

# Uncertainty quantification tools in nanoHUB

Towards predictions with quantified confidence



**Ale Strachan**

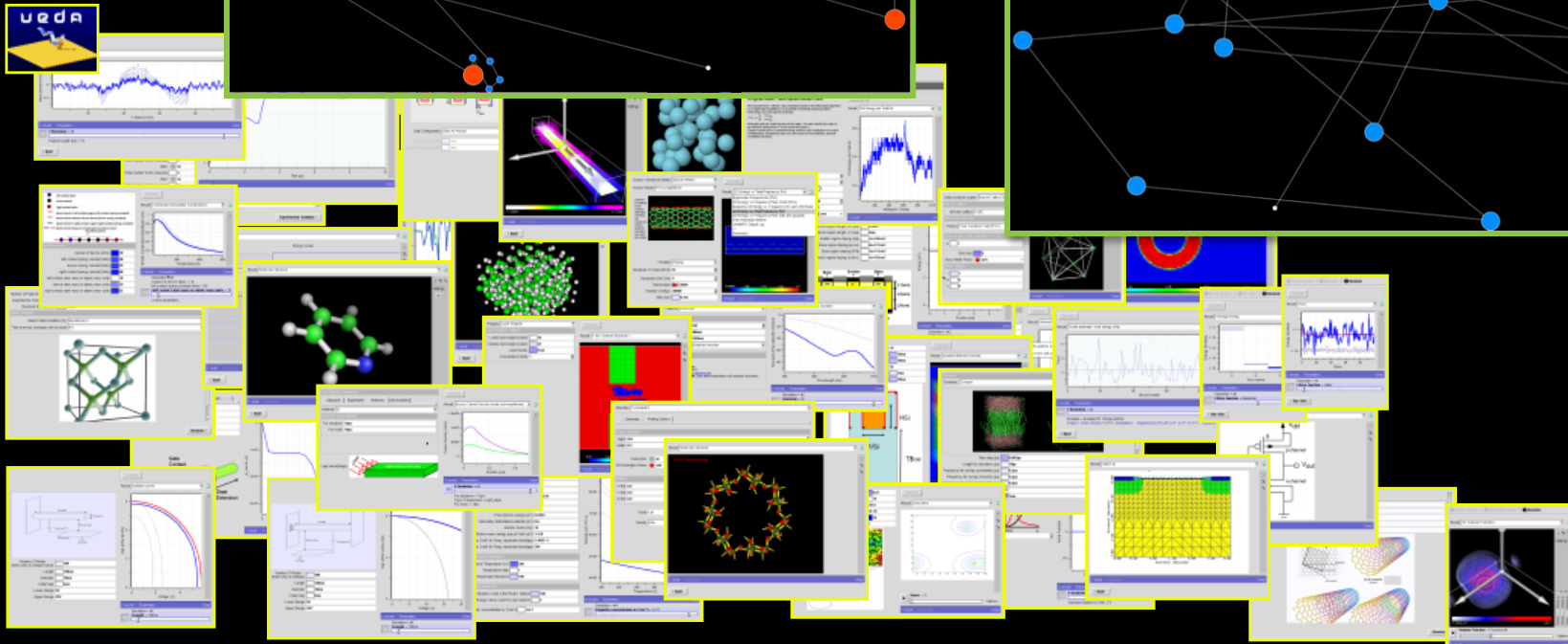
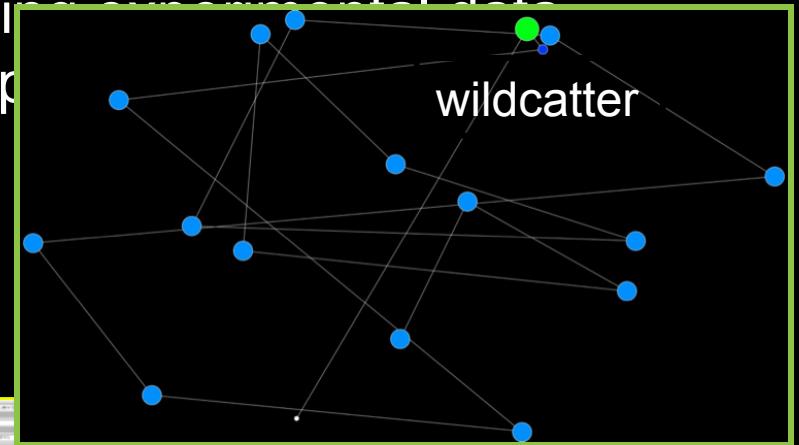
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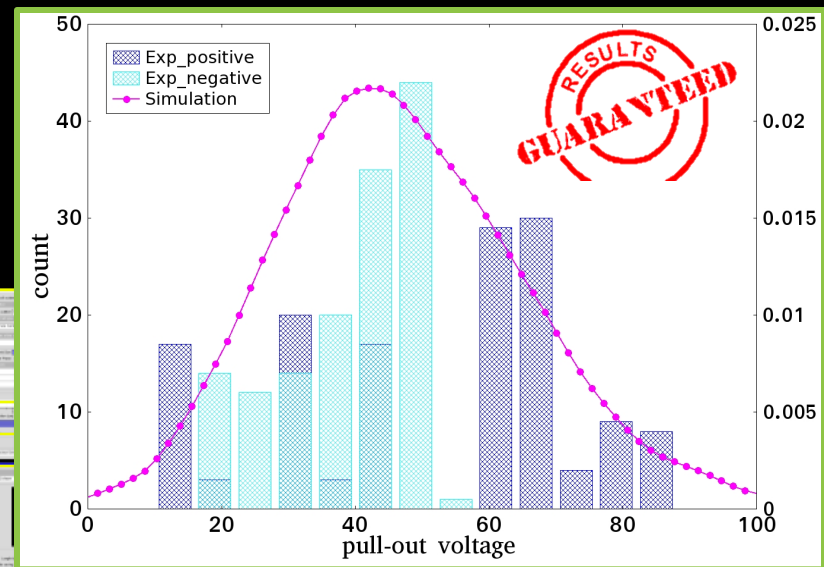
# Enhancing nanoHUB simulations

- Explore parameter space to obtain trends or optimal designs
  - Capture how variations in inputs affect predictions
  - Sensitivity analysis
  - Calibration
  - Rigorous validation
- 
- The diagram illustrates a workflow for model validation and exploration. It starts with a 'searcher' (represented by a green box) which explores the parameter space and captures how variations in inputs affect predictions. This leads to a 'wildcatter' (represented by a green box) which performs rigorous validation. The workflow is supported by 'allocation' and 'usage' (represented by green boxes) and 'exp' (represented by a green box).

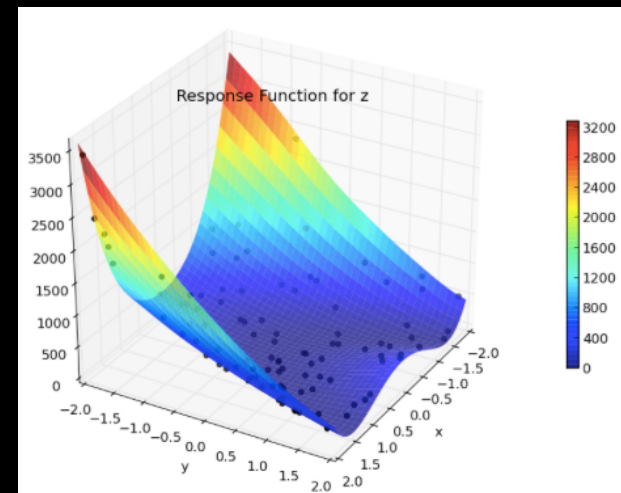
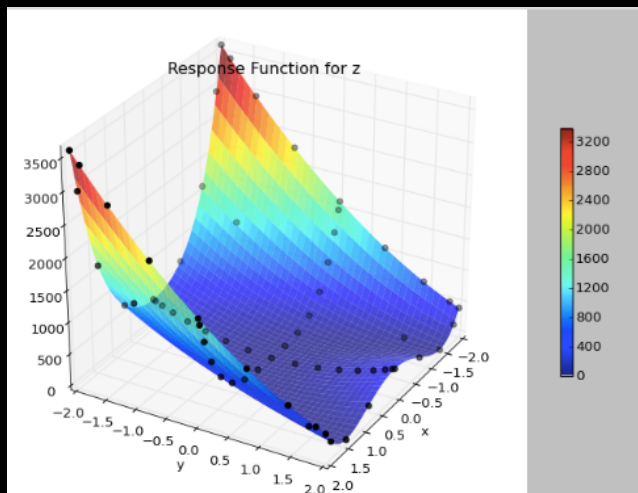


- Explore parameter space to obtain trends or optimal designs
- Capture how uncertainties in inputs affect predictions
- Sensitivity analysis for resource allocation
- Calibration of model parameters using experimental data
- Rigorous model validation using experimental data

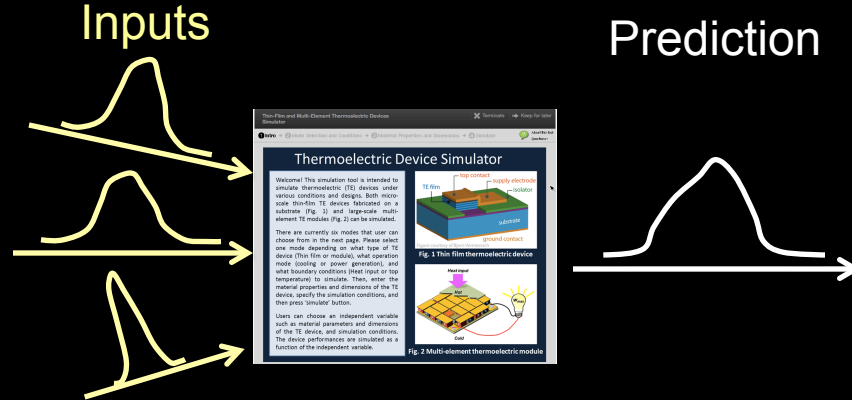
Uncertainty  
quantification



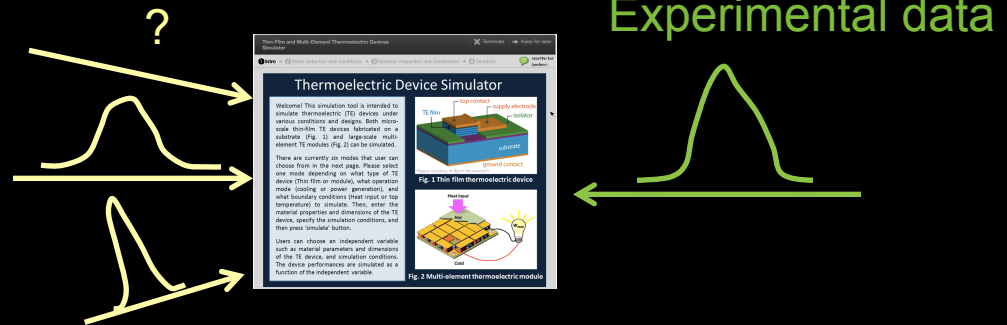
- NNSA PSAAP Center PRISM
  - 2008-2014
  - \$17M investment by NNSA, \$20 M total
- Open source – MIT license
  - <http://c-primed.github.io/puq/>



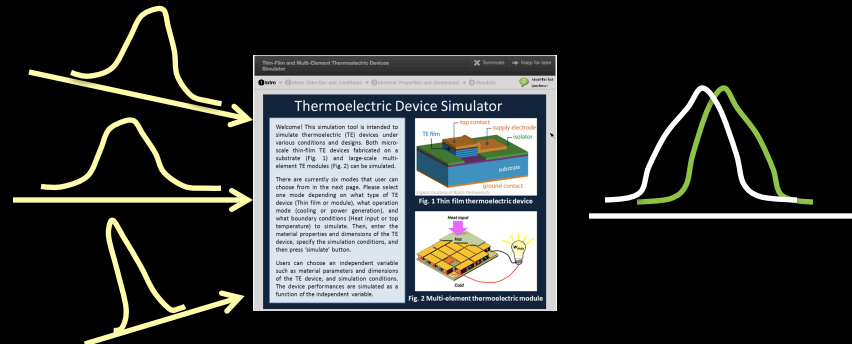
Uncertainty propagation



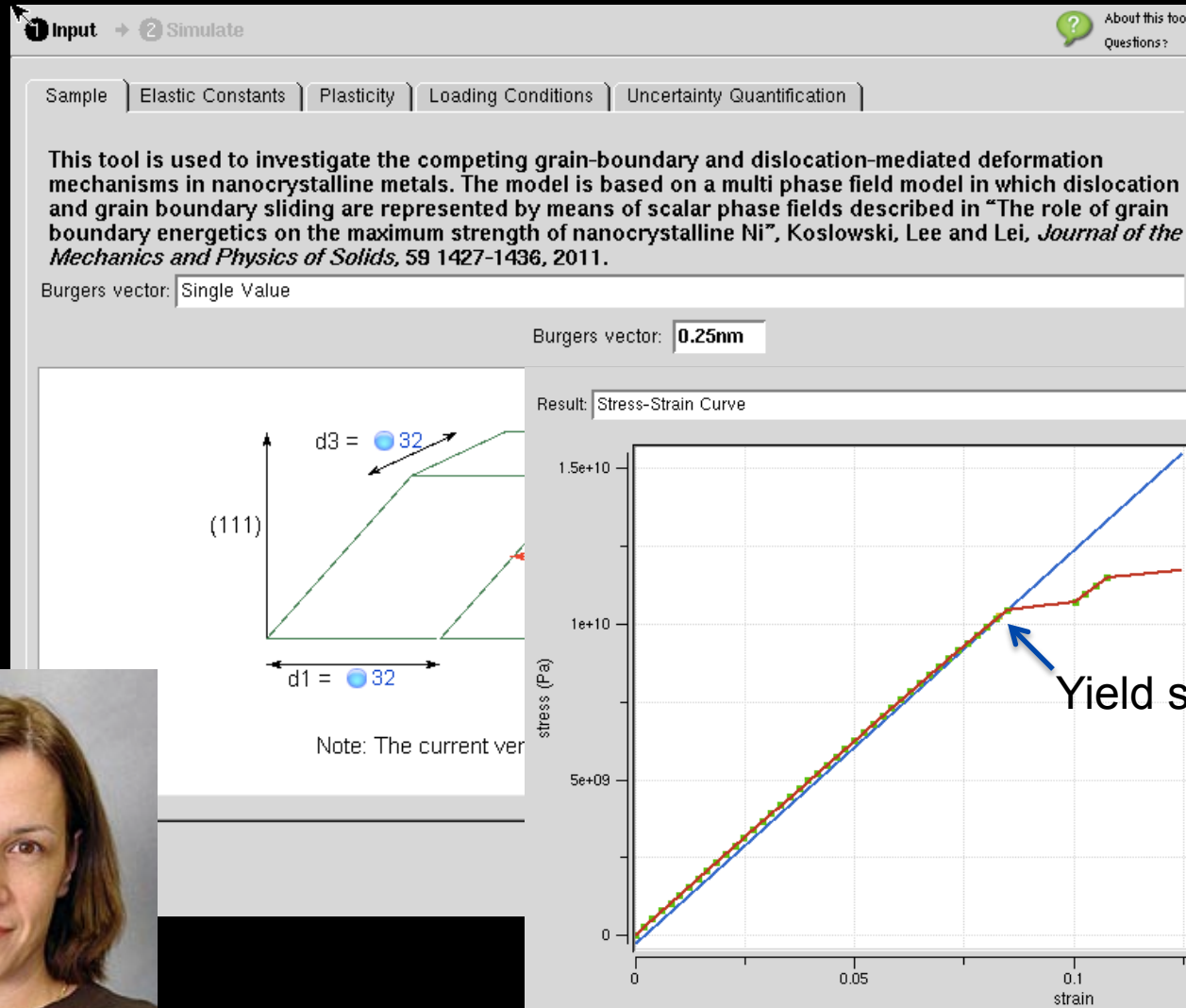
Parameter calibration



Model validation

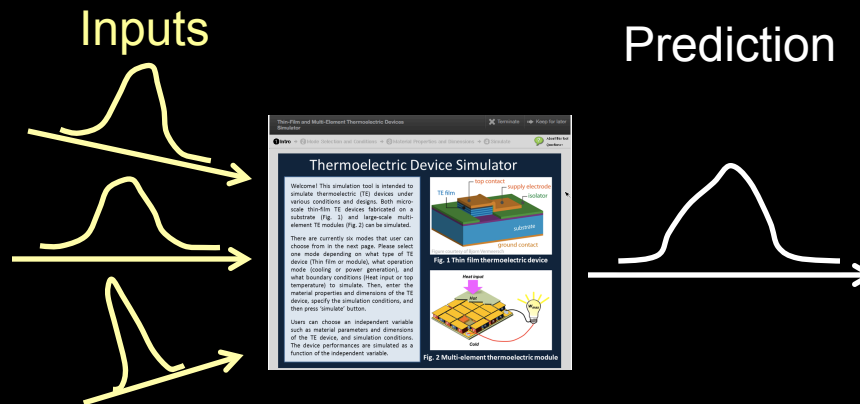






Marisol Koslowski, Mechanical Engineering @ Purdue

# Uncertainty propagation



## Requirements

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

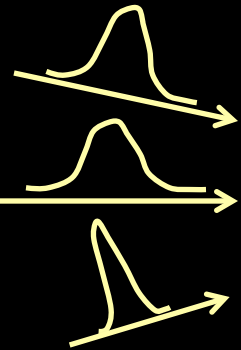
## Our solutions

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





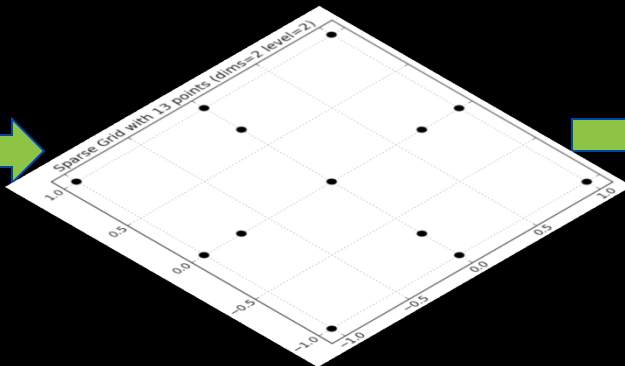
Inputs



PUQ



Sparse Smolyak grid



PUQ

+  
submit

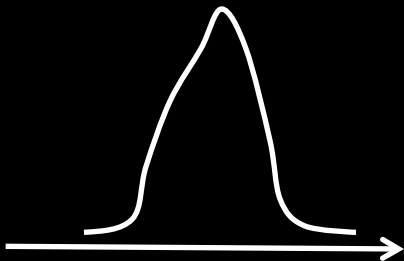


PUQ



Orthogonal polynomials

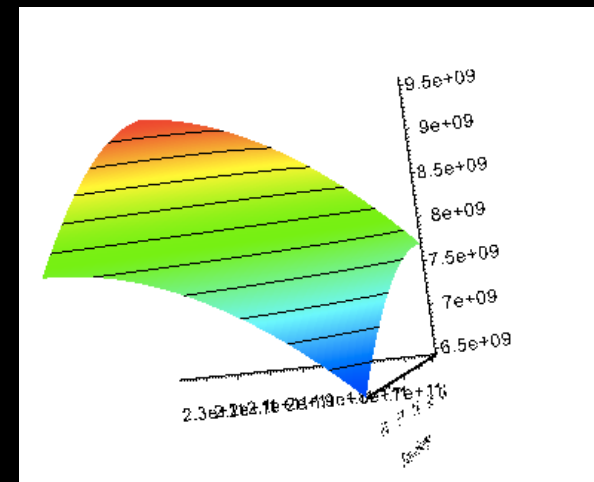
Prediction



PUQ



Monte Carlo Sampling



NanoPlasticity Lab

×

 Terminate
 

⇌

 Keep for later

1 Input

→

2 Simulate

?

 About this tool
 

?

 Question?

Sample

Elastic Constants

Plasticity

Loading Conditions

Uncertainty Quantification

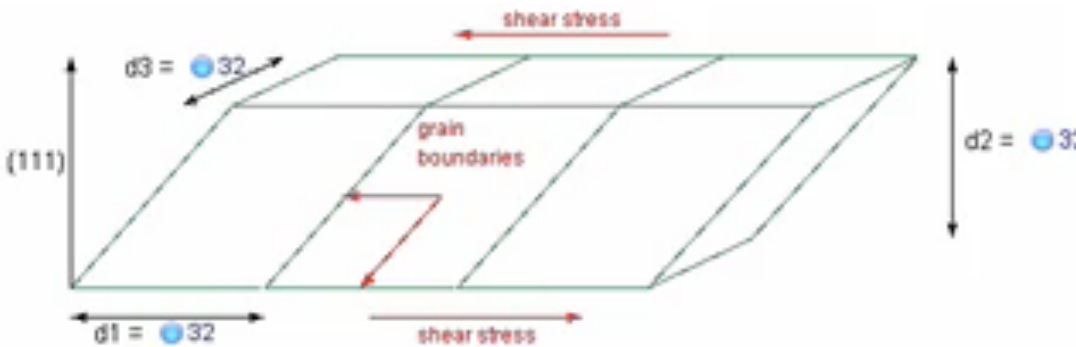
This tool is used to investigate the competing grain-boundary and dislocation-mediated deformation mechanisms in nanocrystalline metals. The model is based on a multi phase field model in which dislocation and grain boundary sliding are represented by means of scalar phase fields described in "The role of grain boundary energetics on the maximum strength of nanocrystalline Ni", Kosłowski, Lee and Lei, *Journal of the Mechanics and Physics of Solids*, 59 1427-1436, 2011.

Burgers vector:

Single Value

Burgers vector:

0.25nm



$d3 = 32$   
 $d1 = 32$   
 $d2 = 32$

(111)  
 grain boundaries  
 shear stress

Note: The current version of this tool requires  $d1=d2=d3$ .

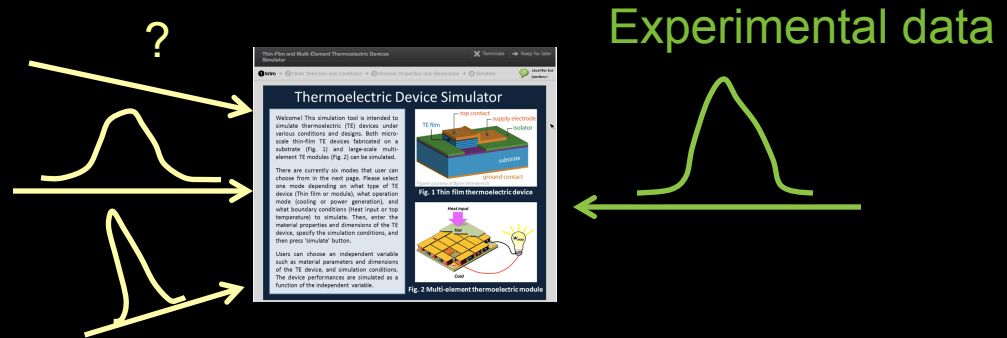
Simulate >

Storage (manage)

59% of 20GB

780 x 600

Parameter calibration



Bayesian theorem & calibration

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

$$P(A | B) = P(A) P(B | A) / P(B)$$

$$P(\text{Param} | \text{Data}) \propto P(\text{Param}) P(\text{Data} | \text{Param})$$

## 1. Specify model

Bayesian Calibration ✕ Terminate ➡ Keep for later

Introduction Model Data **Calibration Parameters**

Number of Calibration Variables

**Calibration Type**

☐ Stochastic

☒ Deterministic

Variable Name

**Prior**

Distribution	Min	Max
<input type="text" value="Uniform"/>	<input type="text" value="1e12"/>	<input type="text" value="1e15"/>

**Calibration Type**

☐ Stochastic

☒ Deterministic

Variable Name

**Prior**

Distribution	Mean	Dev
<input type="text" value="Normal"/>	<input type="text" value="-1"/>	<input type="text" value="0.3"/>

[Help](#) [Options](#) [Run](#)

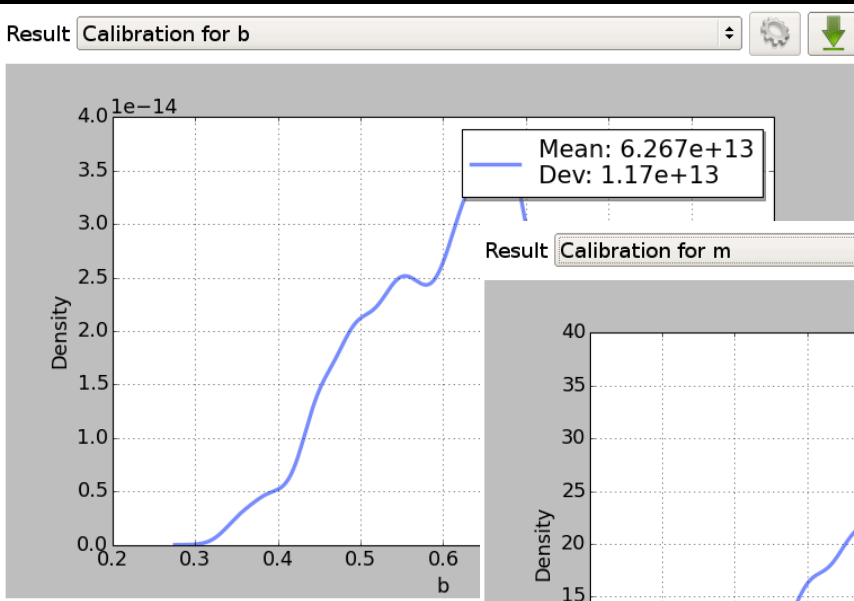
Storage (manage)  780 x 600

## 2. Upload data

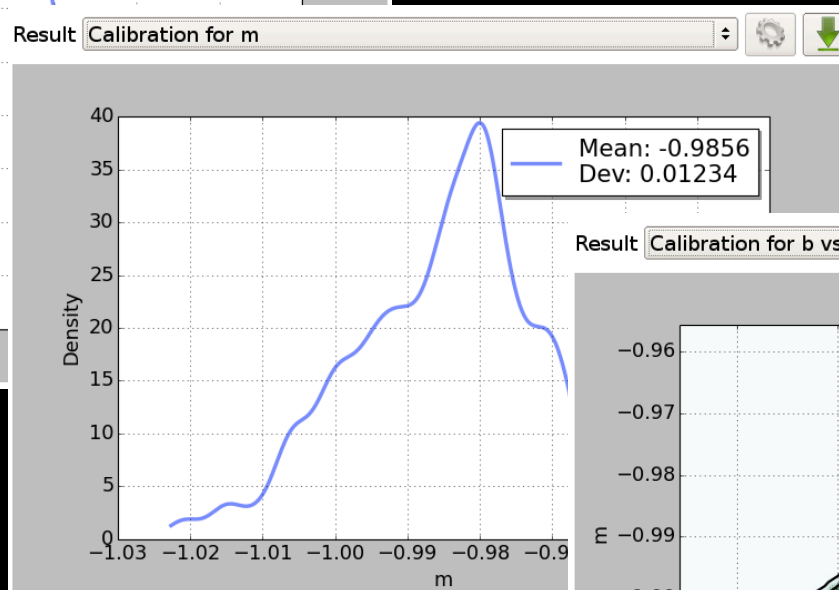
## 3. Setup prior information

## 4. Run calibration

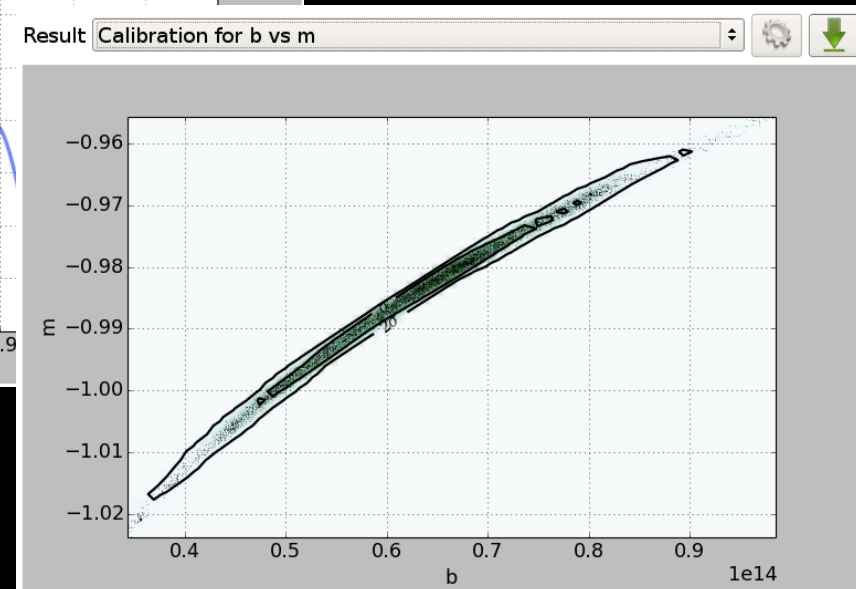
## Distributions of calibrated inputs



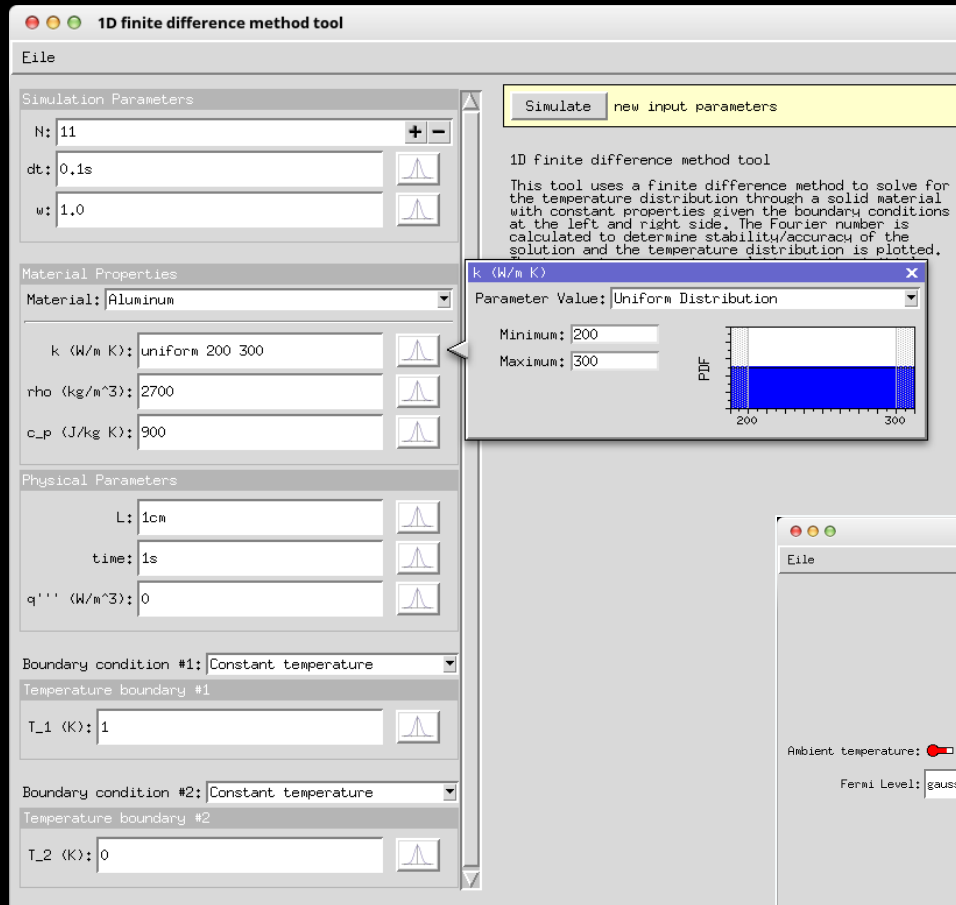
$$N_B(x) = bx^m$$



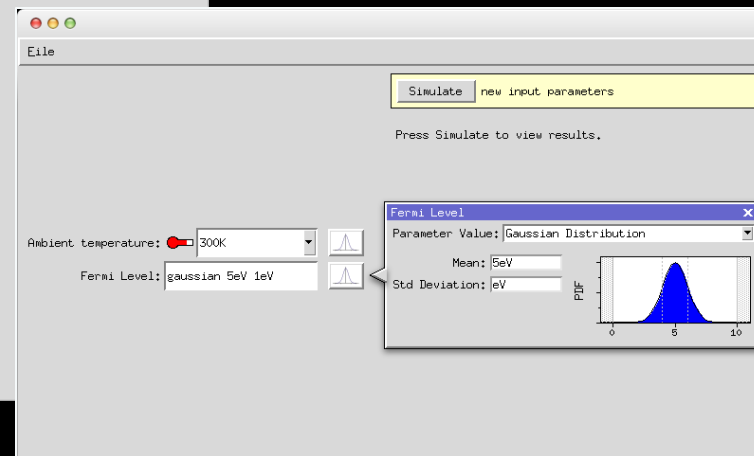
Including  
correlations



## Integration of PUQ and Rappture (Rapid application infrastructure)



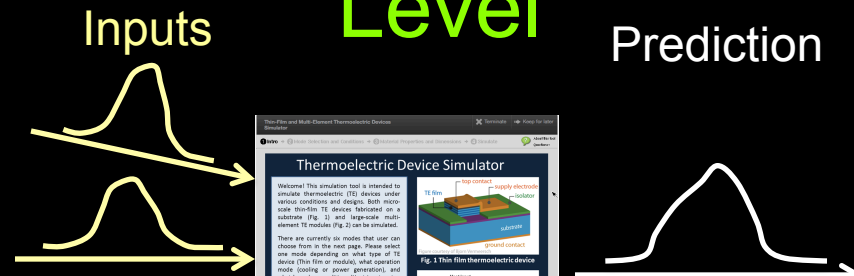
Uncertainty propagation  
with no intervention from  
tool developers





# Elevating nanoHUB to the Next Level

Uncertainty propagation



Pa

- 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

Model validation

