Designing Critical Experiments using Gaussian Process Optimization

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2019 ANS Winter Meeting

11/19/19

Los Alamos NATIONAL LABORATORY EST. 1943

NNSA National Nuclear Security Administration

Managed by Triad National Security, LLC for the U.S. Department of Energy's NNSA

Background

- k_{eff} is the effective neutron multiplication factor of a system
- The number of fission neutrons in one generation compared to the previous generation
  - $k < 1$ is subcritical
  - $k = 1$ is critical
  - $k > 1$ is supercritical
- MCNP6.2® predicts k_{eff}
- WHISPER-1.1 predicts upper subcritical limit (USL)
- A configuration above the USL is not guarantee to be subcritical
- 1101 benchmark experiments weighted by similarity to application

Benchmark Similarity c_k

- Nuclear data sensitivities

$$S_{k,x} = \frac{\partial k_{\text{eff}}/k_{\text{eff}}}{\partial x/x}$$

- Application - A
- Benchmark - B
- Nuclear data covariance matrix - C_{xx}

$$Cov_k(A,B) = S_A C_{xx} S_B^T$$

$$c_k(A,B) = \frac{Cov_k(A,B)}{\sqrt{Var_k(A)Var_k(B)}}$$

- Higher c_k results in higher weighting in computing USL
- If all benchmark have $c_k < 0.9$ the USL is conservatively penalized

ARCHIMEDES Goals

- Long Term Goal: perform critical experiments which result in direct nuclear data improvements for specific applications.
  - What is the "ideal critical experiment" for a given application?

- This Work: Develop/refine advanced tools and a framework that enables optimized design of new benchmark experiments for validation of predictive simulations.

Application Relevant Critical/Subcritical HEU/Pu-based Integral Measurements for Enhancing Data and Evaluating Sensitivities

ARCHIMEDES Project flow

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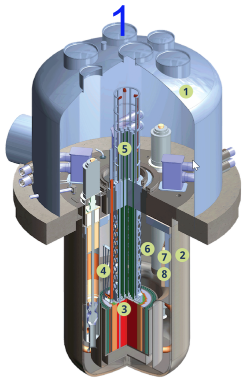

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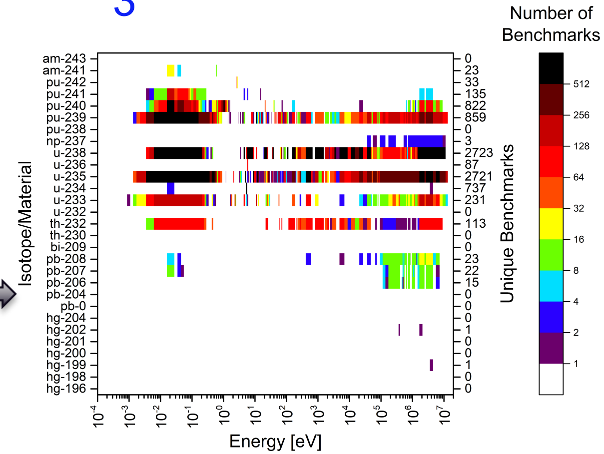
MCNP6

$$S_{k,x} = \frac{dk/k}{dx/x} = -\frac{\left\langle \psi^{\dagger}, \left(\Sigma_x - S_x - k^{-1}F_x\right)\psi \right\rangle}{\left\langle \psi^{\dagger}, k^{-1}F\psi \right\rangle}$$

3



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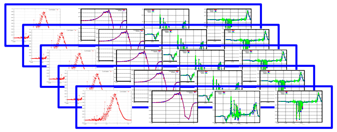
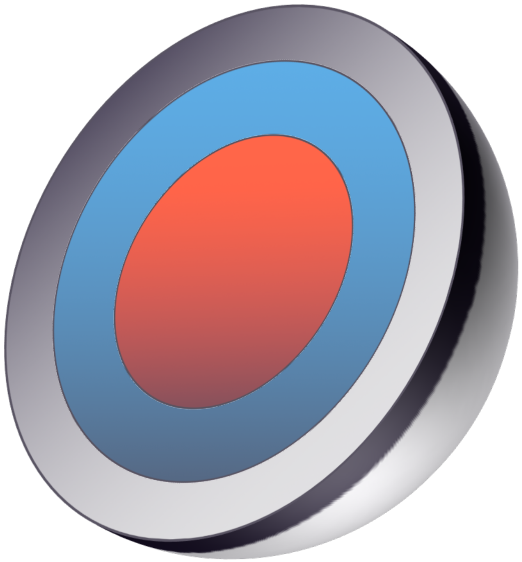
1: **Generate model** (Monte Carlo or deterministic) of application for radiation transport simulations.
2: Perform cross-section **sensitivity simulations**.
3: Perform a **gap analysis** to investigate if similar benchmarks exist.
4: Perform **optimization** to design new experiments that are more sensitive to the application than existing benchmarks.

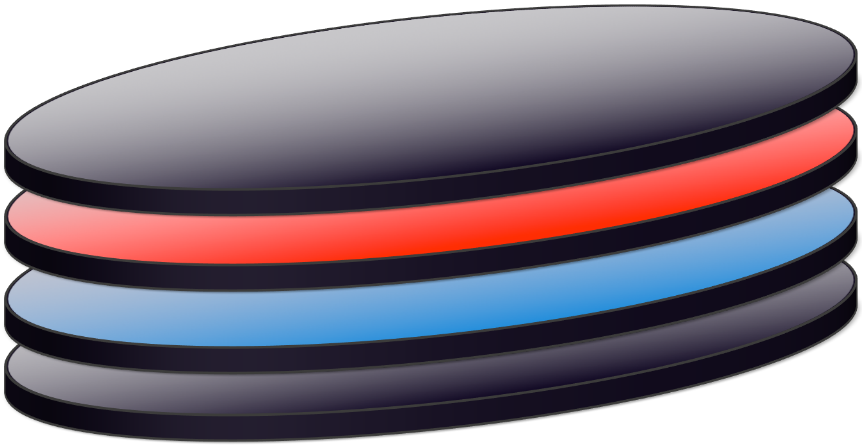


Catalog of Whisper sensitivity profiles for 1100+ experiments

Design Parameters: Geometry, Materials, and Dimensions



Spherical



Cylindrical

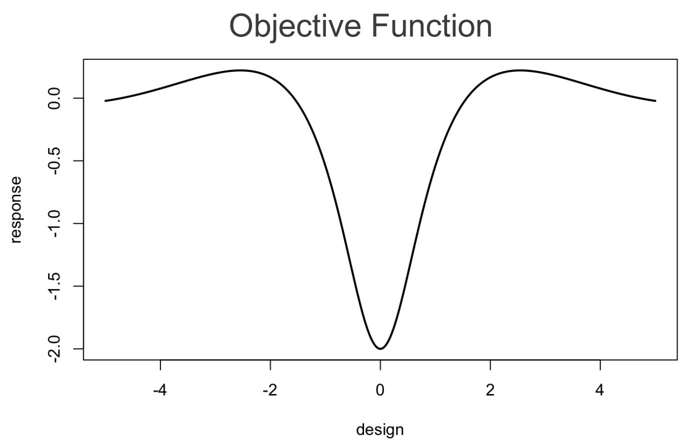
Materials: Pu, U, graphite, polycarbonate, steel, water, etc.

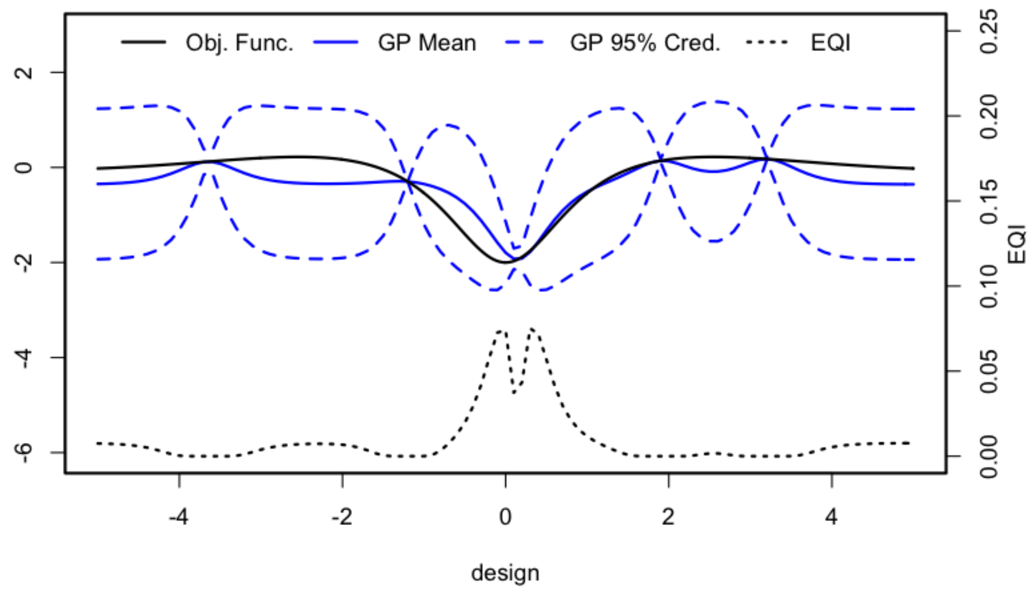
$$\eta = (g, m_1, d_1, m_2, d_2, \dots) \longrightarrow S_\eta \longrightarrow c_k$$

MCNP6 WHISPER1.1

Gaussian Process (GP) Optimization

- Optimize a surrogate function for c_k over the design space
- Use a probabilistic model to inform guesses of optimum
- Sample a Latin hypercube sample (LHS) of experiments (≈ 30 MCNP evaluations)
- Fit a GP model to observations
- For example: $f(x) = -\frac{2\cos(x)}{x^2+1}$

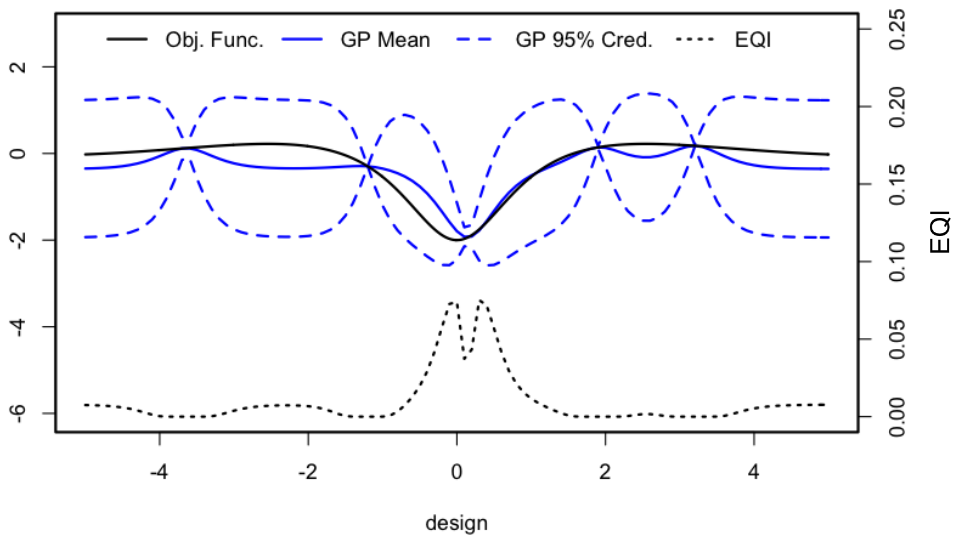


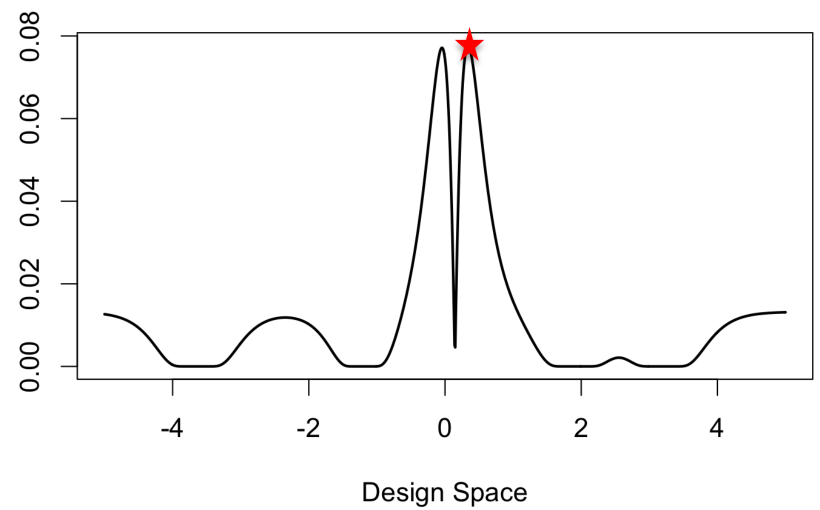


Expected Quantile Improvement (EQI)

$$EQI(\eta, \tau^2) = E\left[\max\left(0, Q_{\beta,min} - Q_\beta(\eta)\right)\right]$$

- Tuning parameters determine exploration/exploitation tradeoff
  - β quantile
  - τ^2 assumed future expected variance

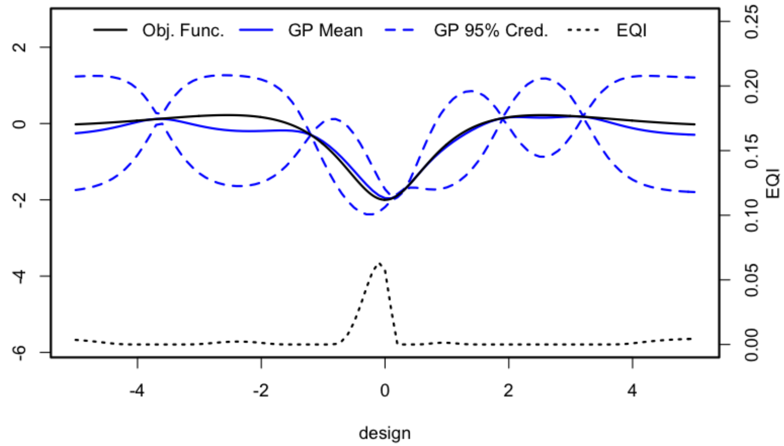




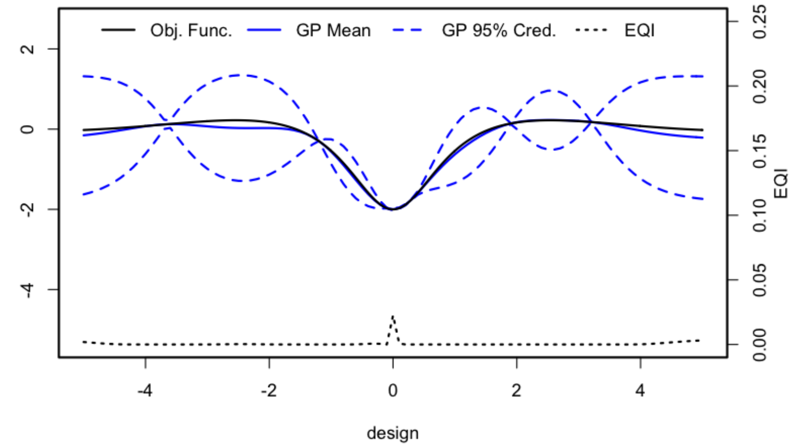
- Maximize EQI with genoud (genetic algorithm with local gradient opt.)
- Next: evaluate obj. function at $x = 0.331$

Repeated EQI Sampling

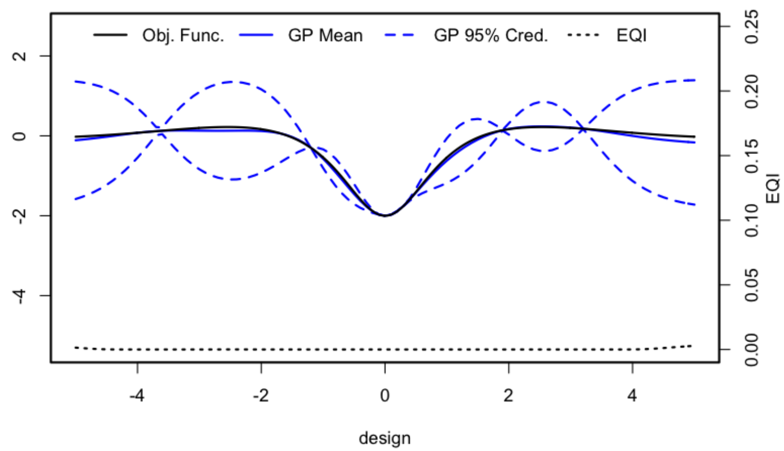
(1) $x_{\max EQI} = -0.088$



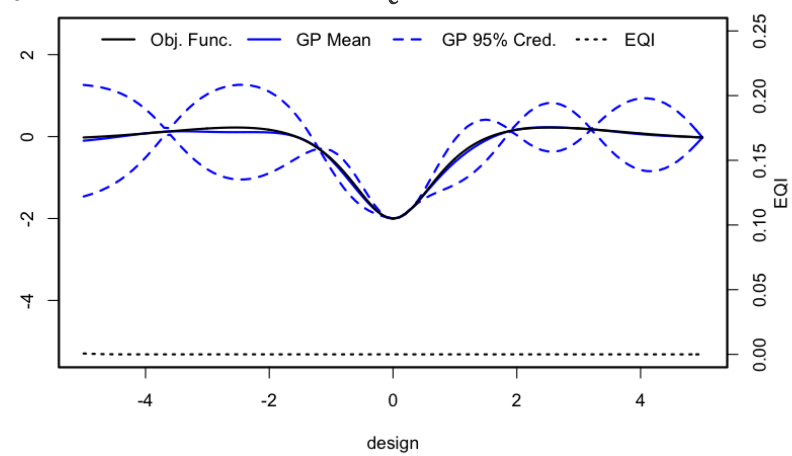
(2) $x_{\max EQI} = 0.0016$



(3) $x_{\max EQI} = 5$



(4) $x_{\max EQI} = -5$



PF-4 Application: Plutonium Casting (Tantalum)

Aliquot Casting: 2,000 g cylindrical α–phase Pu metal, 3 pieces, surrounded by 5 cm Ta on all sides, further surrounded by 1-inch water (computed k_{eff} 0.97927± 0.00008)

List of ranked reactions for Ta example (based on $|k_{eff}$ sensitivities$|$)

		Aliquot Casting		
Nuclide	Reaction	keff sensitivity		
94239.80c	nu	1.00E+00	±	7.47E-04
94239.80c	fission	7.31E-01	±	7.95E-04
94239.80c	elastic	3.68E-02	±	6.79E-04
73181.80c	inelastic	9.57E-02	±	3.52E-04
94239.80c	inelastic	2.67E-02	±	3.83E-04
73181.80c	elastic	8.96E-02	±	5.97E-04
94239.80c	n,gamma	-1.20E-02	±	2.60E-05
73181.80c	n,gamma	-2.11E-02	±	6.41E-05

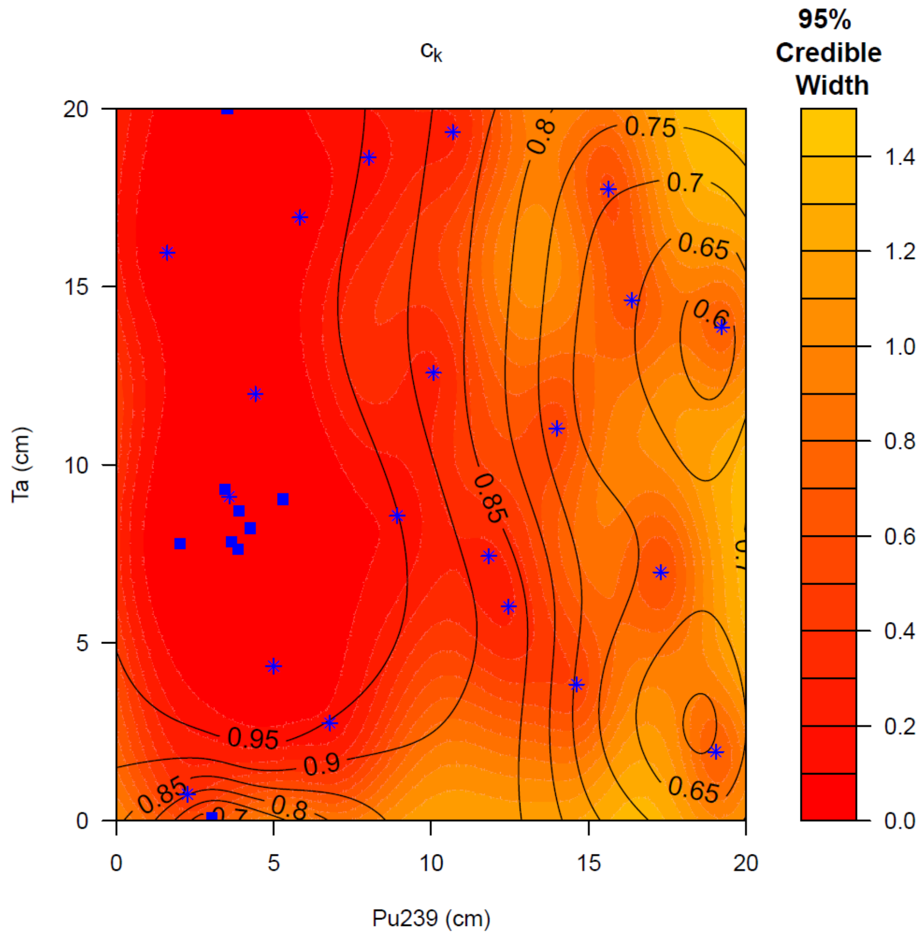
List of ICSBEP cases ranked by c_k

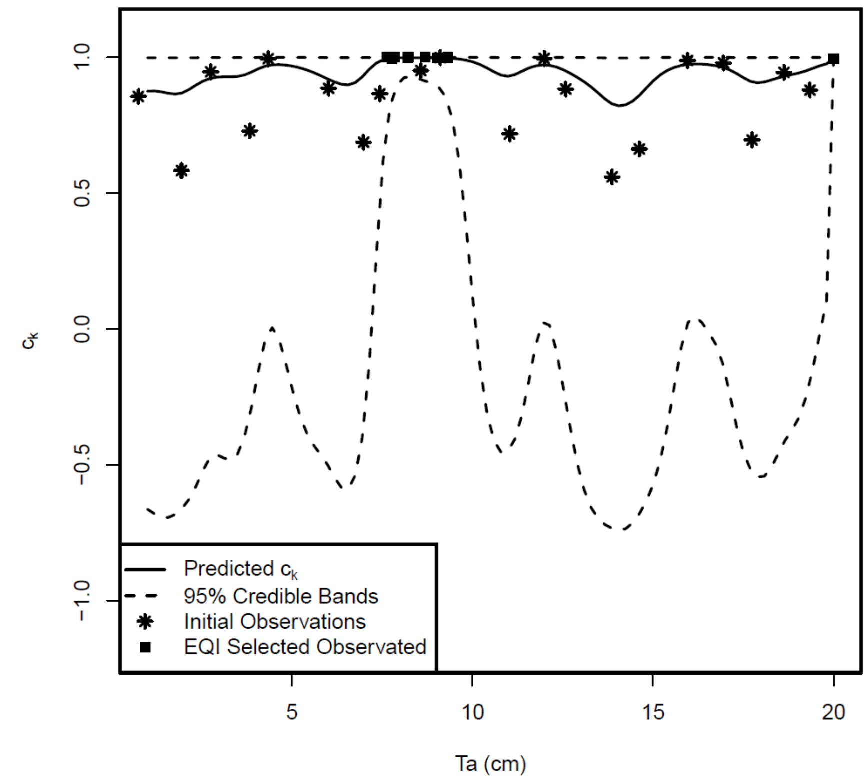
- Fairly low c_k values. Not surprising since there are few benchmarks with Ta.

*IRPhEP Benchmarks

Benchmark	c_k
	Aliquot Casting
LAMPRE-FUND-RESR-001-006*	0.6442
LAMPRE-FUND-RESR-001-004*	0.6445
PMF045-006	0.6401
PMF045-004	0.6394
LAMPRE-FUND-RESR-001-003*	0.6413

PF-4 Application: Plutonium Casting (Tantalum)





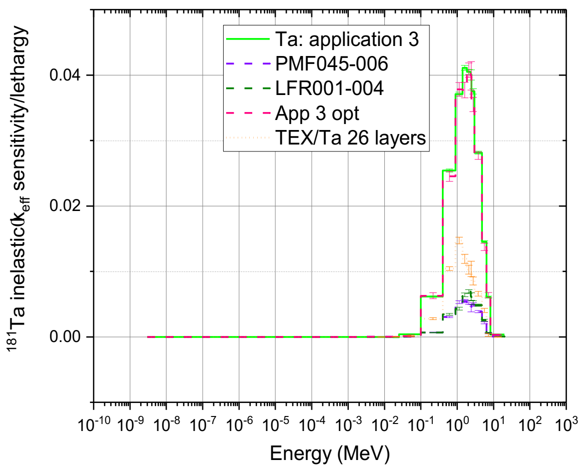
Initial LHS Points

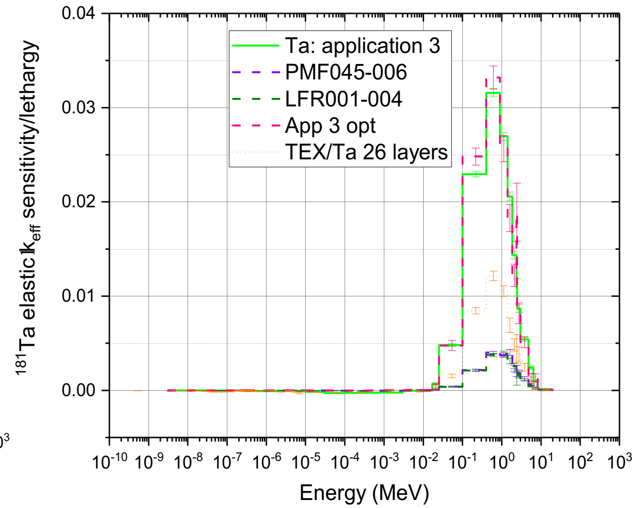
EQI Selected Points

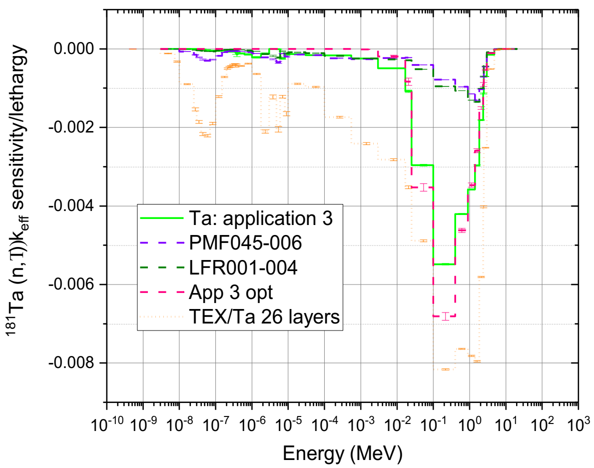
- Fisher transform $z_k = \log\left(\frac{1+c_k}{1-c_k}\right)$ is modeled instead of c_k

Optimized configuration (4.25 cm ^{239}Pu surrounded by 8.24 cm Ta) for aliquot casting yielded c_k of 0.9997.

PF-4 Application: Plutonium Casting (Tantalum)





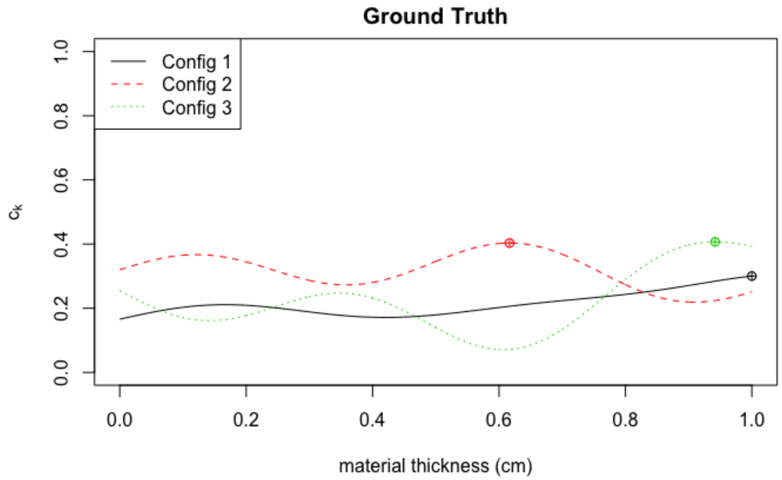


- Solid line is the aliquot casting Ta application.
- Dashed lines include the highest c_k including 1000+ ICSBEP and IRPhEP configurations.
- Dotted line is the TEX configuration with the highest c_k
- App 3 opt is the optimization result for the aliquot casting application.

Extending to Discrete Optimization

- What if we want to optimize over a discrete sets of materials?
- Option 1: Independent optimization for each configuration
- Option 2: Simultaneous optimization over all configurations
- Algorithm:
  1. Initial LHS and fit GP for each configuration
  2. Optimize EQI for each configuration
     - Let $q_{n,i}(\eta_j)$ predicted β-quantile at stage n of config i at design η_j
     - Define $Q^{\star}_{\beta,min} = \min_{i=1,\ldots,m;j=1,\ldots,n_i} \{q_{n,i}(\eta_j)\}$
     - $EQI^{\star}_i(\eta,\tau^2) = E\left[\max\left(0, Q^{\star}_{\beta,min} - Q_{\beta,i}(\eta)\right)\right]$
  3. For i=1,…,m
     1. Run MCNP for best config
     2. Update GP, optimize EQI for chosen config
     3. Recompute maximum EQI for other configs
  4. Return best configuration

Discrete Optimization Demonstration



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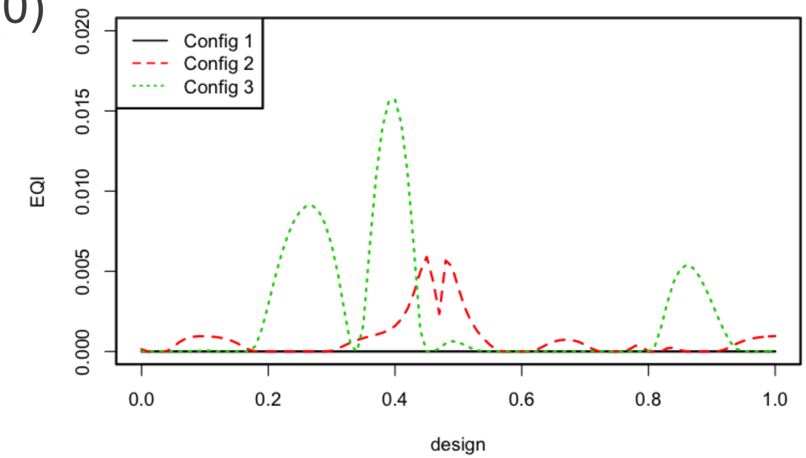
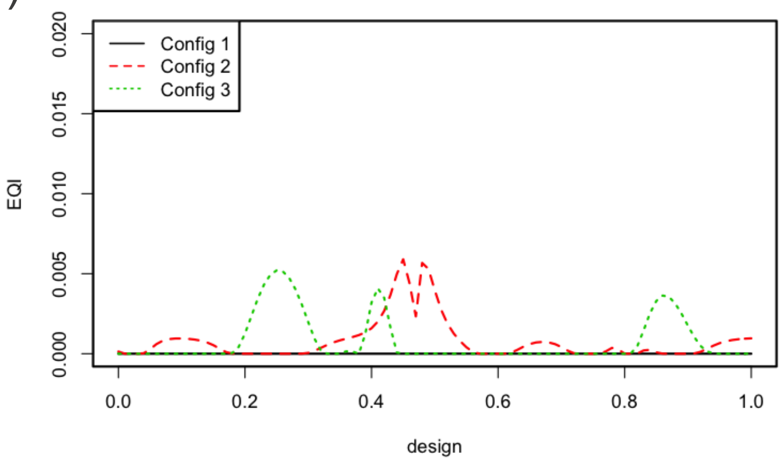


(1)



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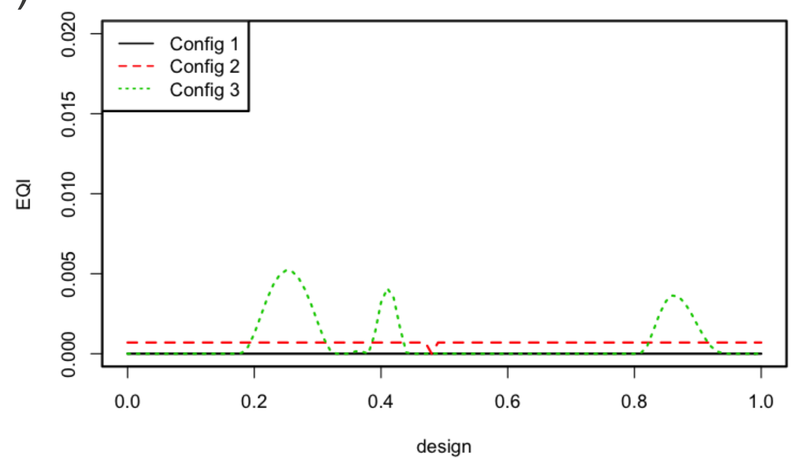


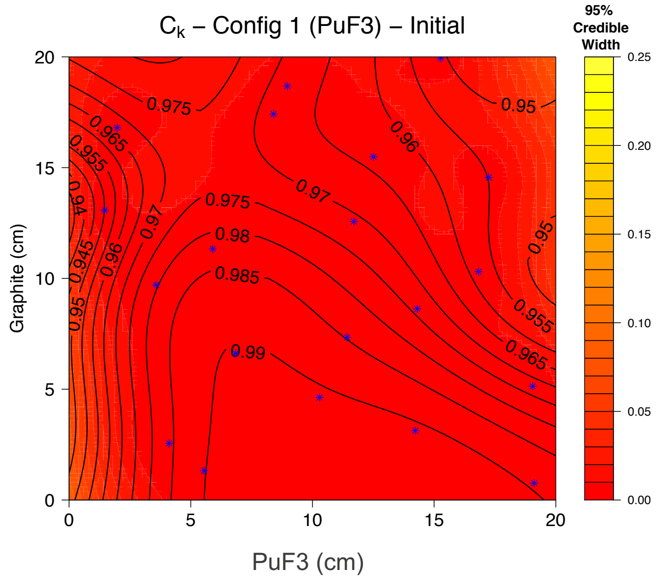
Blind Experiment Example

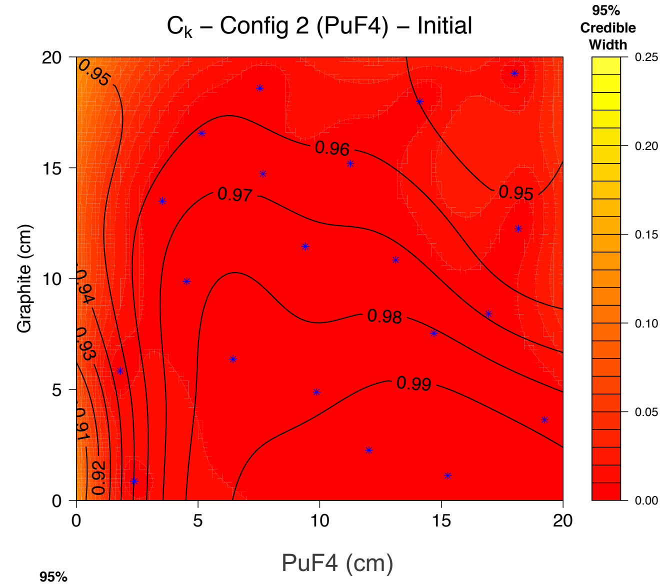
- Given MCNP sensitivity profile for unknown application
- Optimization should reproduce the sensitivities of the unknown application

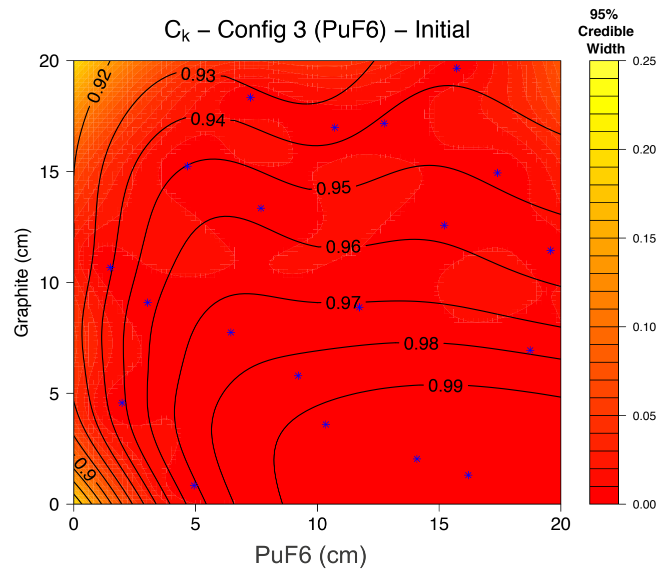
<u>Optimization Steps:</u>

- Identify nuclides: Application is sensitivity to C, F, and Pu
- Identify materials: graphite, Pu, PuF3, PuF4, PuF6, and Teflon (PTFE)
- Enumerate potential configurations:
  1. PuF3, with/without graphite reflector
  2. PuF4, with/without graphite reflector
  3. PuF6, with/without graphite reflector
  4. Pu, with/without PTFE, with/without graphite reflector
- Run initial LHS on each configuration
- Run EQI optimization across all configurations

Blind Experiment: Initial Evaluation

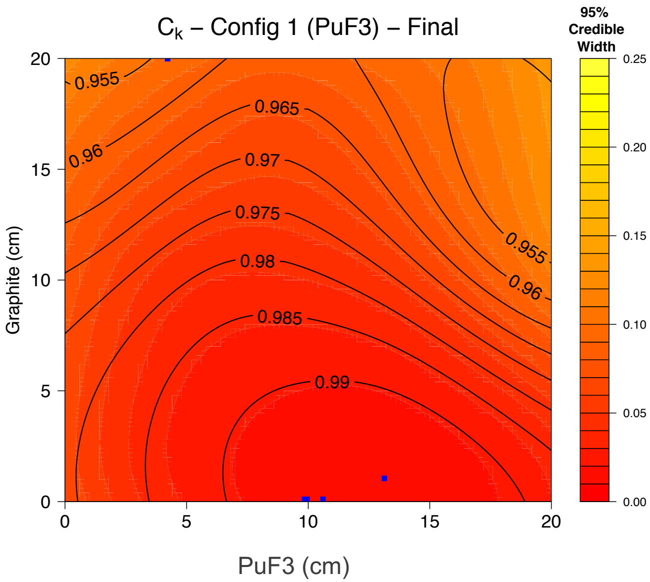


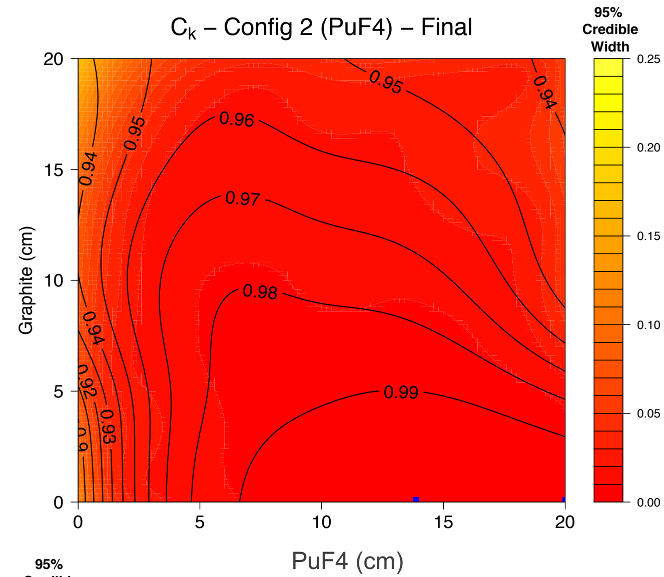


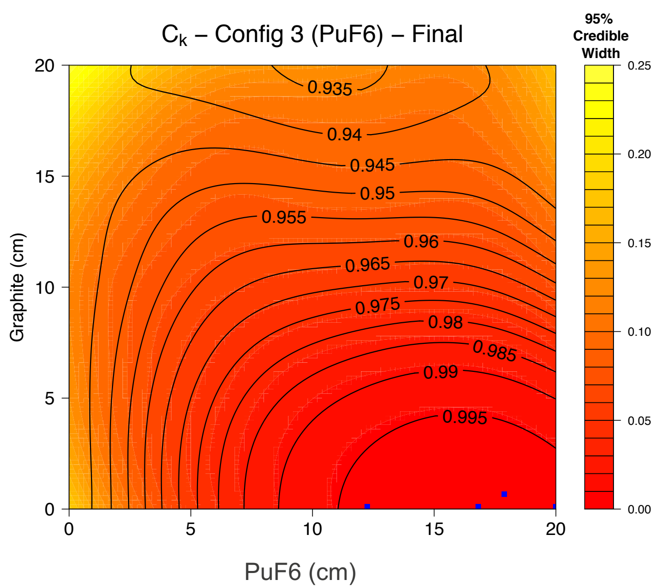


Run 20 initial MCNP runs for each of 3 SNM types

Blind Experiment: EQI Optimization







Optimal Config

PuF6 - 17.88 cm
Graphite - 0.68 cm
c_k = 0.9992

But…
pu-met-fast-023-001.i
c_k = 0.9921

True Config

Pu - 4.16 cm
PTFE - 1.00 cm
Graphite - 1.00 cm

Conclusions

- Optimization technique for mixed continuous and discrete variables
- Optimize over geometries (spherical and cylindrical) and multiple material configurations
- Black-box optimization, so objective can easily be swapped
- GP/Bayesian optimization reduces the number of MCNP evaluations

Acknowledgements

- Research reported in this publication was supported by the U.S. Department of Energy LDRD program at Los Alamos National Laboratory.

References

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