LA-UR-24-28975

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Title: Thales: Designing a New Fast Tantalum Benchmark Experiment for Criticality Safety

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Intended for: 2024 MCNP® User Symposium, 2024-08-19/2024-08-22 (Los Alamos, New Mexico, United States)

Issued: 2024-08-20 (Draft)

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Thales: Designing a New Fast Tantalum Benchmark Experiment for Criticality Safety

2024 MCNP User Symposium

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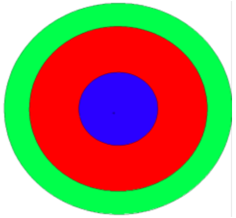
LA-UR-XX-XXXX

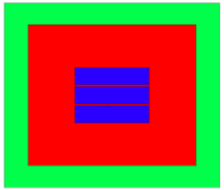
The Thales Project

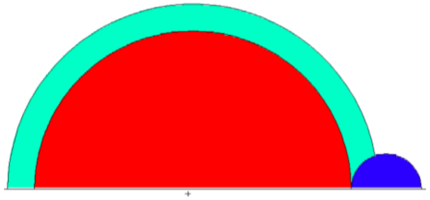
- Ta is a refractory metal with high melting point and high corrosion resistance.
  - Useful as a mold material for plutonium casting.
- There are very limited integral validation data for Ta applications
  - Until 2022, there was 1 experiment sensitive to Ta. Currently there are 6 experiments.
  - There is still a gap in coverage at fast energies
- New criticality experiments are needed to validate casting applications
- We will cover the conceptual design for these new criticality experiments
  - Down-selection of applications and materials using sensitivity correlations (c_k)
  - Iterative design process and a new design criterion for multiple target applications
- See also:
  - *"Impact of Higher Fidelity Design Iteration on Critical System Criteria"* by Peter Brain
  - "*Low-fidelity MCNP Integral Experiment Model Optimization* " by Noah Kleedtke

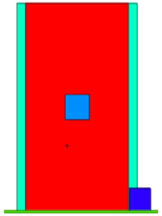
Ta Applications

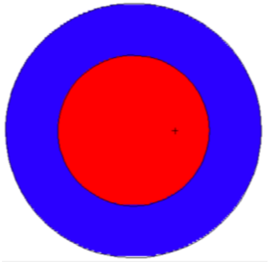
- PF-4 applications: 5 examples provided 2019-2024
- SRS applications: 34 files created given SRS input
- Fictitious sphere application (critical sphere of 100% ^{239}Pu with infinite Ta reflection)
- We will refer to these with labels A01 – A40
- All applications contain Pu and Ta
- A mixture of nominal and credible upset conditions

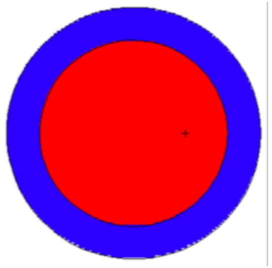












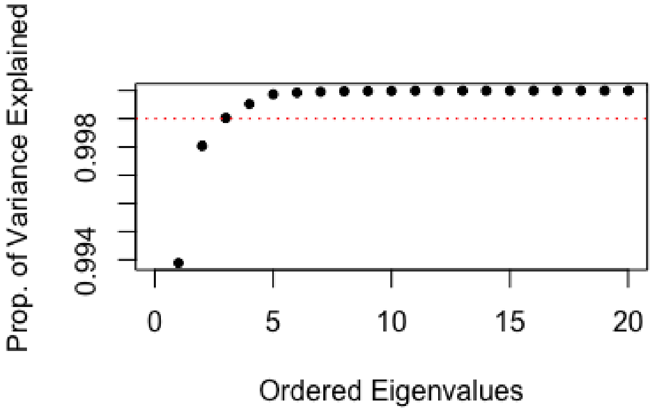
Application Down-select using c_k

- All pairwise c_k for 40 applications
- A 40x40 correlation matrix
- Diagonal elements are 1 by definition
- A01 has $c_k > 0.99$ for A04 and A05
- A02 has $c_k < 0.99$ to other applications
- A03 has $c_k > 0.99$ for A06-A40
- At most <u>three application (A01, A02, and A03)</u> are needed
- Alternatively, PCA gives:

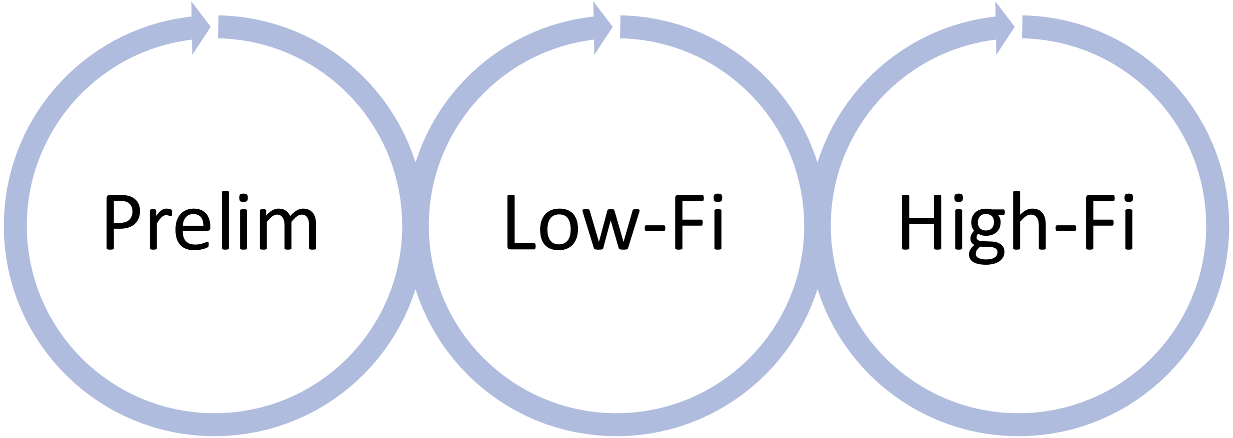
All values with $c_k > 0.99$ are shown in green

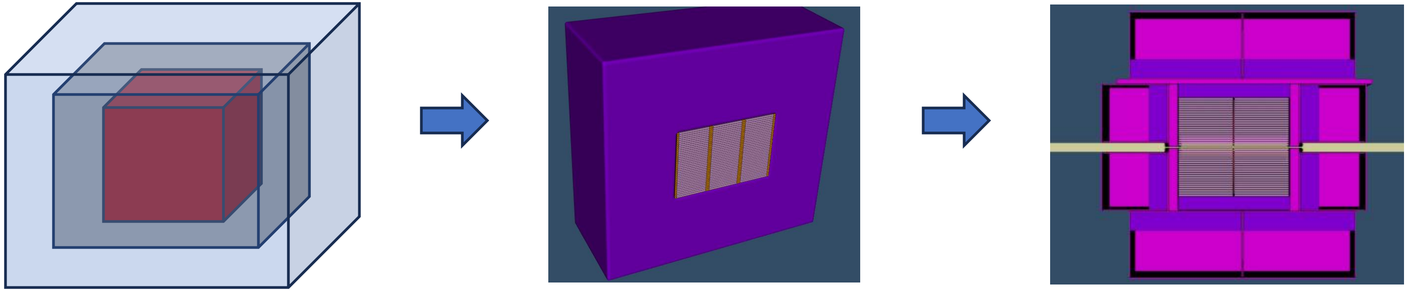
Application #	1	2	3
1	**1.000**	0.901	0.971
2	0.901	**1.000**	0.973
3	0.971	0.973	**1.000**
4	**0.995**	0.898	0.975
5	**0.997**	0.910	0.970
6	0.966	0.980	**0.998**
7	0.969	0.969	**0.998**
8	0.973	0.970	**0.998**
9	0.972	0.966	**0.999**
10	0.973	0.963	**0.996**
11	0.974	0.965	**0.999**
12	0.977	0.965	**0.998**
13	0.974	0.965	**0.999**
14	0.980	0.958	**0.996**
15	0.975	0.964	**0.999**
16	0.978	0.964	**0.998**
17	0.976	0.964	**0.999**
18	0.980	0.961	**0.998**
19	0.976	0.964	**0.999**
20	0.981	0.961	**0.998**
21	0.976	0.964	**0.999**
22	0.980	0.957	**0.997**
23	0.977	0.962	**0.999**
24	0.980	0.960	**0.997**
25	0.977	0.964	**0.999**
26	0.980	0.960	**0.997**
27	0.977	0.963	**0.999**
28	0.979	0.965	**0.998**
29	0.977	0.963	**0.999**
30	0.980	0.962	**0.998**
31	0.977	0.964	**0.999**
32	0.975	0.965	**0.997**
33	0.977	0.964	**0.999**
34	0.979	0.960	**0.997**
35	0.977	0.964	**0.999**
36	0.979	0.964	**0.998**
37	0.976	0.965	**0.999**
38	0.981	0.959	**0.998**
39	0.976	0.965	**1.000**
40	0.979	0.963	**0.998**

Three applications cover 99.9% of the variance among applications



Progressive Design Process



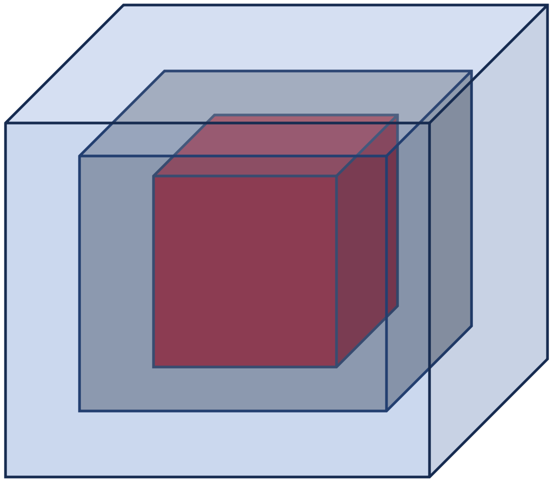


Conceptual Design

Engineering Design

Simple Rectangular Parallelepiped (RPP) Geometry

- Early calculations showed that ZPPR plates offer the greatest flexibility in achieving criticality with multiple reflector thicknesses
- Nested RPP shells
- Pu fuel
  - ℓ, w, h between 0 to 20 cm
  - ZPPR alloy (10% Al)
  - Stainless steel cladding
- Inner Ta reflector (mold material)
  - 0 to 20 cm thick
- Outer $H_2 0$ reflector (upset condition)
  - 0 to 20 cm thick



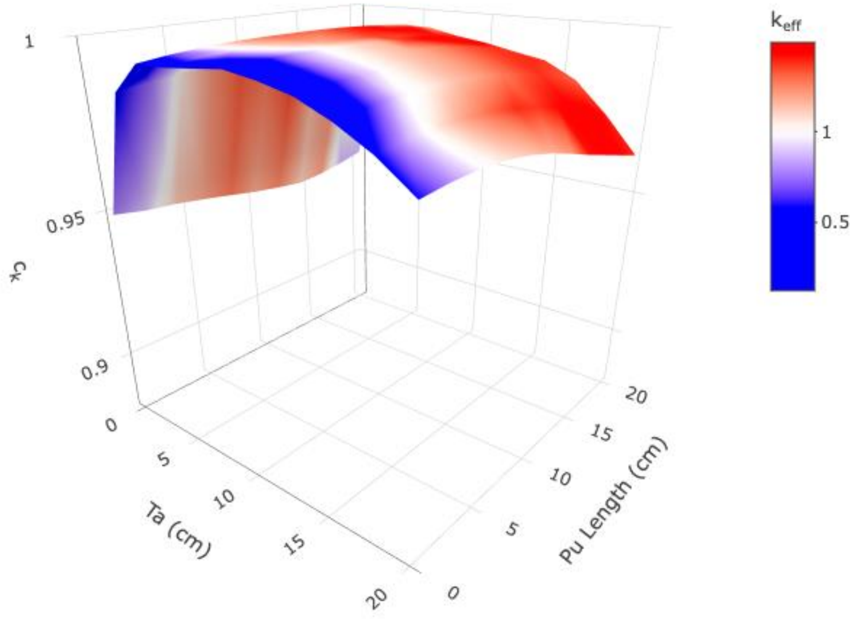
Exploratory c_k Analysis

- **Profiling:** Select two variables, maximize c_k with respect to all the others, and plot the resulting function.

$$f(\theta;\lambda), \text{where } \theta = (x,y) \text{ and } \lambda = (z,w)$$
$$\hat{\lambda}_\theta = argmax\, f(\theta;\lambda)$$
$$\hat{f}(\theta) = f\left(\theta;\hat{\lambda}_\theta\right)$$

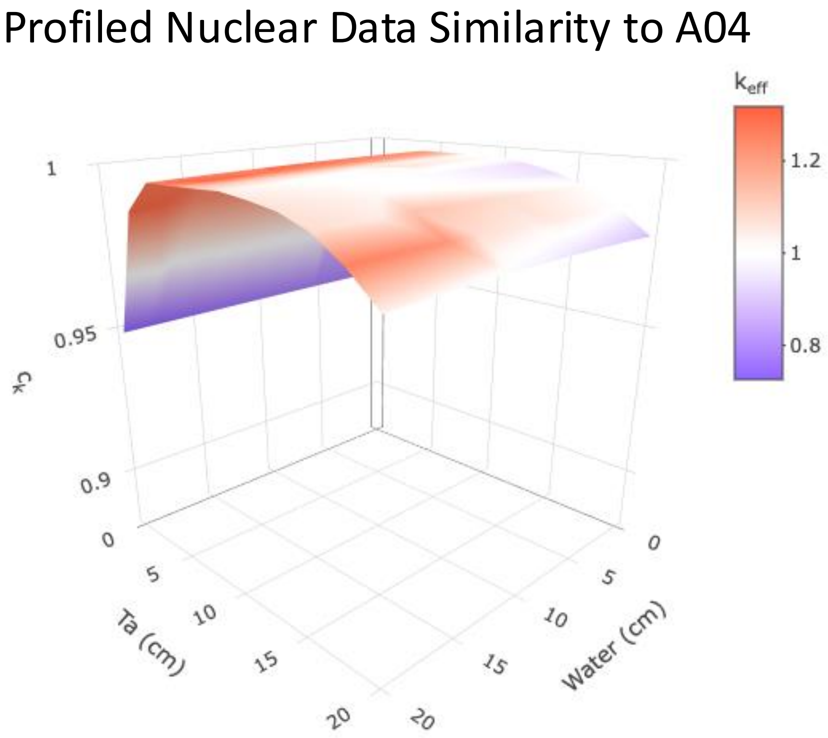
- Application A04 is an upset condition
- Relatively large region where $c_k > 0.99$
- Two ridges for high (15 cm) and lower (5 cm) Ta thicknesses

Profiled Nuclear Data Similarity to A04



Exploratory c_k Analysis

- c_k is insensitive to water
- Corroborates the down-select throwing out all applications with water
- We do not need a water surrogate material in the design
- We will probably get more benefit from having multiple Ta reflector configurations



Posterior Uncertainty Reduction Metric

- **Problem:** c_k only allows pairwise comparisons between sensitivity vectors
- We need a metric that will optimize multiple experiments for three applications
- The posterior application covariance matrix is

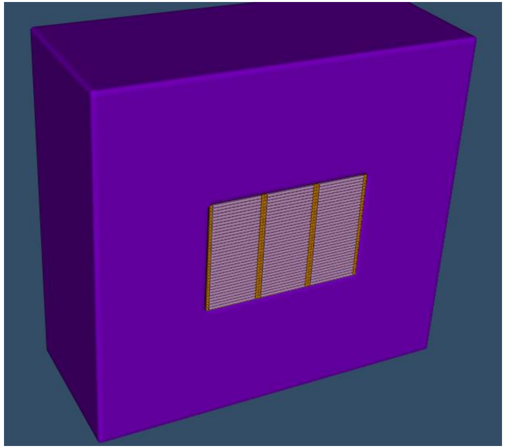
$$\Sigma'_A = S_A \Sigma' S_A^T = S_A \left(\Sigma - (\Sigma S_B)(S_B^T \Sigma S_B + \Sigma_e)^{-1} (\Sigma S_B)^T\right) S_A^T,$$

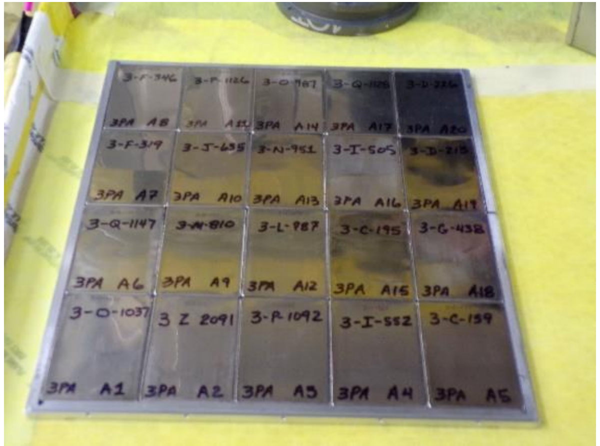
for sensitivity matrix S_B of proposed experiments and nuclear data covariance Σ

- We can then compute $\phi(S_B) = \log\det\Sigma_A - \log\det\Sigma'_A$
- Related to D-optimality criterion used in the EUCLID experiment
- The criterion $\phi(S_B)$ is the mutual information between the proposed experiment and the target applications

Low-Fi ZPPR Simulations

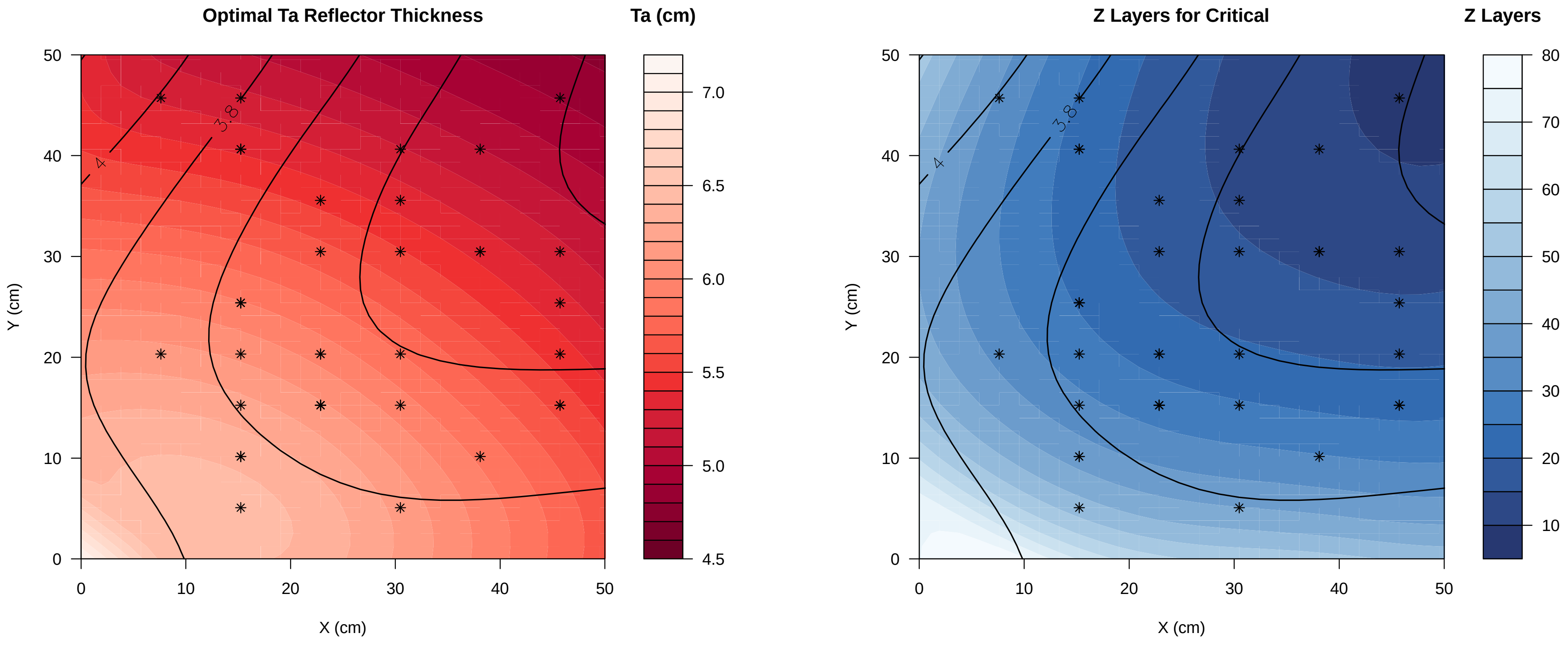
- Pu fuel
  - Discrete ZPPR plates (3” x 2”)
  - (X,Y) cross-section
  - X and Y (1 to 9 plates)
  - Z (10 to 100 layers)
- Ta reflector
  - 0 to 20 cm thick
  - Solid, no gaps





Ex: 4 x 5 Cross-sectional layer

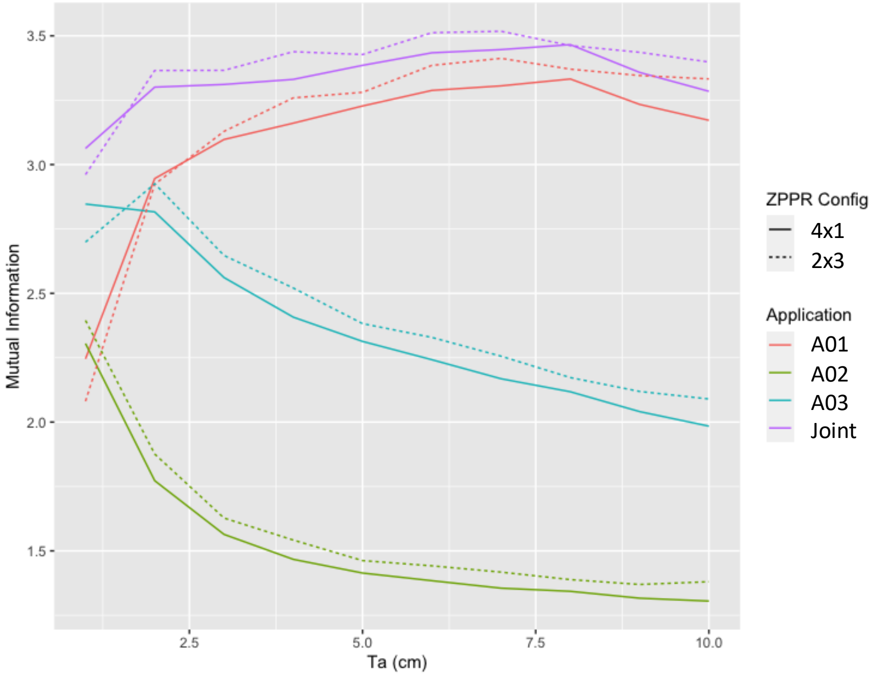
Profiled Gaussian Process Response Surfaces



Mutual information ranges from 3.2 to 4 (higher is better)

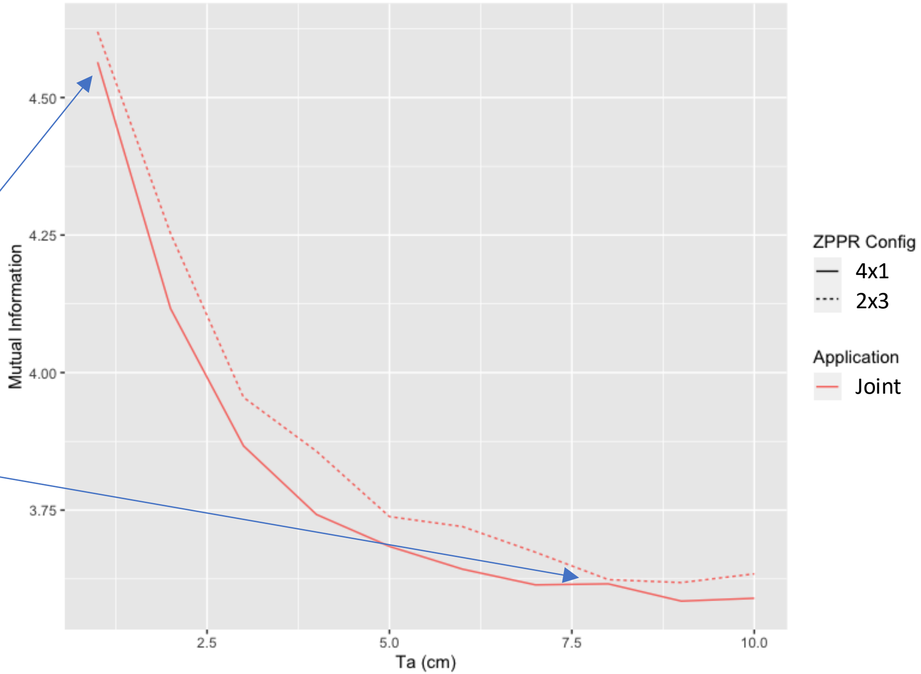
Joint Criterion is Dominated by Application A01

- Joint criterion is driven by A01
- Mutual information is not additive because the applications are correlated
- Best experiment does not necessarily match Ta dimensions exactly
- A01 has 20 cm Ta reflector whereas the best experiment is only about 8 cm
- Great news because <u>we can minimize weight</u>!
- Symmetric cross-section slightly better than Asymmetric, but noisy



Added 3x2 + 8 cm Ta Experiment

- Include the optimal experiment
- Next best experiment minimizes the Ta reflector
- Mutual information is cumulative (previously ≈ 3.5)
- Diminishing returns for future experiments
- Getting +1 for 1 cm reflector
- Getting +0.125 for 8 cm reflector



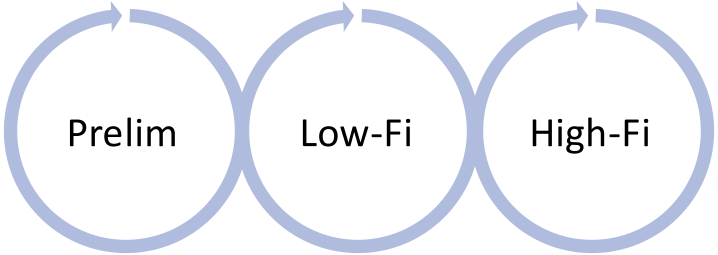
Final Low-Fi Design

- We performed a handful of long simulations to differentiate the best configurations
- 2x2 design is the best (barely)
- We need a series of (Z,R) which are critical with R approximately at 1, 2, 4, 8, and maybe 10 cm
- 2x2 requires 40 layers with max reflection, which will increase with minimum reflection
- 2x3 achieves criticality with less reflection without a large increase in the number of layers
- More margin for error in the experiment

X	Y	Z	R	dc	k
2	2	40	8.89	3.64930917	1.005789
1	3	56	8.14	3.63187	0.988315
2	3	29	8.89	3.61453052	1.01363
2	2	39	10.1	3.60070011	1.003354
1	3	67	5.91	3.55154367	1.003176
1	9	34	7.94	3.53964421	1.009402
2	2	45	5.08	3.53946299	0.999924
1	3	56	10.7	3.52597797	1.000761
2	3	27	11.4	3.49110467	0.99614
1	9	33	8.89	3.48368657	1.006412
2	2	60	2.54	3.45312203	1.001345
2	3	42	1.9	3.41683885	1.001082
1	9	47	3.18	3.39373162	1.013732

Conclusions

- Thales is building validation data for fast Pu systems with tantalum reflection
- We have shown our preliminary and Lo-Fi design stages that rely on MCNP simulations
  - Application down-selection (40 → 3)
  - Exploration of materials (eliminated water)
  - Identification of cross-section configuration (2 x 3 ZPPR plates)
  - A series Ta reflectors that should maximize the information from the experiments



Acknowledgments

- NCERC is supported by the DOE Nuclear Criticality Safety Program, funded and managed by the National Nuclear Security Administration for the Department of Energy.
- Los Alamos National Laboratory is operated by Triad National Security, LLC, for the National Nuclear Security Administration of the US Department of Energy under Contract No. 89233218CNA000001.