Constrained Bayesian Optimization of Criticality Experiments

Presented to WPEC Subgroup 46

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November 12, 2020

LLNL-PRES-XXXXXX

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

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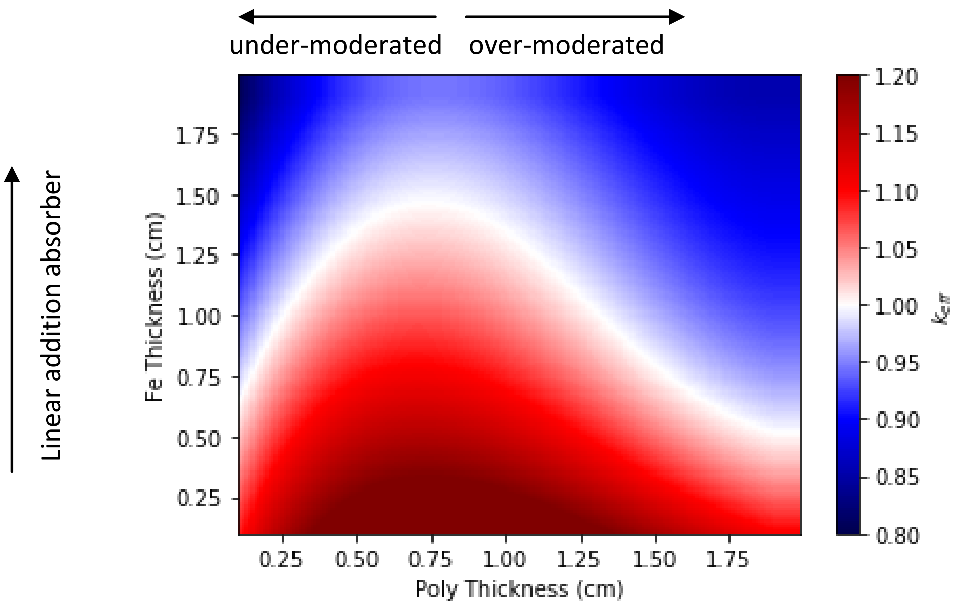
Integral Experiment Design Challenge

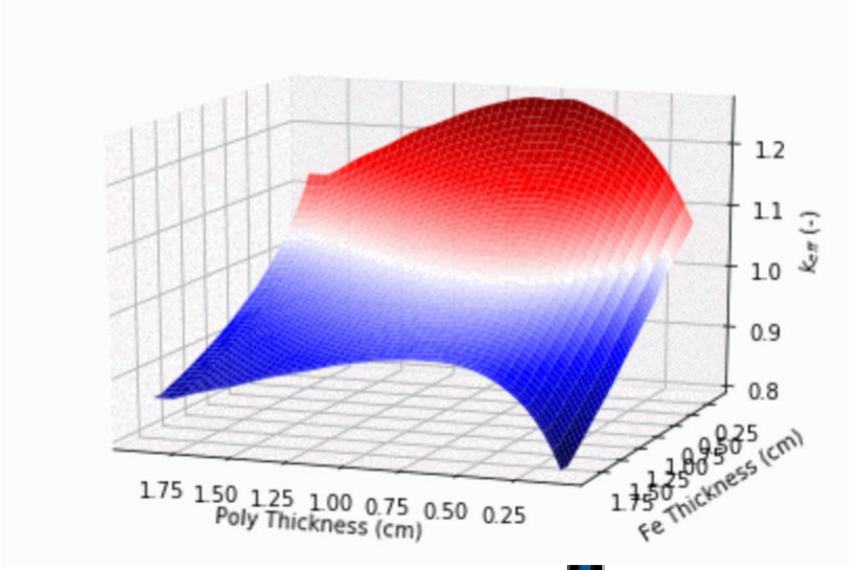
- Must be optimal with respect to a variable (*objective*)
  - Intermediate fission fraction
  - EALF
  - Sensitivity to specific reaction of specific nuclide at specific energy range
  - Representativity of criticality safety application
  - …
- Must respect constraints
  - Criticality
  - Height-to-diameter ratio
  - Weight
  - Cost
  - …

- Designs simulated with Monte Carlo (MC) codes
- **Challenge**: Find best design with least code executions and least headache

What combination makes a critical experiment?

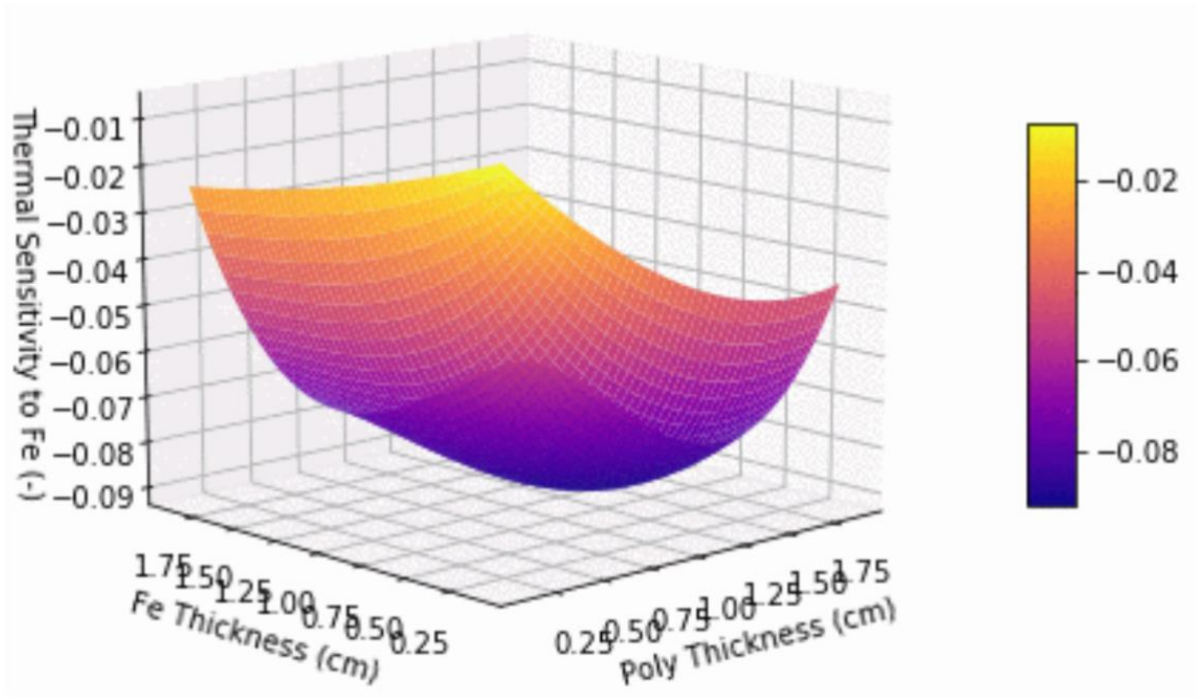
k_{eff} vs. design parameters

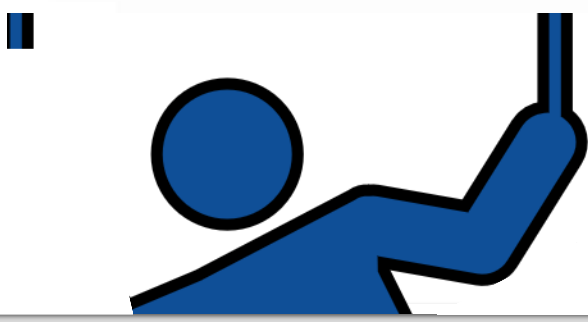




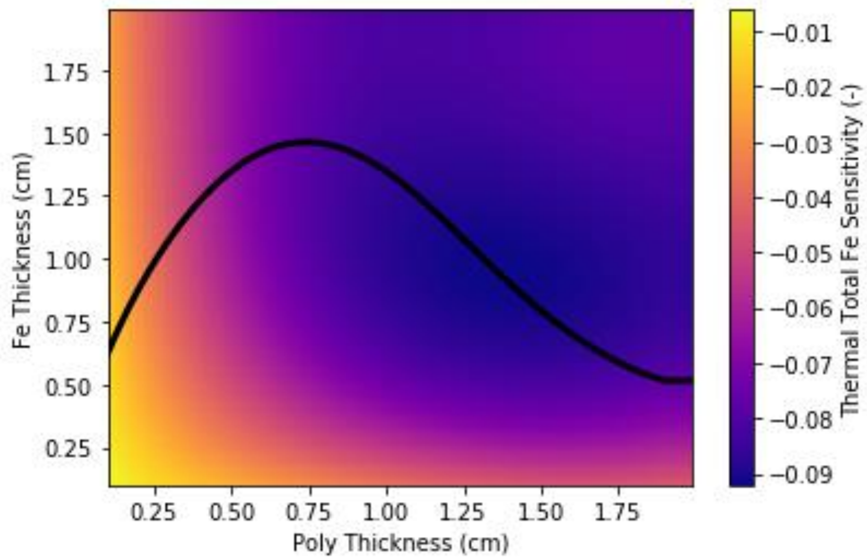
What Combination Maximizes Sensitivity?

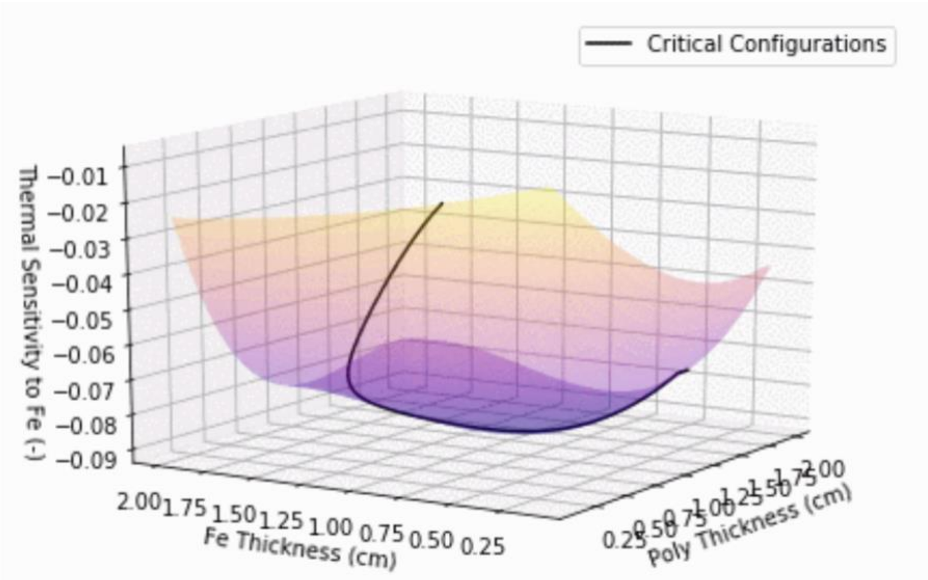
Thermal Iron Sensitivity vs. Design Parameters



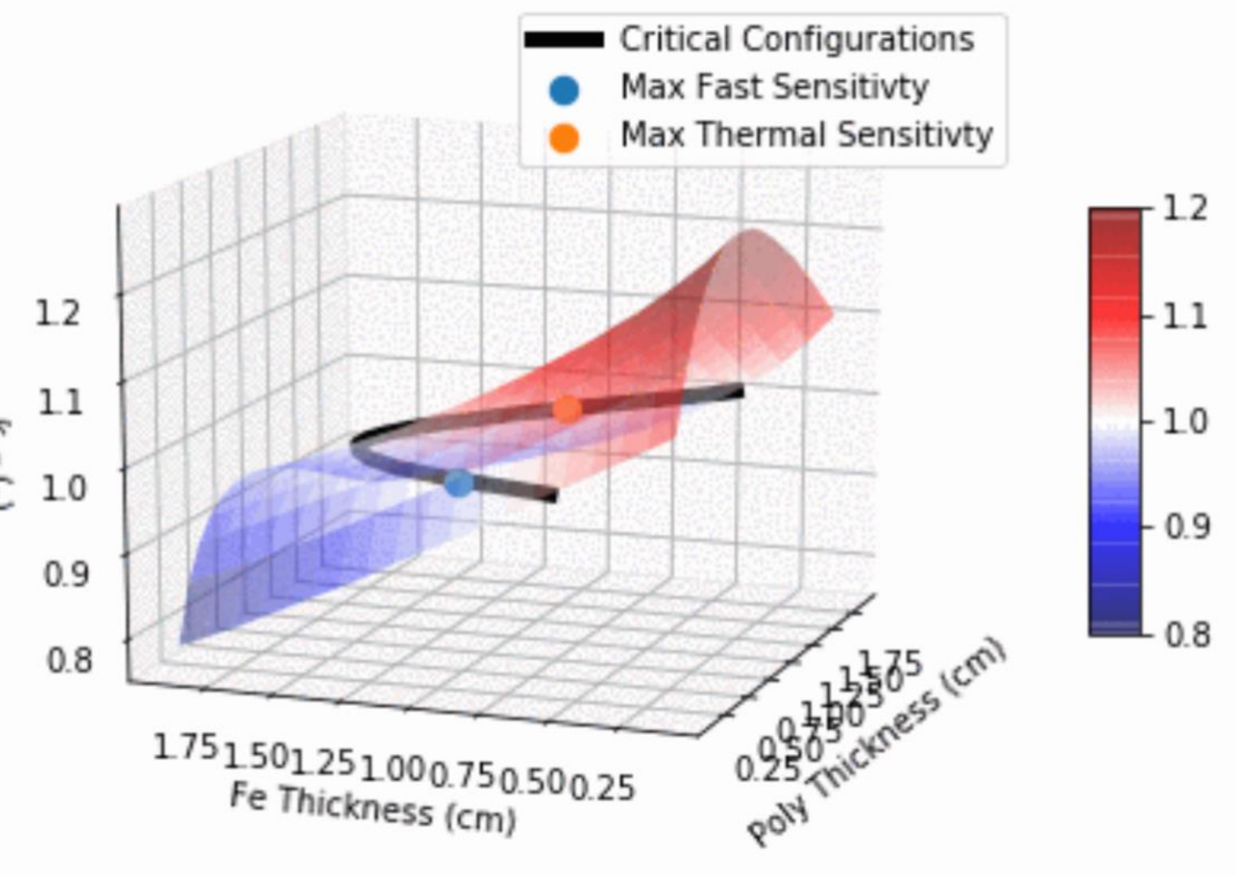


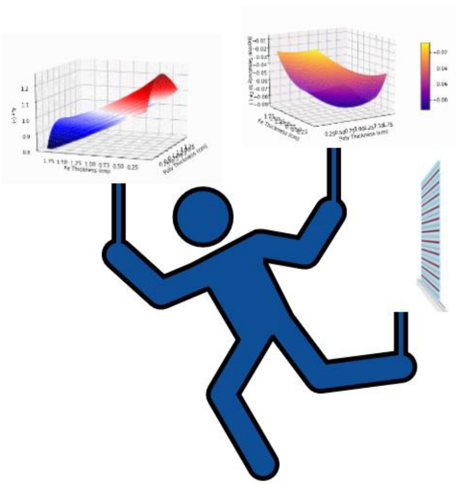
What Does Both?
Critical Configurations in Sensitivity Space





Optimal Designs

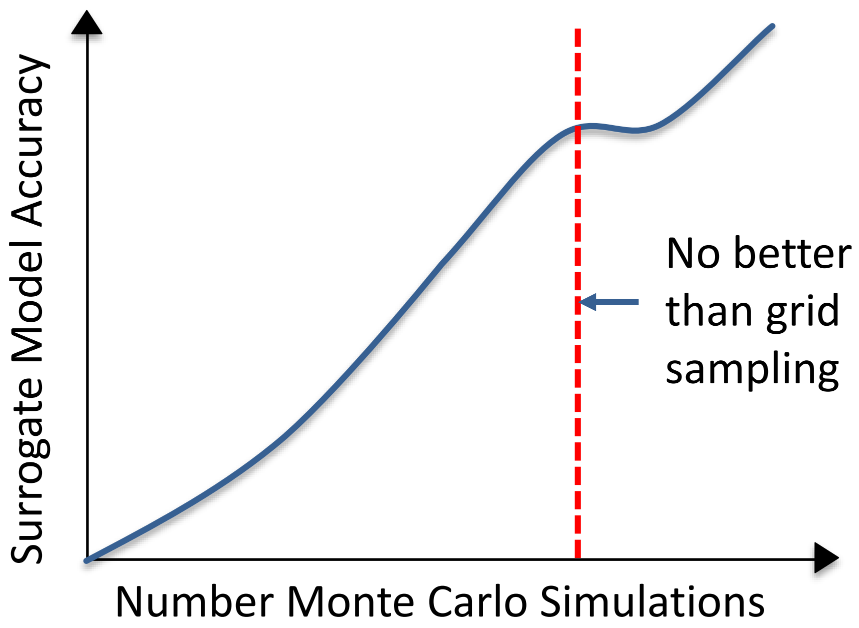




Optimization Strategy

- Idea:
  - Surrogate model of MC code
  - Use model to find the optimal design
  - Avoid expensive MC
- Questions:
  - Which surrogate model?
  - How to minimize MC simulations?
    - Balance between accurate regression and minimizing computational cost
- One Solution:
  - Gaussian processes
  - Efficient global optimization

Competing Desires



Gaussian Process

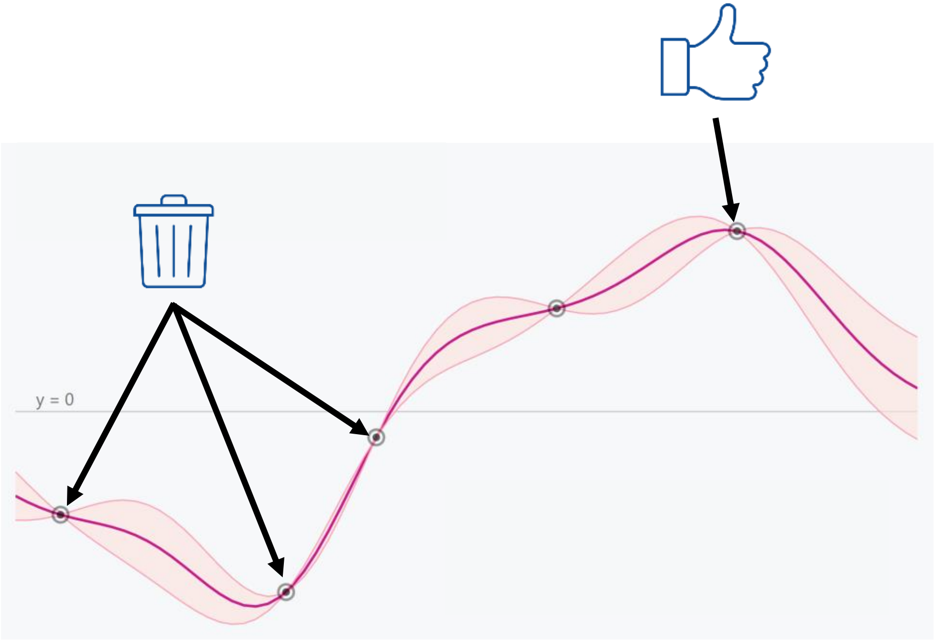
(Kriging Metamodel[1])

- Similar designs have similar underlying physics
  - Highly correlated because the physics is the same
  - Example: If I know k_{eff} at 1.000 cm thick reflector, easy to predict k_{eff} at 1.001 cm
- Dissimilar designs have very different physics
  - Uncorrelated or anti-correlated
  - Example: anti-correlation in under- vs. over-moderated reactor
- **Idea**: Use a probability distribution as the surrogate model
  - 'Gaussian' comes from using normal distribution
  - Analytical solutions are possible
  - Incorporates uncertainty of training data
- Predict variable based on the degree of correlation with training data

[1]*Krige, Danie G. (1951). "A statistical approach to some basic mine valuation problems on the Witwatersrand". J. of the Chem., Metal. and Mining Soc. of South Africa.* ***52*** *(6): 119–139*

How to Add Training Data Efficiently

- Adding training data is expensive
  - MC simulations
  - Experiments
- For optimization, only want to add it near a max or min
- How do we efficiently choose where to add new points?
- An answer: **Bayesian Optimization**



Bayesian Optimization

- Bayesian Optimization: algorithm for finding an optimum
  - Fit GP
  - Choose new training data
  - Find the optimum

- "Bayesian" from the training of GP (prior) with observations (posterior)

- **Acquisition function** used to choose next point

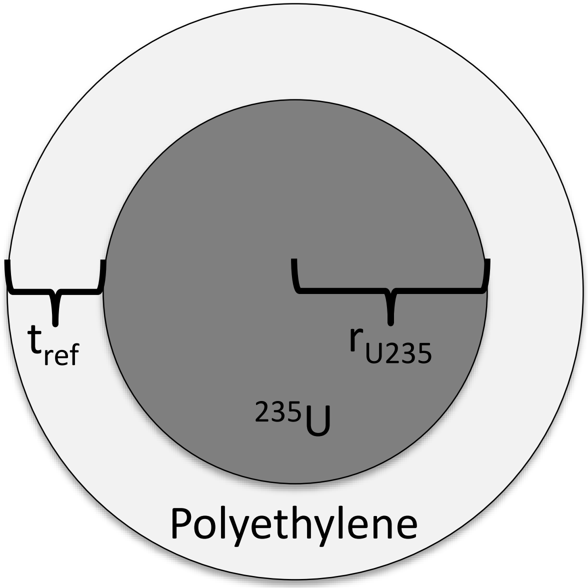
- Balances two important factors:

  1. **Exploitation**: Need training data near optimum

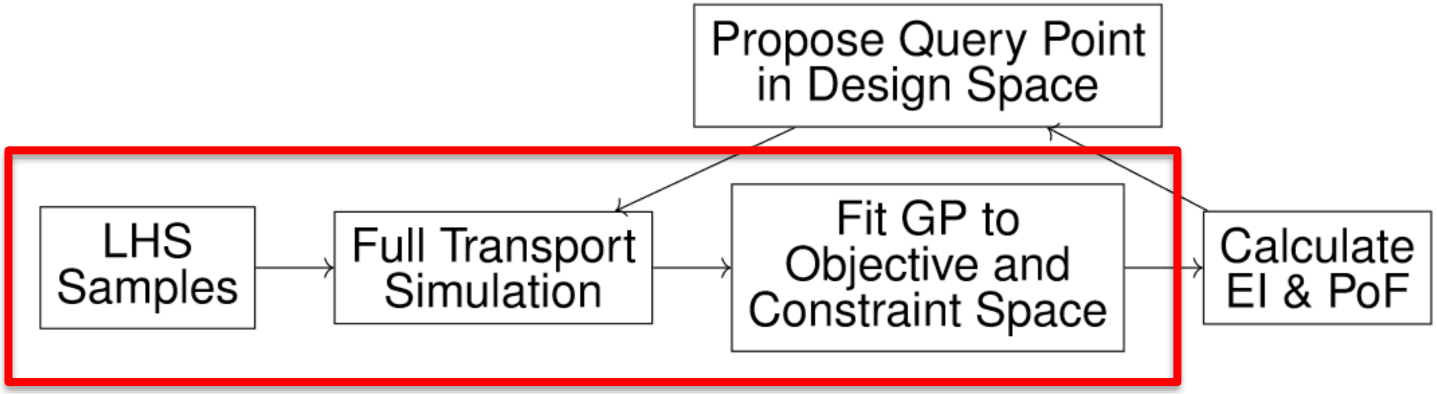
  2. **Exploration**: Need an accurate regression (low uncertainty in GP)

Reflected ^{235}U Sphere

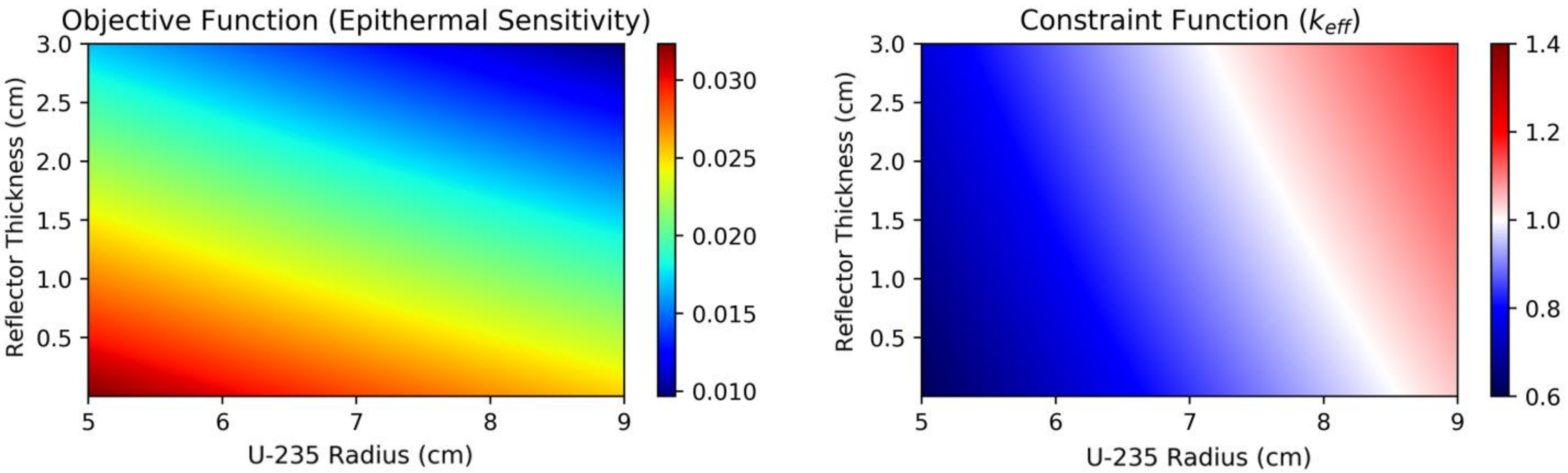
- Where is intermediate sensitivity of ^{235}U maximized but system is critical?
  - Modeled with MCNP6.2
- Free parameters:
  - Radius of U-235 (95 wt%) sphere
  - Thickness of polyethylene reflector
- Known solution!
- Almost bare critical sphere



Initial Fit

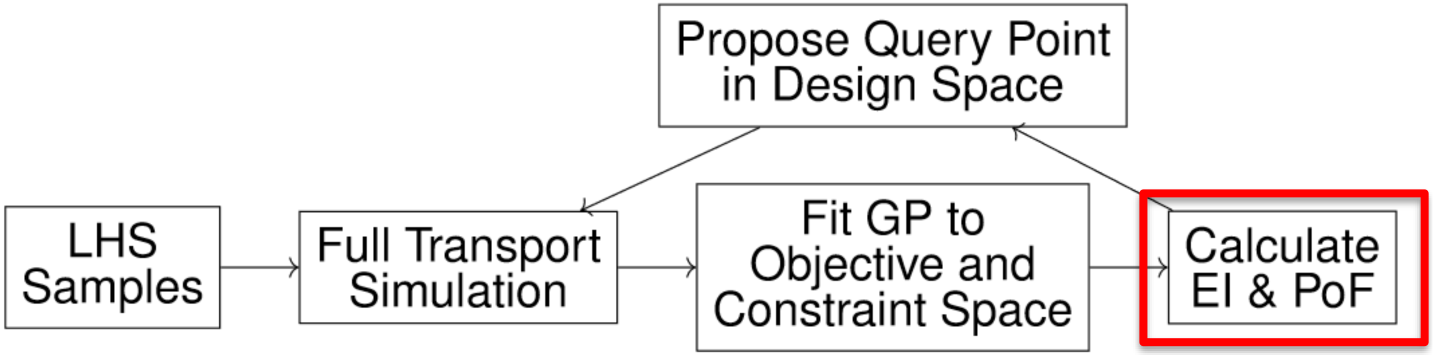


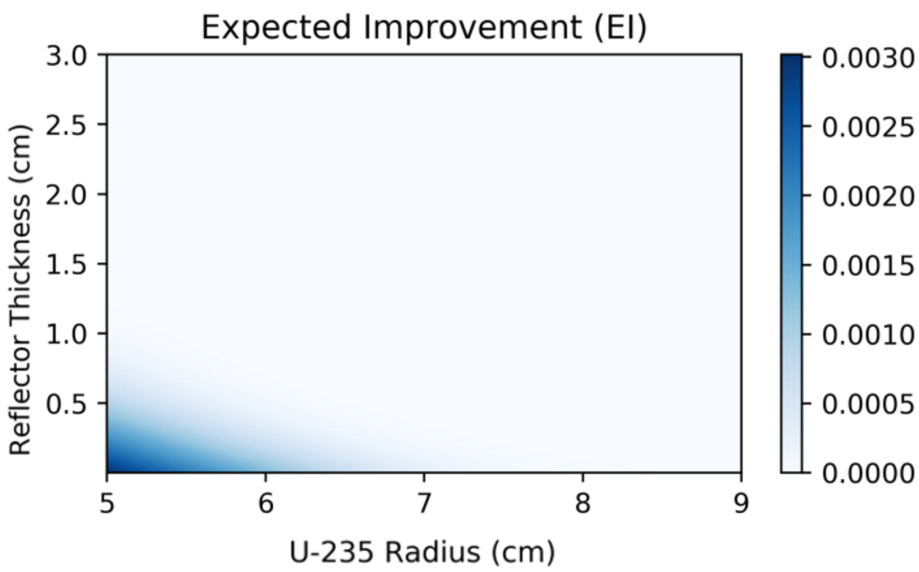
Propose Query Point in Design Space
LHS Samples
Full Transport Simulation
Fit GP to Objective and Constraint Space
Calculate EI & PoF

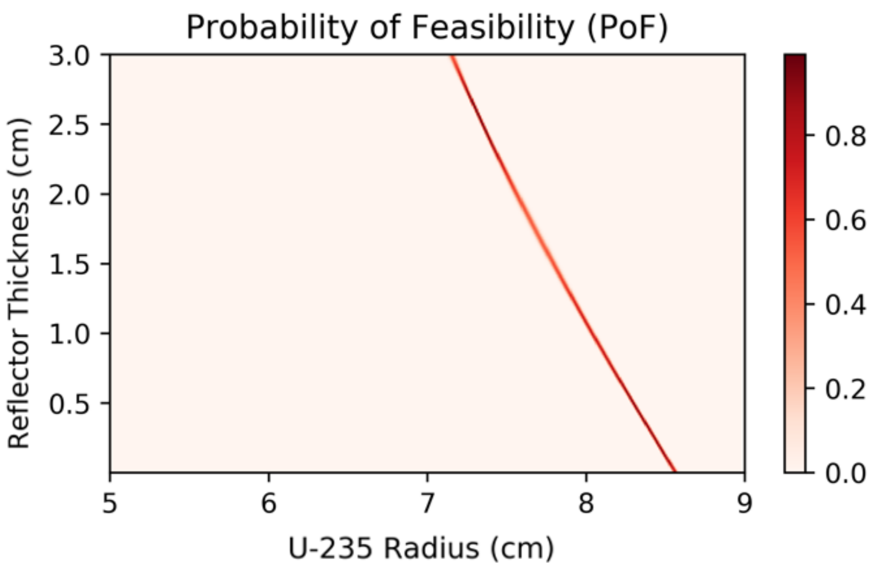


Objective Function (Epithermal Sensitivity)
Reflector Thickness (cm)
U-235 Radius (cm)
3.0
2.5
2.0
1.5
1.0
0.5
5
6
7
8
9
0.030
0.025
0.020
0.015
0.010
Constraint Function (k_{eff})
Reflector Thickness (cm)
U-235 Radius (cm)
3.0
2.5
2.0
1.5
1.0
0.5
5
6
7
8
9
1.4
1.2
1.0
0.8
0.6

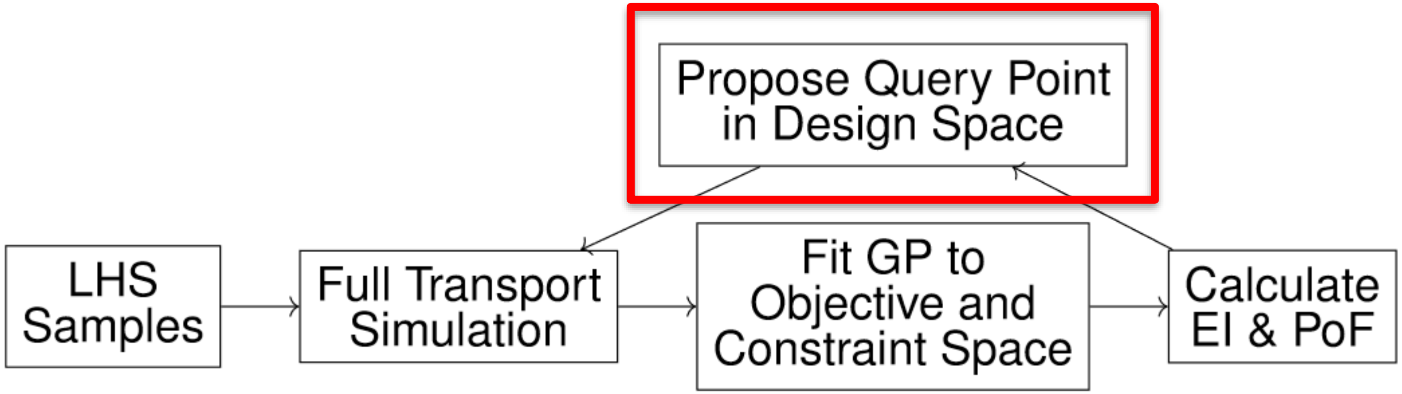
Calculate EI and PoF

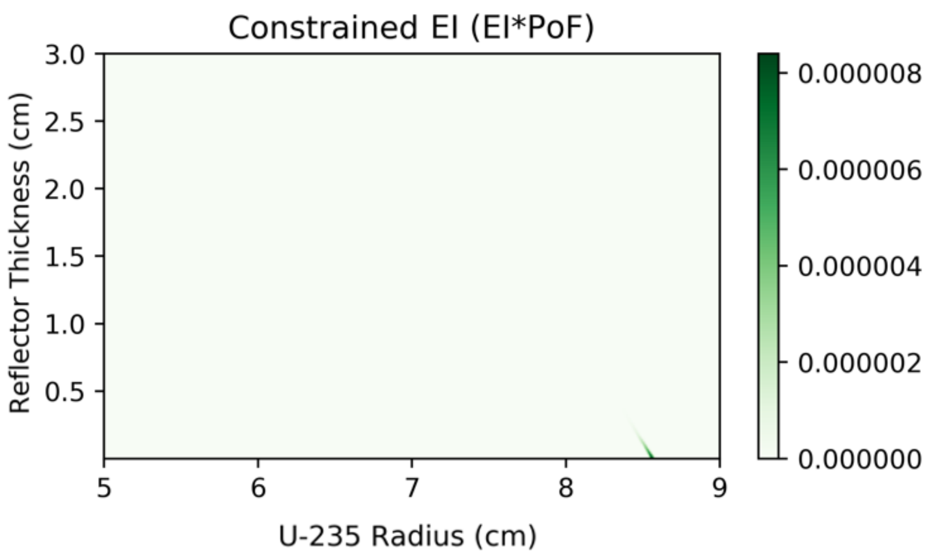


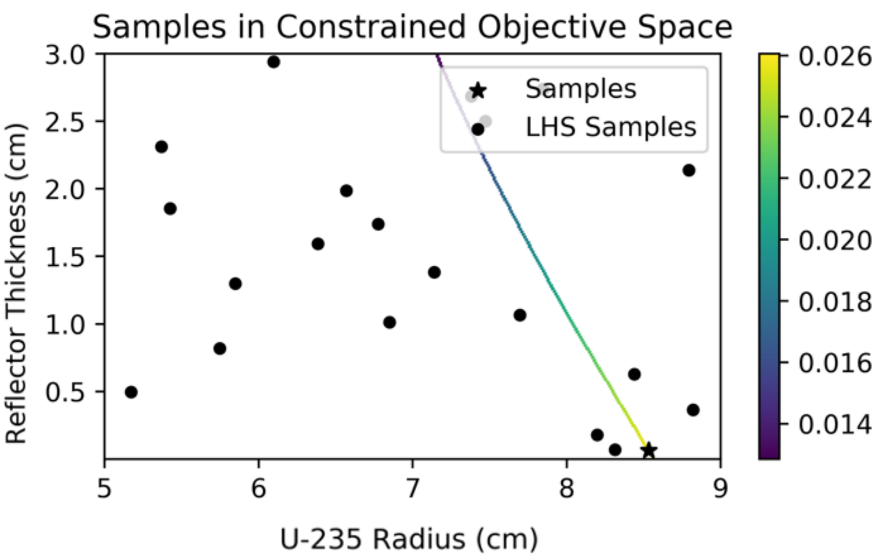




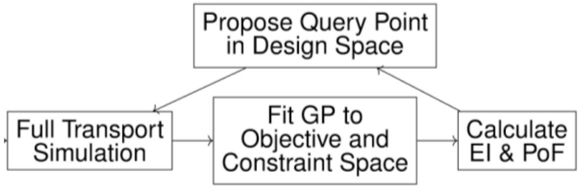
Pick Next MCNP Execution



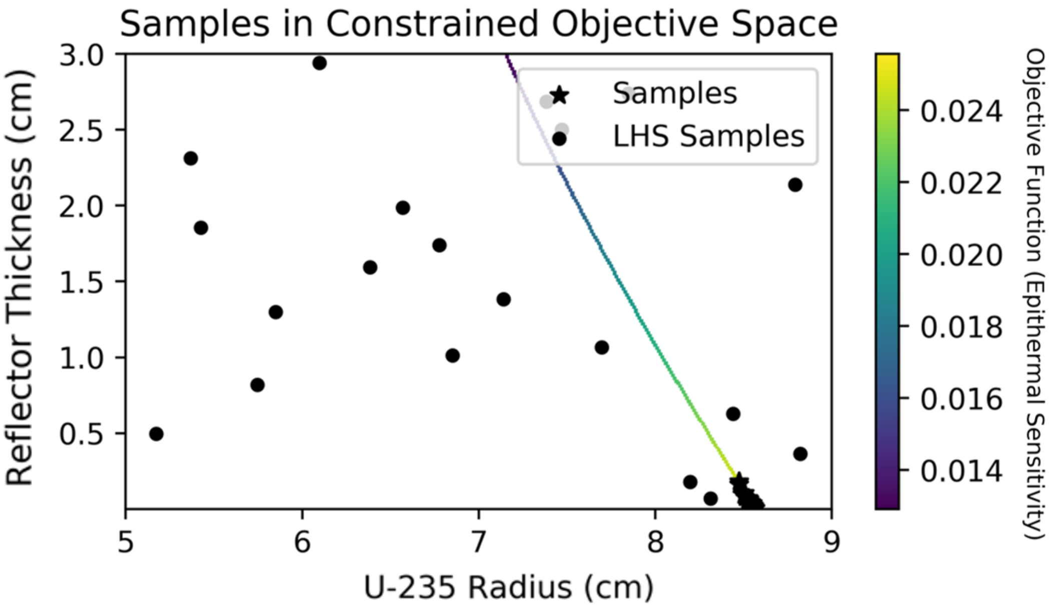




Thirty More Queries



x 15



Design of TEX Experiment

- Make a critical TEX that maximizes similarity with nuclear waste of Hanford Tank Farm
  - For Whisper USL estimations
- Objective is c_k coefficient
  - c_k = 1 if perfect match
  - Advantages:
    - Weighs importance of sensitivities with magnitude of nuclear data uncertainty
    - Directly used in WHISPER and TSURFER
  - Disadvantages
    - Varies with nuclear data covariance matrix: optimization with library will be different from with another library

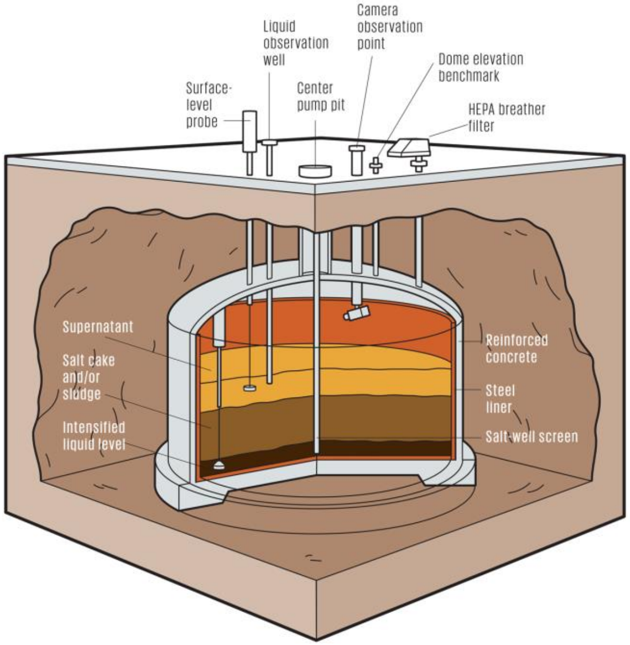
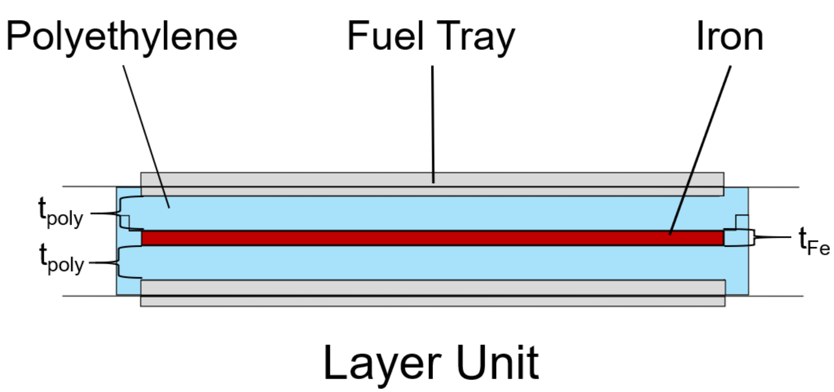


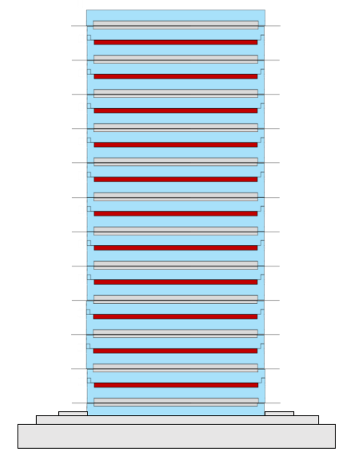
Illustration by J. Provost

$$c_k = \frac{S_A M_\sigma S_B^T}{\sqrt{S_A M_\sigma S_A^T}\sqrt{S_B M_\sigma S_B^T}}$$

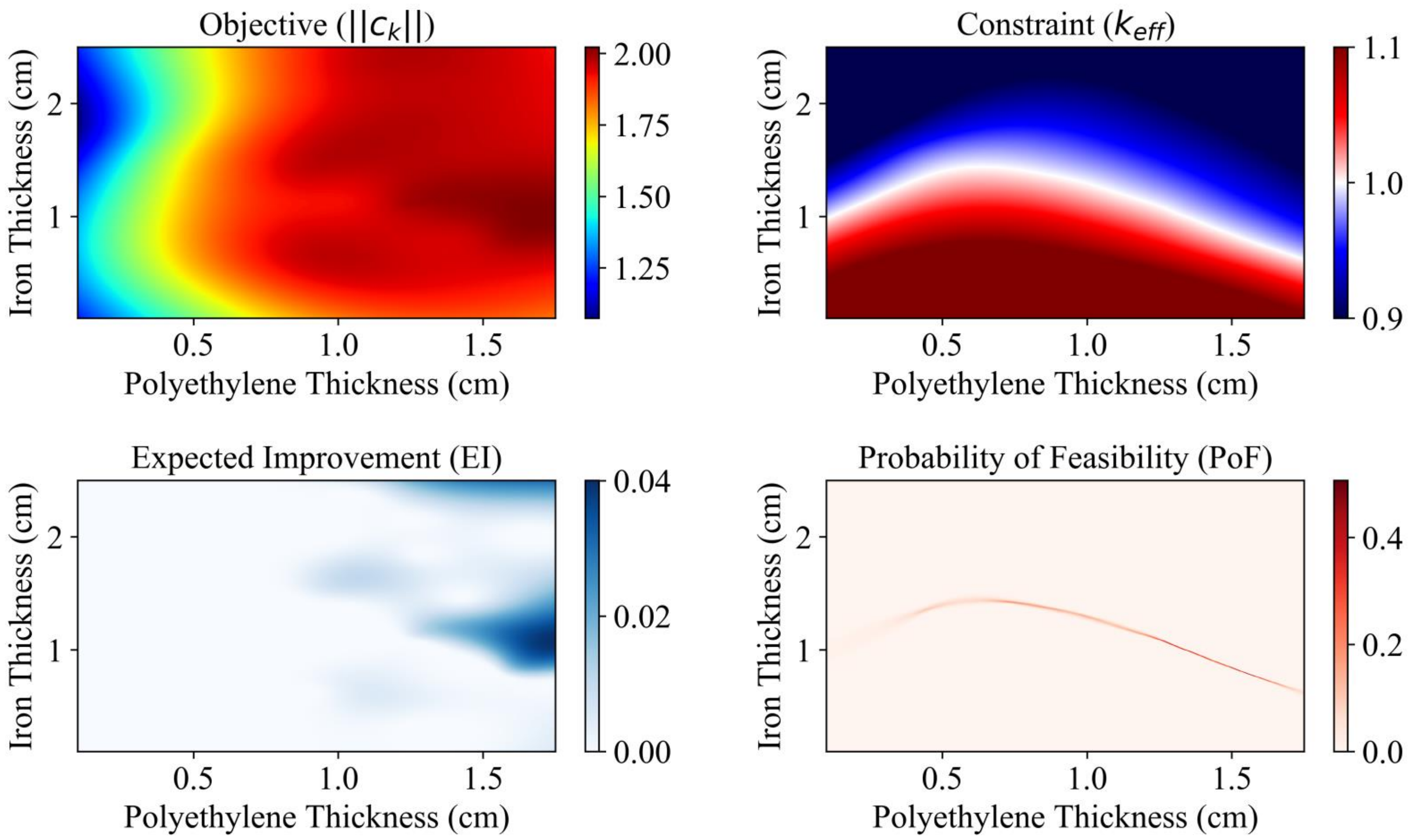
Design Process

- Design parameters:
  - Thickness of polyethylene moderator
  - Thickness of iron/manganese absorber layers
  - Number of layers in stack
- Constraints:
  - MCNP $k_{eff} = 1 \pm 150$ pcm
  - Height/width ratio < 2
  - Separated stack $k_{eff} < 0.9$

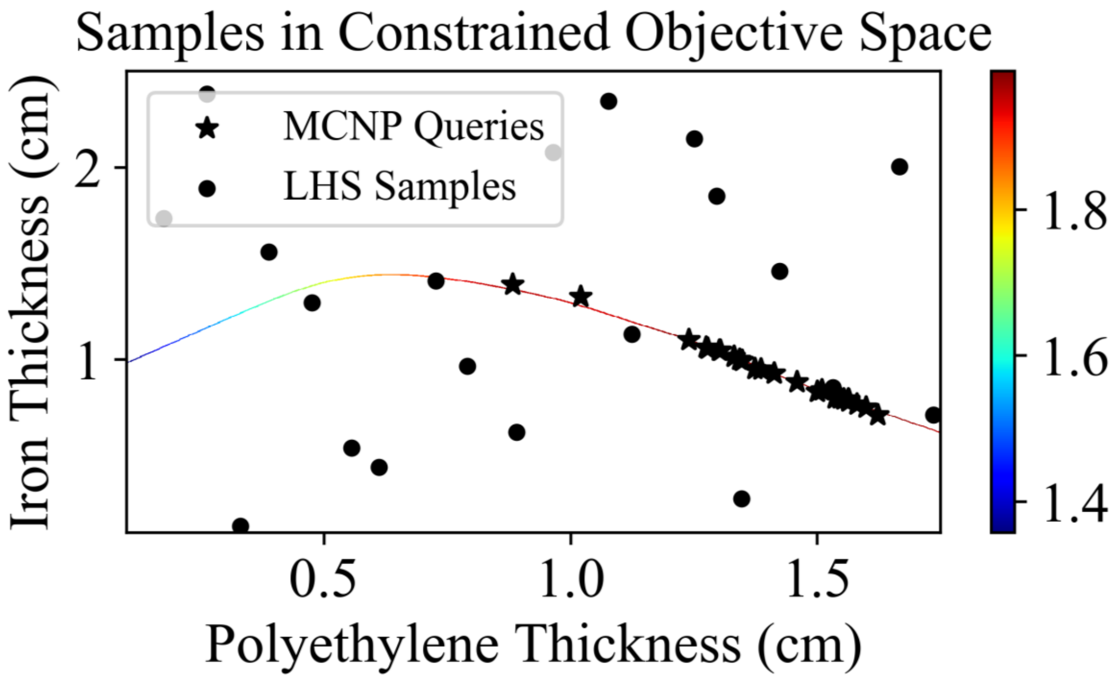




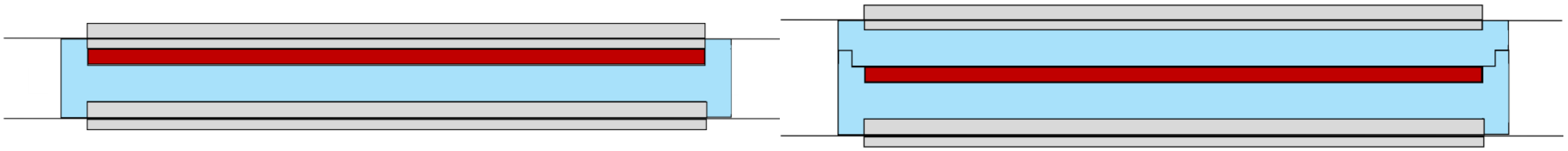
Constrained Bayesian Optimization Results

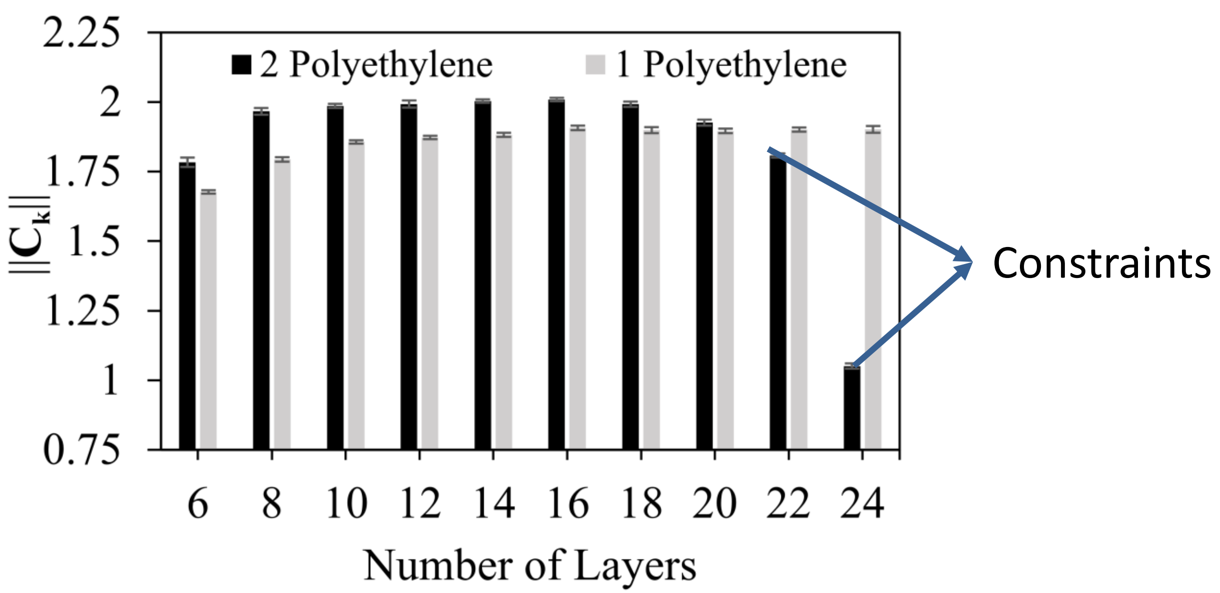


MCNP Queries in Regions of Interest

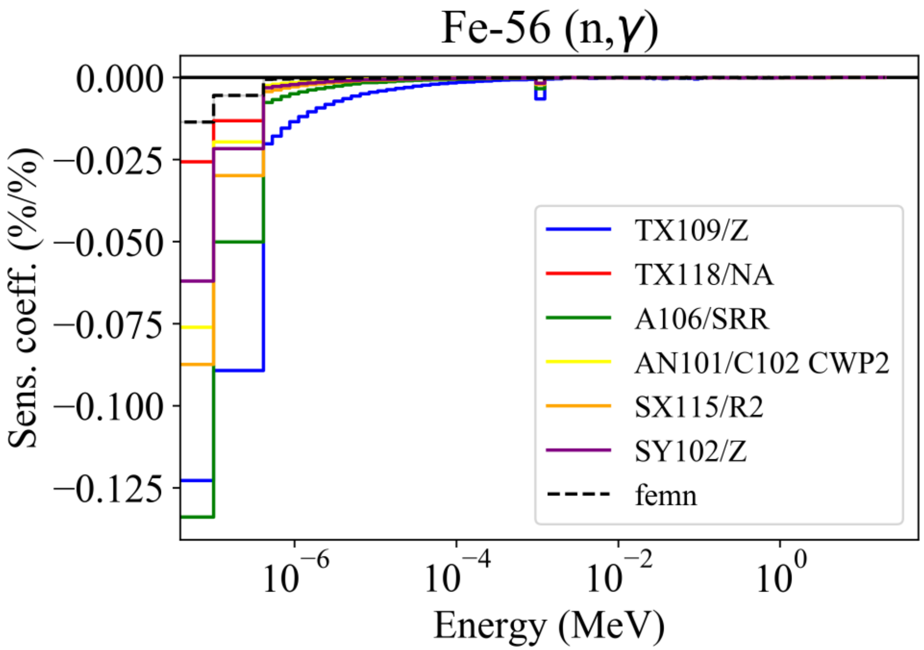


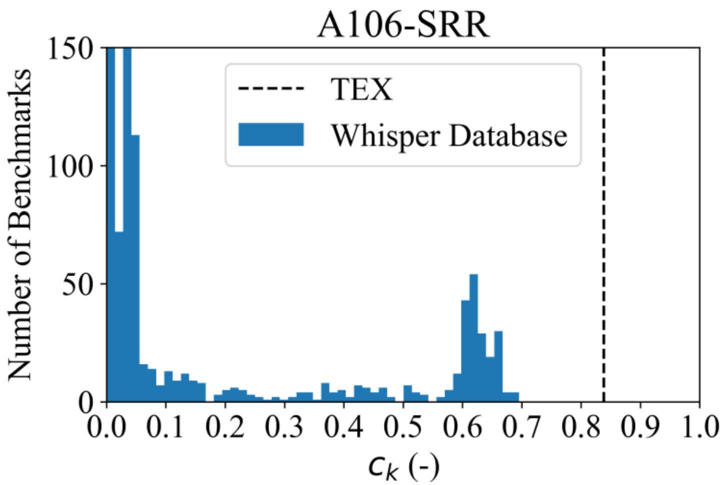
Search Through Design Space

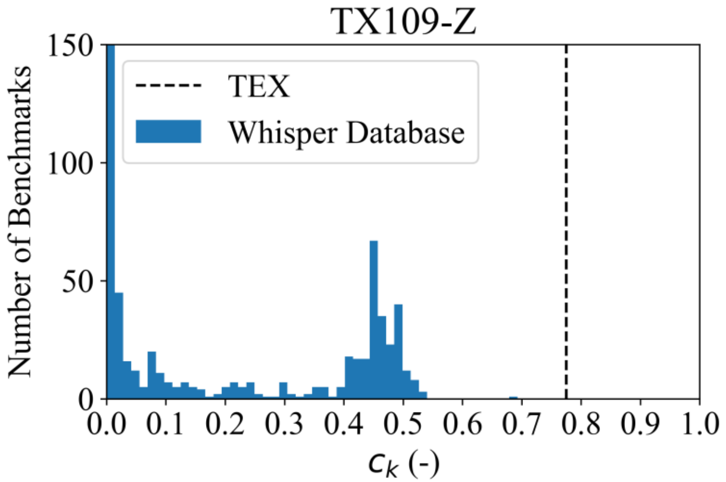




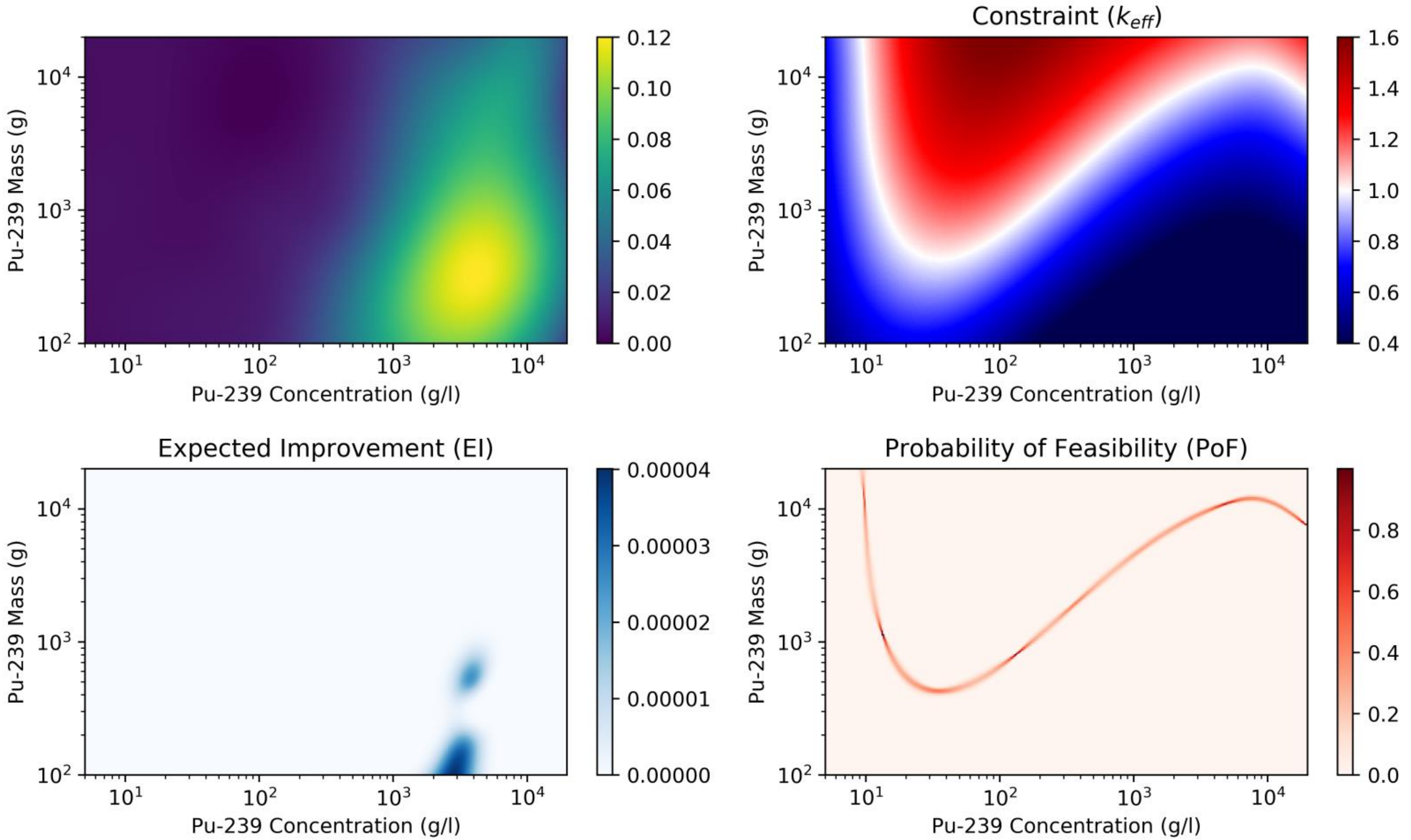
Search Through Design Space



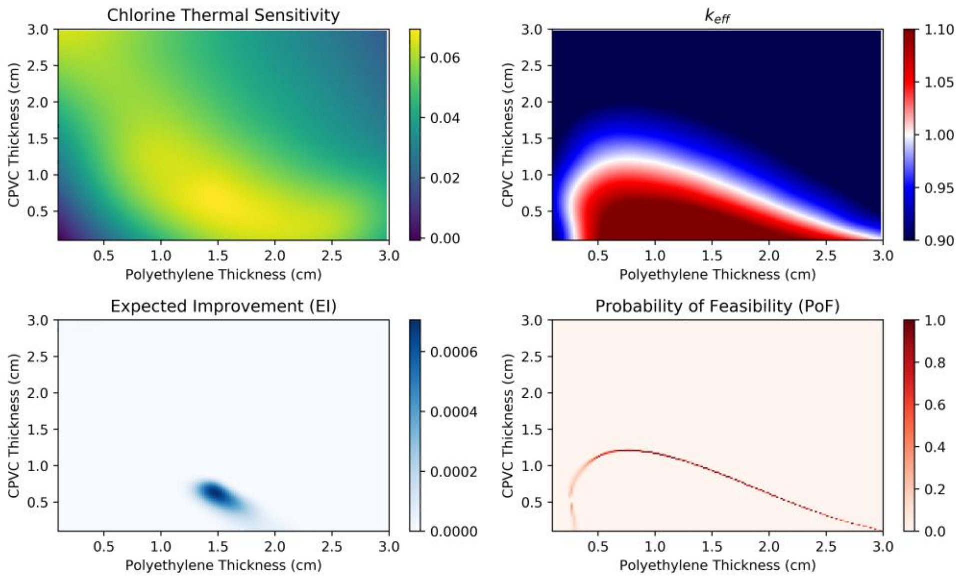


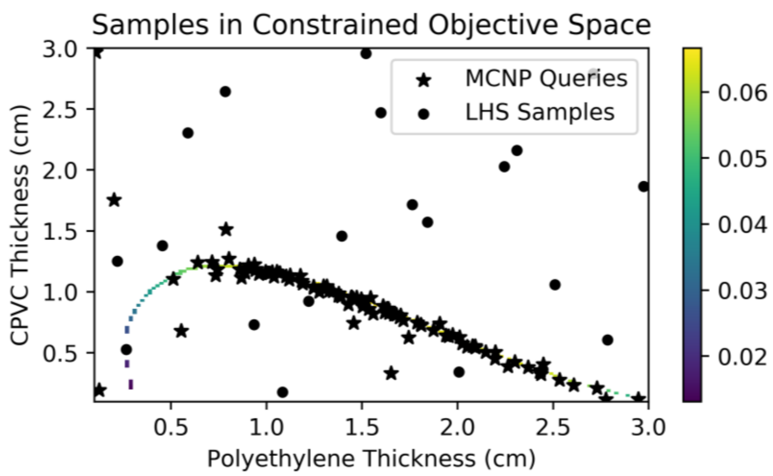


Other Studies: ^{239}Pu/polyethylene dilution



TEX-Chlorine





Questions?

Reference:

Constrained Bayesian optimization of criticality experiments
D Siefman, C Percher, J Norris, A Kersting, D Heinrichs
Annals of Nuclear Energy **151** (2021)

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