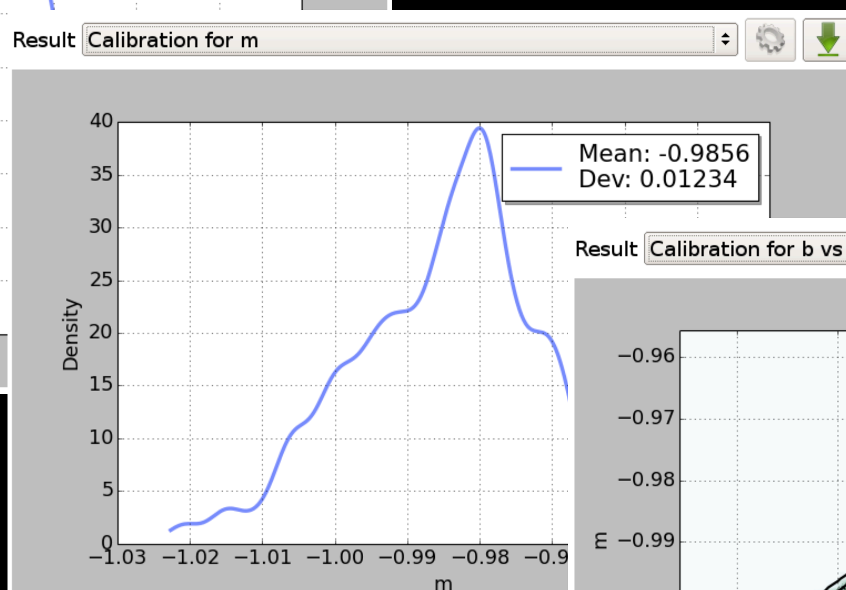
4. Run calibration

Bayesian calibration tool

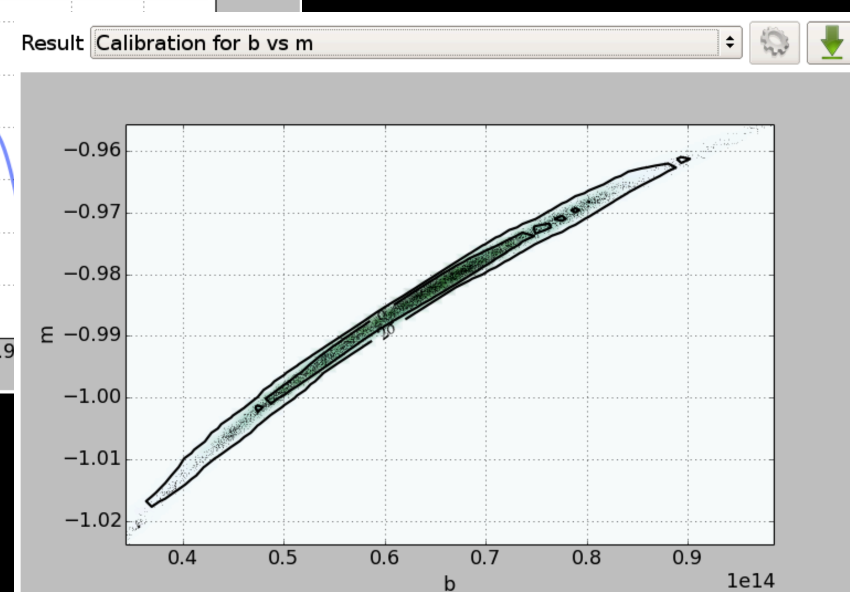
Distributions of calibrated inputs

$$N_B(x) = bx^m$$



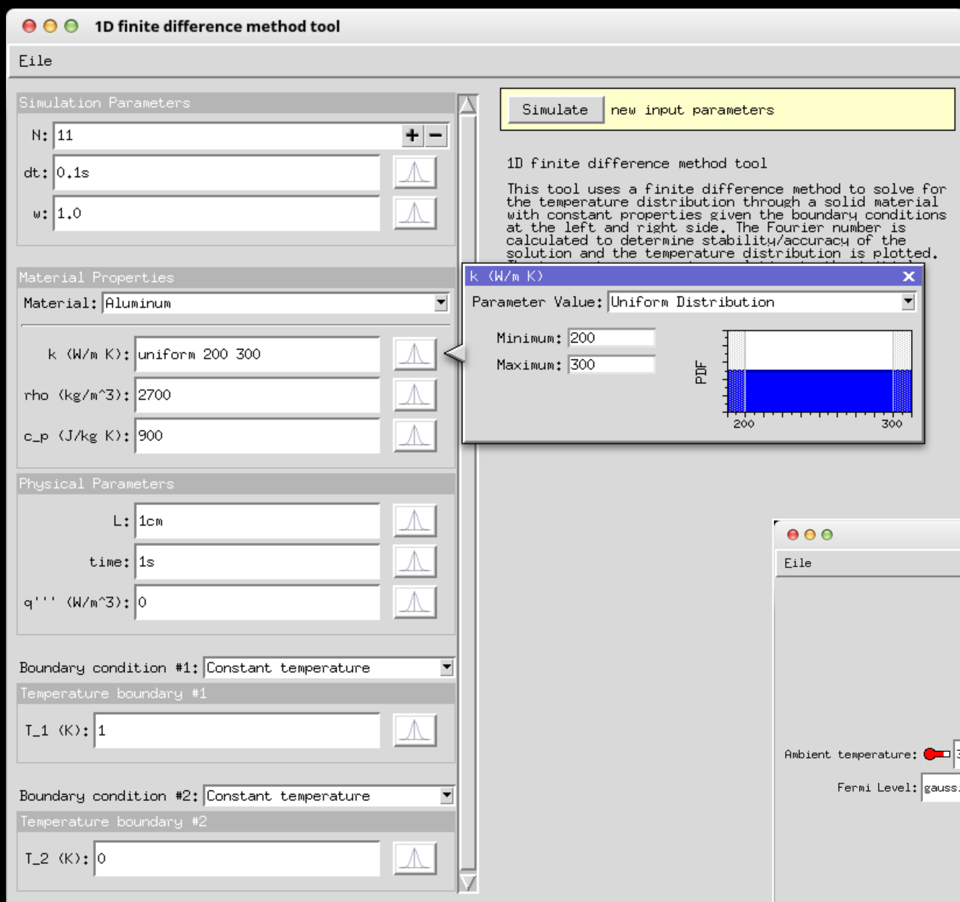


Including correlations

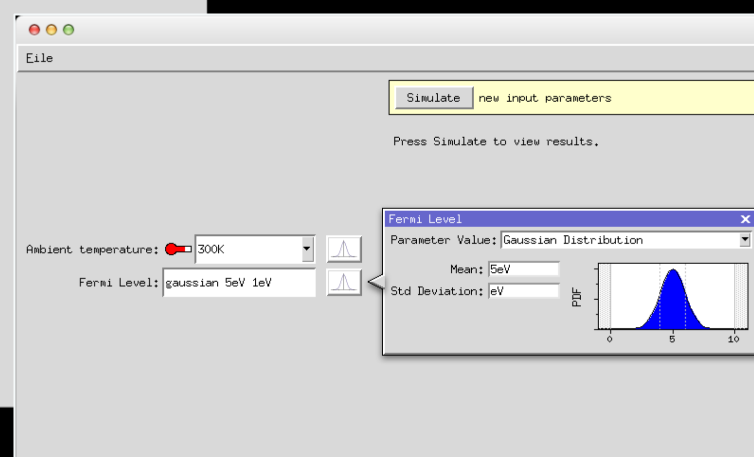


UQ for all tools

Integration of PUQ and Rappture (Rapid application infrastructure)

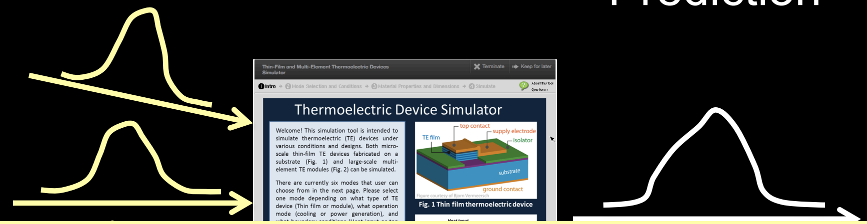


Uncertainty propagation with no intervention from tool developers



Elevating nanoHUB to the Next Level

Uncertainty propagation



- Change the way nanoHUB users perform simulations
- New ways for nanoHUB users to use simulation results
- Powerful analysis tools for experimental data
- New classes of users
  - Expert computational scientists
  - Experimentalists

Pa

Model validation