The Los Alamos ARCHIMEDES Project: Application-specific experiments for nuclear data and analytical methods validation

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Abstract

- ARCHIMEDES is a LANL LDRD reserve project with the goal of designing new integral experiments that match nuclear data sensitivities to specific applications. The process has four main steps: first, computational models are generated, next cross-section sensitivities are investigated, then a gap analysis is performed, and finally experiment optimization takes place. In addition to suggesting new integral experiments that can help address nuclear data needs, this project will also result in better understanding of cross-section sensitivities for specific applications as well as help determine which existing criticality benchmarks are most applicable for specific applications.

ARCHIMEDES Goals

- **Long Term Goal:** perform critical experiments that result in nuclear data improvements that are of high importance for specific applications.
    - What is the “ideal critical experiment” to support a given application?
- **This Project:** Develop and refine advanced tools and a framework that enables optimized design of new benchmark experiments for validation of predictive simulations.
    - Note that this project was an 8-month LDRD reserve funded project (February – September, 2019).

ARCHIMEDES

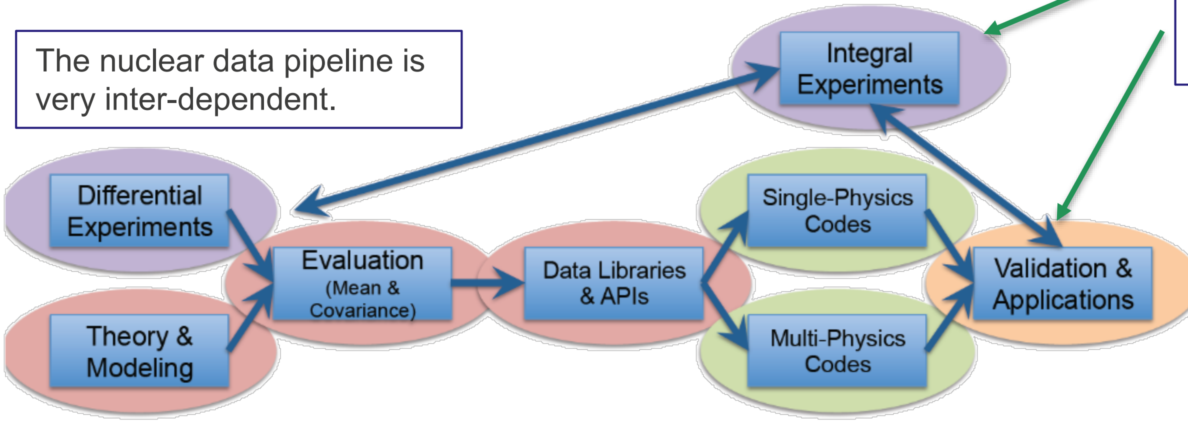
Application Relevant Critical/Subcritical HEU/Pu-based Integral Measurements for Enhancing Data and Evaluating Sensitivities

Outline

- Project background – scope and methods
- Results for one specific application
- Summary and future work

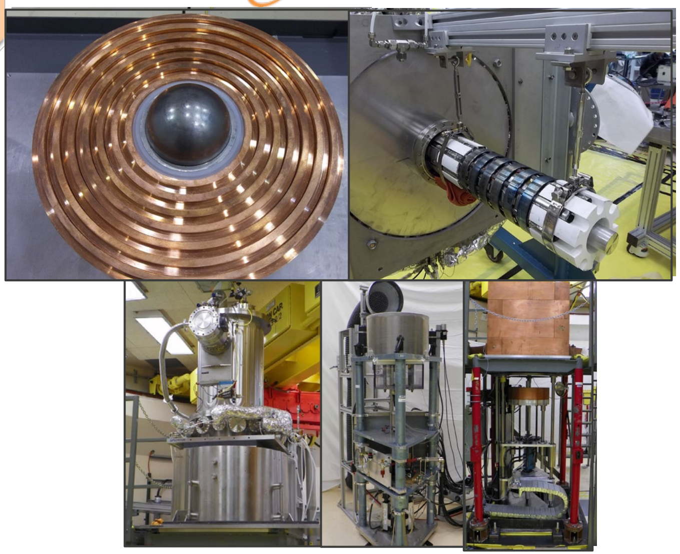
Background

The nuclear data pipeline is very inter-dependent.



The ARCHIMEDES project focuses on activities on the RHS of the pipeline, with an objective of influencing activities further upstream.

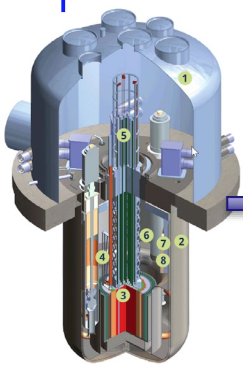
The nuclear data pipeline is also not new!



- Differential and integral experiments to support nuclear data began in the 1940s.
- The first Evaluated Nuclear Data File (ENDF) library was released in 1968.
- The first Monte Carlo and deterministic codes were developed in the 1940s and 1950s respectively.

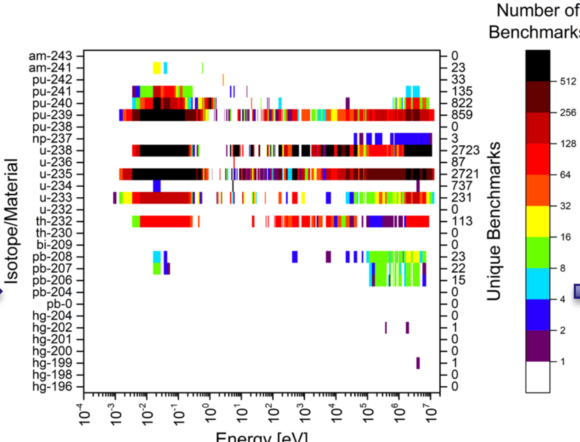
Project flow

1



2

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



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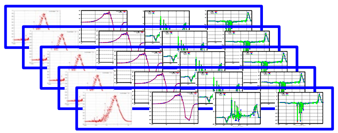

Catalog of Whisper sensitivity profiles for 1100+ experiments

4

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.

Step 2 – Determine Sensitivity

- k_{eff} sensitivity capabilities are present in modern Monte Carlo codes including MCNP®.
- SENSMG (an analysis code that uses results from PARTISN) allows for sensitivities of k_{eff} and α.

ANS
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DOI: http://dx.doi.org/10.1080/00295639.2017.1283153

Review of Early 21st-Century Monte Carlo Perturbation and Sensitivity Techniques for *k*-Eigenvalue Radiation Transport Calculations

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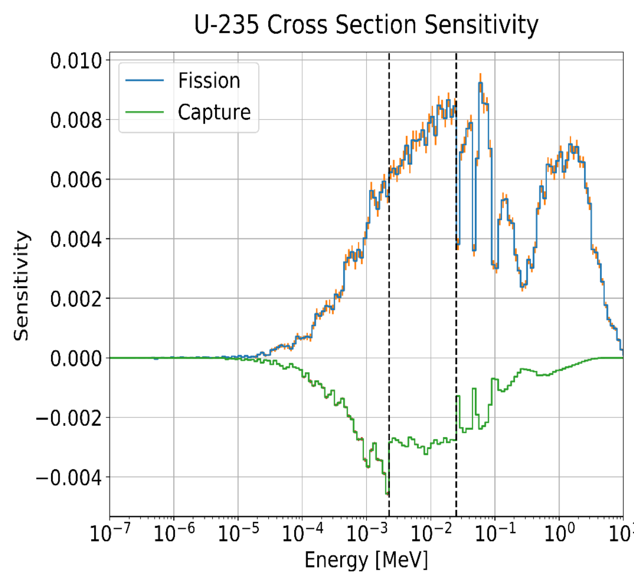
$$S_{k,x} = \frac{dk/k}{dx/x} = -\frac{\left\langle \psi^{\dagger}, \left(\Sigma_x - S_x - k^{-1}F_x\right)\psi \right\rangle}{\left\langle \psi^{\dagger}, k^{-1}F\psi \right\rangle}$$

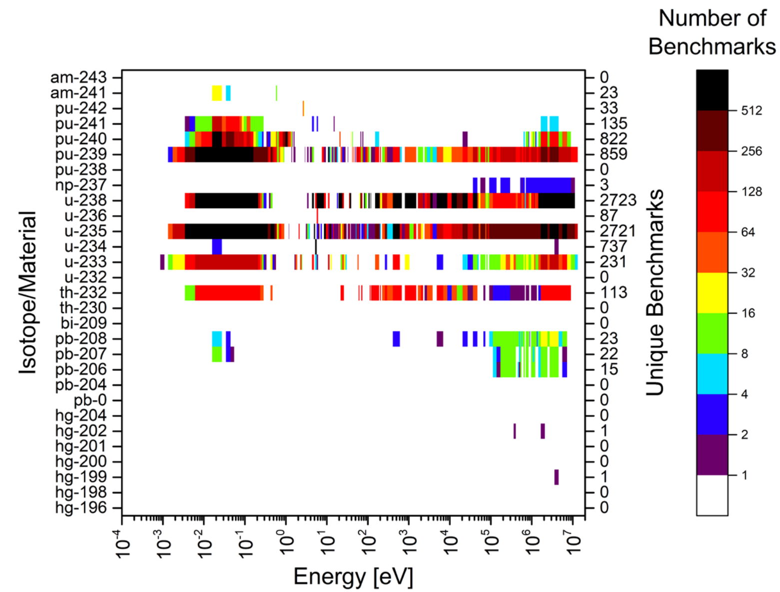
$S_{k,x}$, the sensitivity coefficient, is the ratio of relative change in k-effective to relative change in a system parameter x.



MCNP® and Monte Carlo N-Particle® are registered trademarks owned by Triad National Security, LLC, manager and operator of Los Alamos National Laboratory. Any third party use of such registered marks should be properly attributed to Triad National Security, LLC, including the use of the designation as appropriate. For the purposes of visual clarity, the registered trademark symbol is assumed for all references to MCNP within the remainder of this paper.

Step 3 - Gap Analysis – Method 1 – Heatmaps

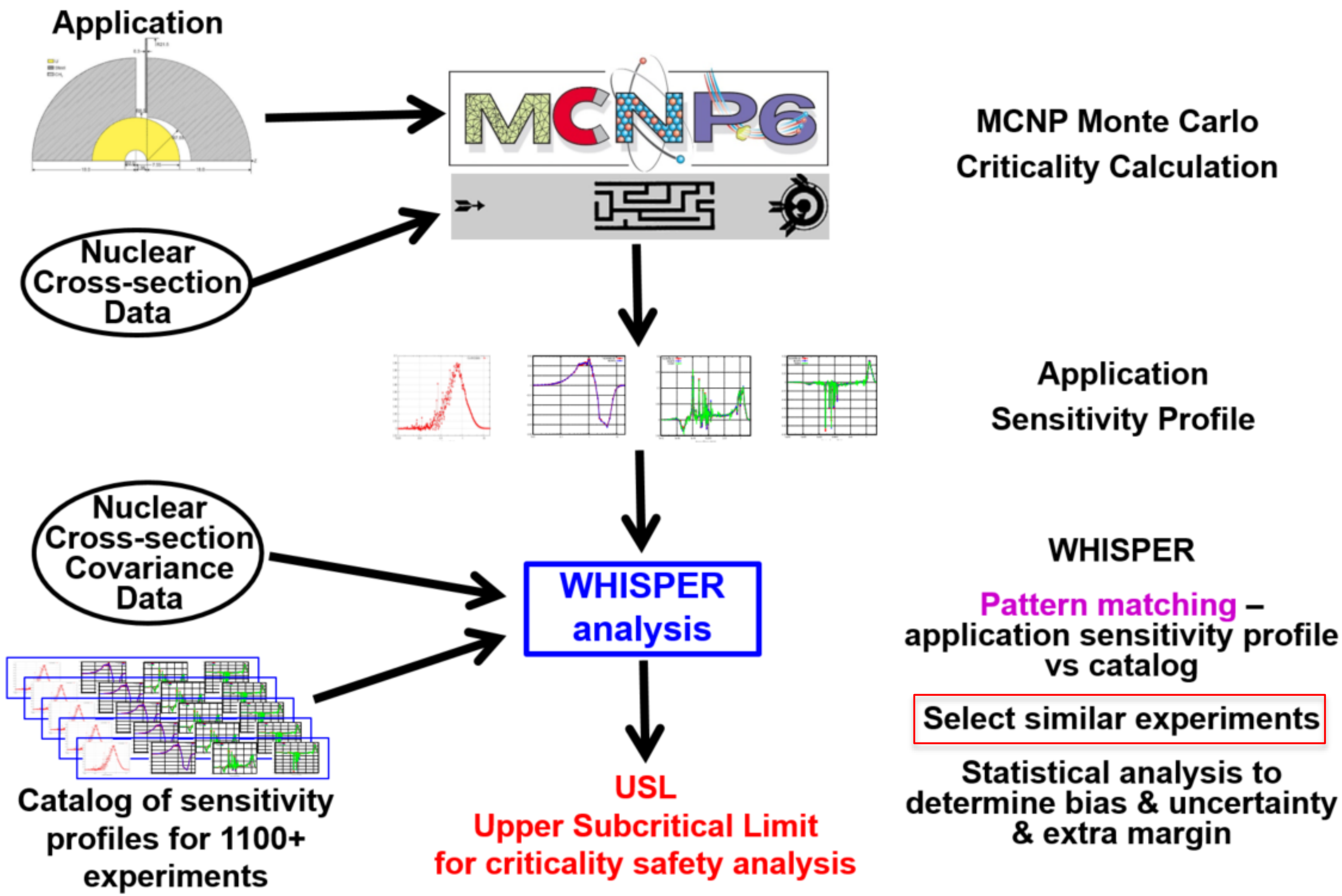
- Look at all existing benchmarks, all isotopes, all reactions, all energies
- Use these existing sensitivity files to determine where gaps exist for application sensitivities
- Distill data down to a readable form (Heatmaps)
- Generic heatmap of the number of benchmarks that have a sensitivity > 10^{-3} for each energy (238 groups), for each isotope (this example is for total cross section).



- Each line is an energy bin
- Each color is how many benchmarks are sensitive to the total cross section of that energy bin of that isotope
- Can do the same for any reaction (scattering, capture, fission, nubar, etc.)

N. Thompson, et. al., “Identifying gaps in critical benchmarks,” Transactions of the American Nuclear Society, 119, 829-832 (2018).

Step 3 - Gap Analysis – Method 2 – Whisper



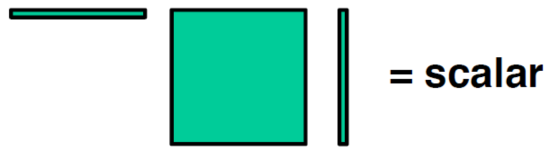
Step 3 - Gap Analysis – Method 2 – Whisper

- **Given:** **Problem A,** **Sensitivity S_A computed by MCNP**
  Problem B, **Sensitivity S_B computed by MCNP**

- **Variance in Keff due to nuclear data uncertainties:**

$$Var_k(A) = \vec{S}_A \bar{C}_{xx} \vec{S}_A^T$$

$$Var_k(B) = \vec{S}_B \bar{C}_{xx} \vec{S}_B^T$$



- **Covariance between A & B due to nuclear data uncertainties:**

$$Cov_k(A,B) = \vec{S}_A \bar{C}_{xx} \vec{S}_B^T$$

- **Correlation between Problems A & B due to nuclear data:**

$$c_k(A,B) = \frac{Cov_k(A,B)}{\sqrt{Var_k(A)} \cdot \sqrt{Var_k(B)}} = \frac{\vec{S}_A \bar{C}_{xx} \vec{S}_B^T}{\sqrt{\vec{S}_A \bar{C}_{xx} \vec{S}_A^T} \cdot \sqrt{\vec{S}_B \bar{C}_{xx} \vec{S}_B^T}}$$

For ARCHIMEDES:
- Problem A is the Application
- Problem B is one of the 1100+ benchmarks in the Whisper catalog

The S's are vectors of sensitivity coefficients calculated per slide 9

The C's are nuclear data covariances from ENDF/B evaluations

$Cov_k(A,B)$ and $c_k(A,B)$ are computed for each of the 1100+ benchmarks

We are not as focused on Whisper's USL as criticality safety analysts are, but:
- We can use the maximum value of $c_k(A,B)$ found by Whisper to determine whether there are gaps in existing benchmarks for the application of interest, and
- We can add candidate "optimized" experiments to the Whisper catalog and compare new c_k's from these candidate experiments to c_k's from existing benchmarks

F. Brown, "Sensitivity-Uncertainty Techniques for Nuclear Criticality Safety," LA-UR-17-27058, 2017.

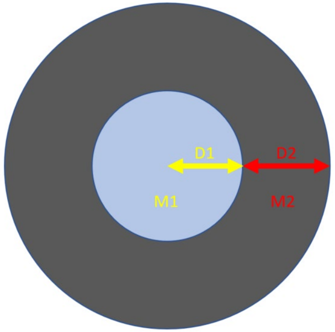
Step 4 - Experiment Optimization

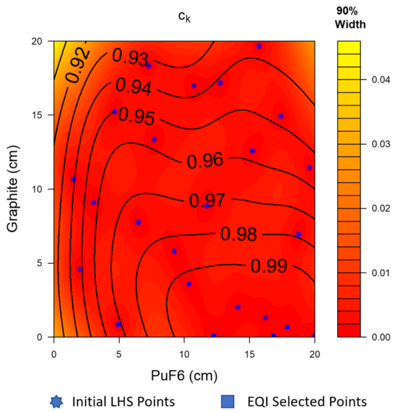
- Uses a probabilistic model to make informed global guesses of optimum
- Model c_k as a function of configuration η using a Gaussian process (GP)
- GP model is sequentially refined and maximized using the Expected Quantile Improvement

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

- Algorithm:
    1. Initial Latin Hypercube Sample (LHS) of MCNP runs
    2. For i=1,…,n
        1. Optimize EQI over all configurations
        2. Run MCNP for best configuration
        3. Update GPs
    3. Return best configuration
    4. (optional) Run physical experiment

- Configurations are described as
  $$\eta = [(M1, D1), (M2, D2), \ldots]$$
- M1, M2,… are material types (discrete)
- D1, D2,… are thicknesses (continuous)





Weaver, Brian P., et al. "Computational enhancements to Bayesian design of experiments using Gaussian processes." *Bayesian Analysis* 11.1 (2016): 191-213.

Test cases

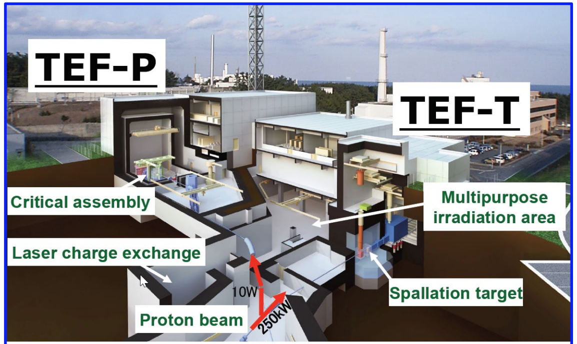
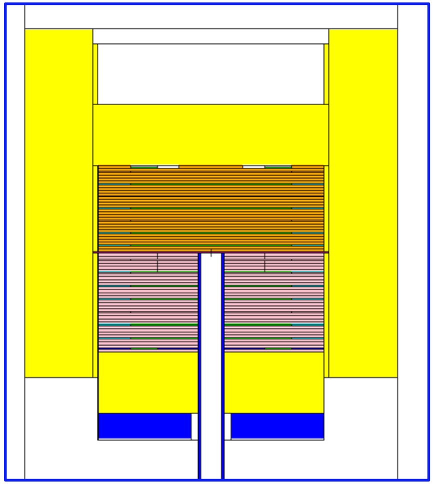
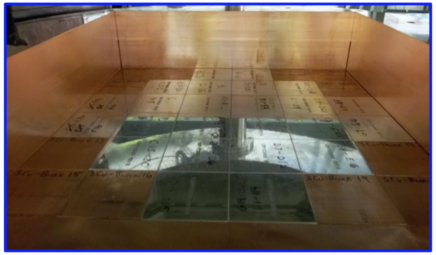
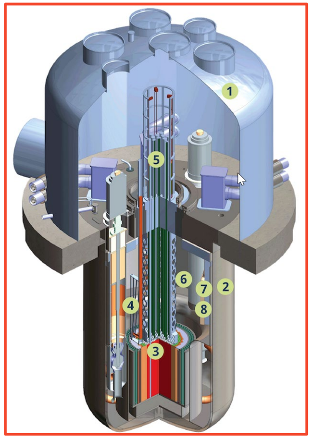


Figure 2. Transmutation Experimental Facility (TEF)

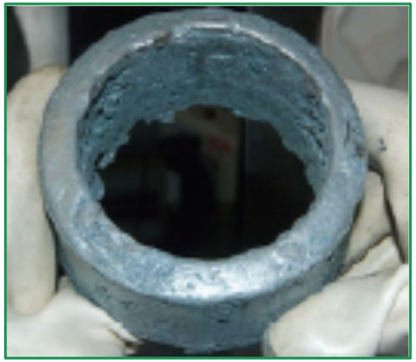


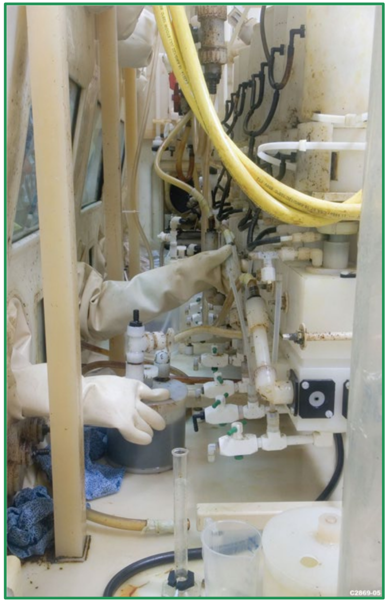




Travelling Wave Reactor.

JAEA collaboration.





Kilopower/KRUSTY.

LANL PF-4 applications.

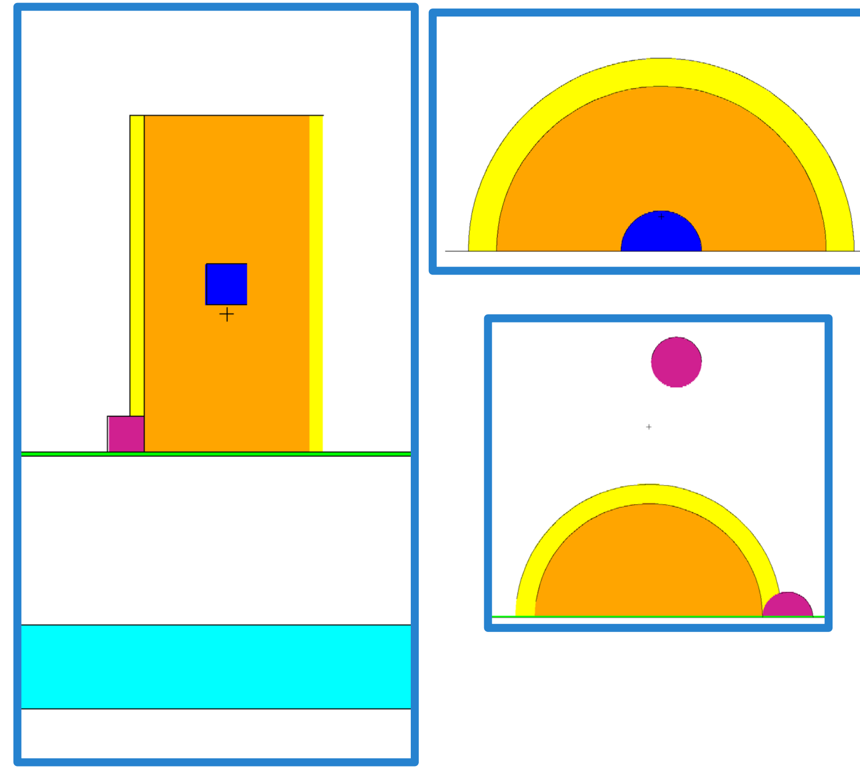
PF-4 Applications

- Aqueous Chloride
- Plutonium Casting
  - Tantalum
  - Graphite

PF-4 Applications: Plutonium Casting (Tantalum)

- Simplified Single Piece Casting: 4,500 g Pu spherical α–phase metal reflected by 1-2 cm thick Ta
- 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
- Single Piece Casting(shown right): 6,000 g Pu metal, surrounded by 5 cm Ta on all sides, further surrounded by 1-inch water, beside 4,500 g Pu cylinder and additional 4,500 g cylinder located 30-cm away, with reflection from stainless steel glovebox surface and concrete floor. Reflected surface down center of model.

Application	Condition	Plutonium	Reflector	keff		
Simplified Single Piece Casting	Normal	4.5 kg α-Pu	1 cm Tantalum	0.84563	±	0.00007
		4.5 kg α-Pu	2 cm Tantalum	0.87726	±	0.00007
Aliquot Casting	Normal	3 x 2.0 kg α-Pu	5 cm Tantalum	0.97927	±	0.00008
Single Piece Casting	Abnormal	6.0 kg α-Pu	5 cm Tantalum & Incidental	0.97087	±	0.00008



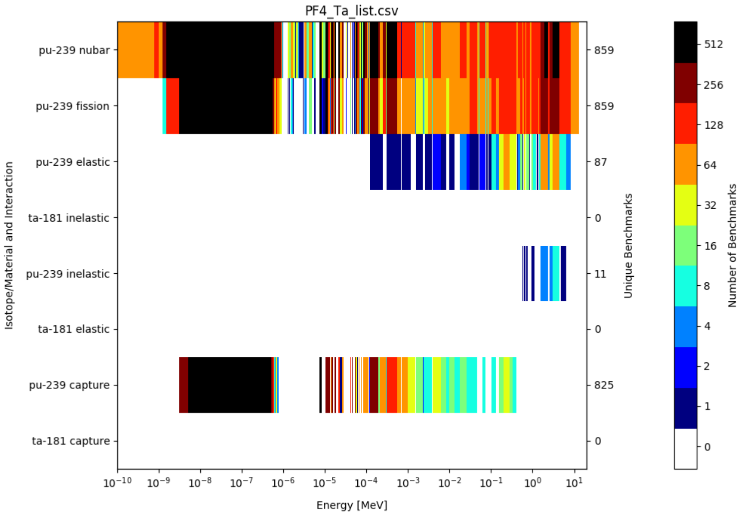
MCNP6 Illustration of Example 4: Pu (blue) surrounded by Ta (orange) and water (yellow), next to cylinders of Pu metal (magenta), with stainless steel (green) and concrete (turquoise) floor.

PF-4 Applications: Plutonium Casting (Tantalum)

File		Simplified Single Piece 1cm			Simplified Single Piece 2cm			Aliquot Casting			Single Large Piece Cast		
Nuclide	Reaction	keff sensitivity			keff sensitivity			keff sensitivity			keff sensitivity		
94239.80c	nu	1.00E+00	±	8.21E-04	1.00E+00	±	7.90E-04	1.00E+00	±	7.47E-04	1.00E+00	±	2.83E-03
94239.80c	fission	7.88E-01	±	8.59E-04	7.74E-01	±	8.14E-04	7.31E-01	±	7.95E-04	7.28E-01	±	2.86E-03
94239.80c	elastic	5.02E-02	±	6.00E-04	4.72E-02	±	6.23E-04	3.68E-02	±	6.79E-04	3.08E-02	±	2.25E-03
73181.80c	inelastic	4.13E-02	±	1.73E-04	6.27E-02	±	2.33E-04	9.57E-02	±	3.52E-04	7.42E-02	±	1.60E-03
94239.80c	inelastic	3.43E-02	±	3.48E-04	3.23E-02	±	3.33E-04	2.67E-02	±	3.83E-04	2.14E-02	±	1.22E-03
73181.80c	elastic	3.24E-02	±	1.89E-04	5.29E-02	±	2.78E-04	8.96E-02	±	5.97E-04	7.87E-02	±	2.51E-03
94239.80c	n,gamma	-6.94E-03	±	1.70E-05	-8.02E-03	±	1.86E-05	-1.20E-02	±	2.60E-05	-1.45E-02	±	1.64E-04
73181.80c	n,gamma	-1.04E-03	±	5.65E-06	-3.17E-03	±	1.26E-05	-2.11E-02	±	6.41E-05	-4.09E-02	±	3.54E-04

List of most sensitive reactions for the four Ta examples (based on $|k_{eff}$ sensitivities$|$).

Heatmaps for the top 8 reactions. Benchmarks included are those that exceed a sensitivity threshold of > 10^{-3} for that energy bin.
Note the lack of relevant benchmarks for Ta!



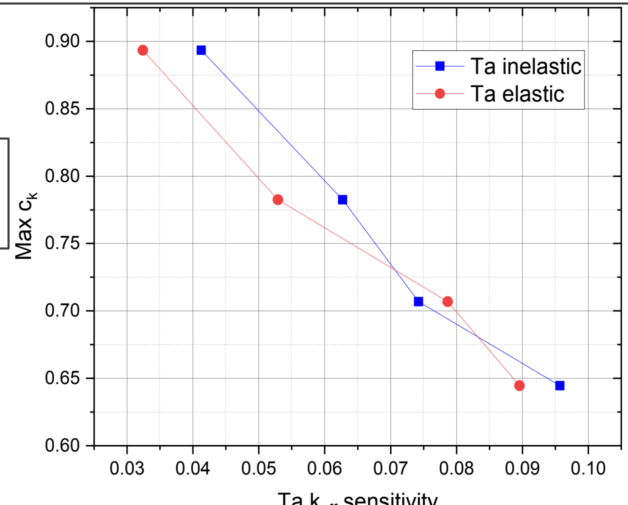
PF-4 Applications: Plutonium Casting (Tantalum)

benchmark	c_k			
	Simplified Single Piece 1cm	Simplified Single Piece 2cm	Aliquot Casting	Single Large Piece Cast
LAMPRE-FUND-RESR-001-006*	0.8933	0.7824	0.6442	0.7069
LAMPRE-FUND-RESR-001-004*	0.8915	0.7815	0.6445	0.7068
PMF045-006	0.8904	0.7789	0.6401	0.7040
PMF045-004	0.8884	0.7774	0.6394	0.7025
LAMPRE-FUND-RESR-001-003*	0.8879	0.7780	0.6413	0.7045

List of benchmarks ranked by maximum c_k for the four Ta applications.
- Fairly low c_k values. Not surprising since there are few benchmarks with Ta.
- The top 5 benchmarks were the same for all 4 application models (although the order is slightly different).

*IRPhEP Benchmarks (same series as PMF045, however modeled with more experimental detail)

As the Ta sensitivities (both elastic and inelastic) increase, the maximum c_k values go down as expected.



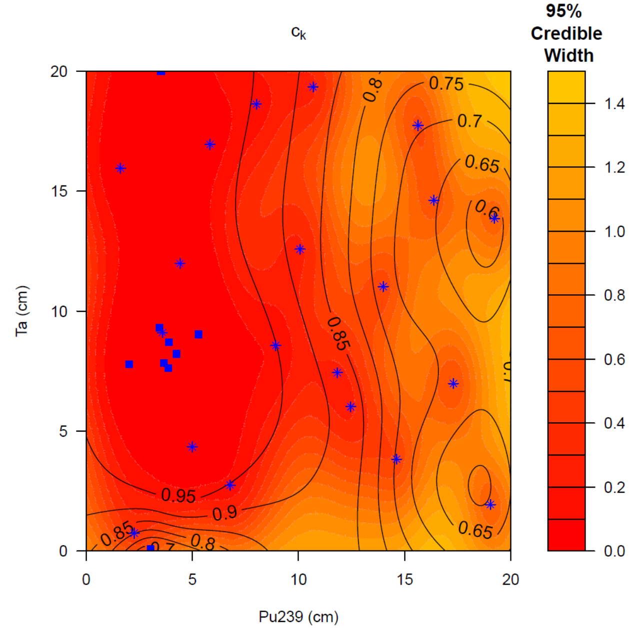
PF-4 Applications: Plutonium Casting (Tantalum Aliquot Casting Example)

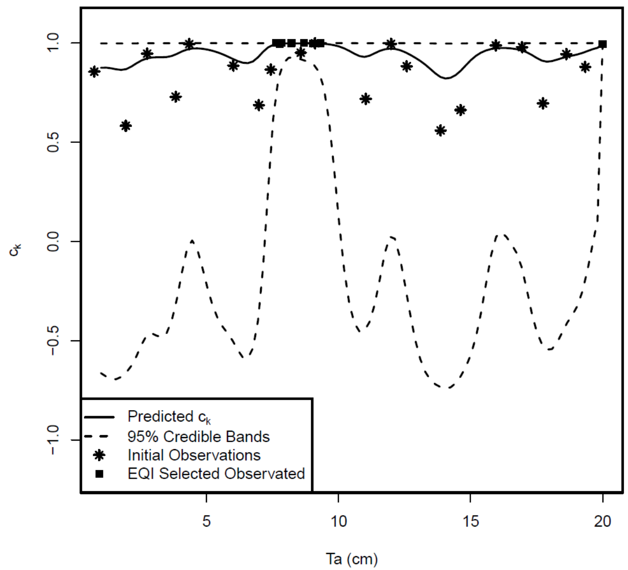
Recall that the maximum value of c_k from the existing benchmark suite was 0.6442.

The TEX/Ta models (not in ICSBEP yet) were then also included in an expanded benchmark suite.

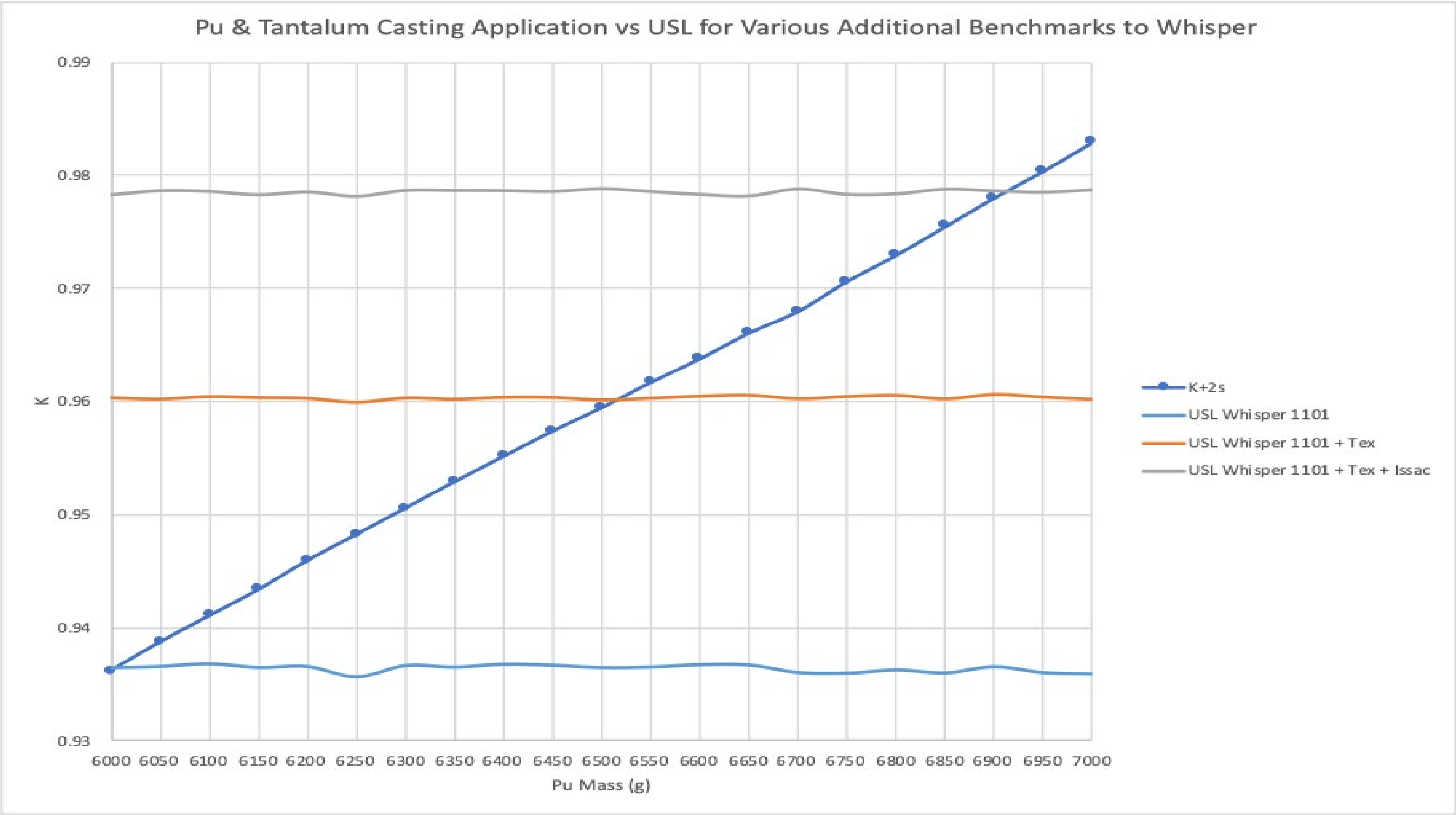
- The highest c_k was for the configuration with 26 units (which has no HDPE moderation).
- The c_k for that configuration was 0.8981 (much higher than any current benchmark).
- The other TEX/Ta configurations had low c_k values for the aliquot casting example (all < 0.5).

- We then applied the optimization tool. 2D (left) and 1D (right) optimization results are shown.
- The optimized configuration is 4.25 cm ^{239}Pu surrounded by 8.24 cm Ta).
- This configuration yielded a c_k of 0.9997.
- Might any of this matter in the real world? See next slide.

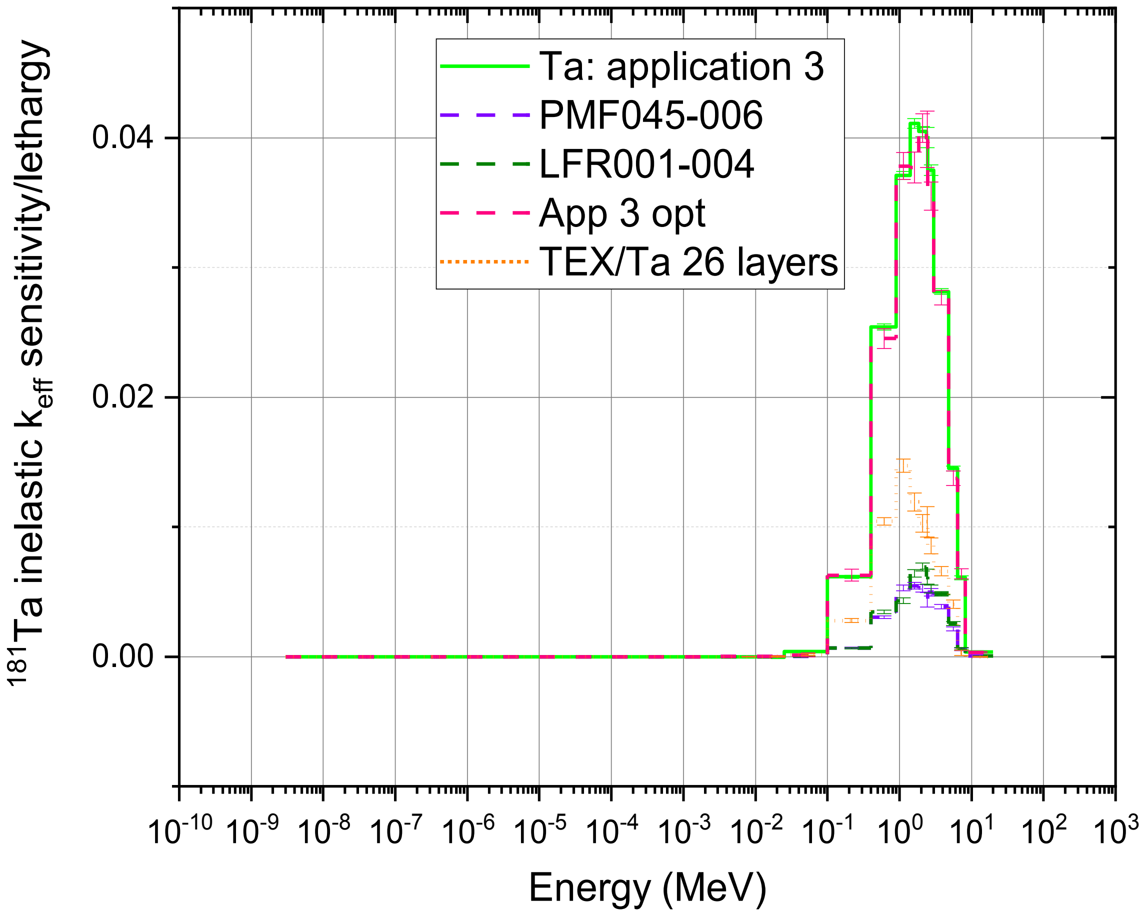




Possible Operational Impact of Additional Benchmarks



Why Would Optimized Experiment Help?



- 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.

Summary

- **All steps in the ARCHIMEDES process have been successfully demonstrated.**
- **Initial results indicate that operational improvements are possible.**
- **It is possible to design an experiment which matches k_{eff} sensitivities of an application very well but has different geometry and/or material form.**
    - What matters is having the correct combination of the right materials in the right location.
    - This is great news as it is likely that we can design experiments to meet many different applications using the existing NCERC nuclear material inventory.
- **Ongoing efforts are progressing on sensitivity simulations, gap analysis, optimization, and documentation.**
- **A long term goal is to perform benchmark experiments to meet nuclear data needs of specific applications.**

Future Work

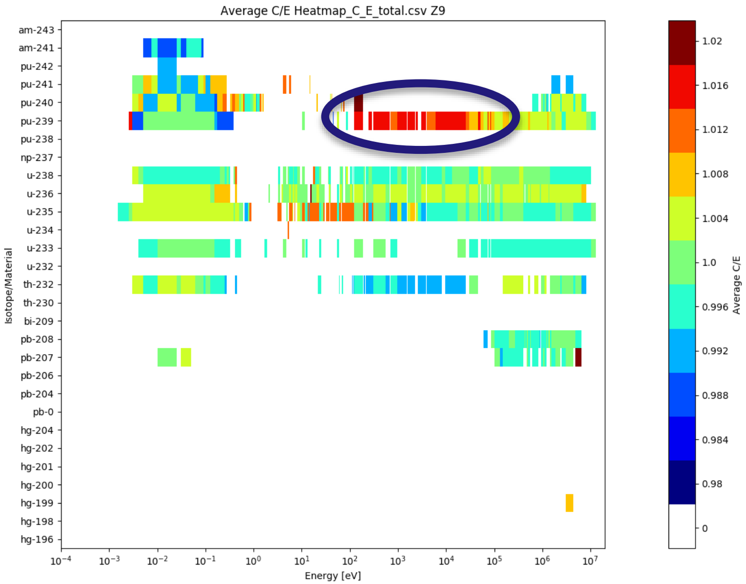
- **Compare k_{eff} sensitivities from MCNP and SENSMG**
- **Explore other options for determining similarity, including the E_{sum} method (that does not rely on covariance data)**
- **Research on other parameters to optimize against (in addition to c_k)**
  - Also other features: k_{eff} filter, removal of nuclides / reactions, contribution from a single nuclide / reaction, etc.
- **Create a more modern covariance library for MCNP / Whisper**
- **Enable calculation of sensitivities to reactivity coefficients**
- **Incorporate fixed-source sensitivities in MCNP**
- **Look at sensitivities to more than just cross-sections and nubar: angular / energy distributions, higher P_ν moments, etc.**
- **Conduct experiments and use results in future nuclear data libraries**

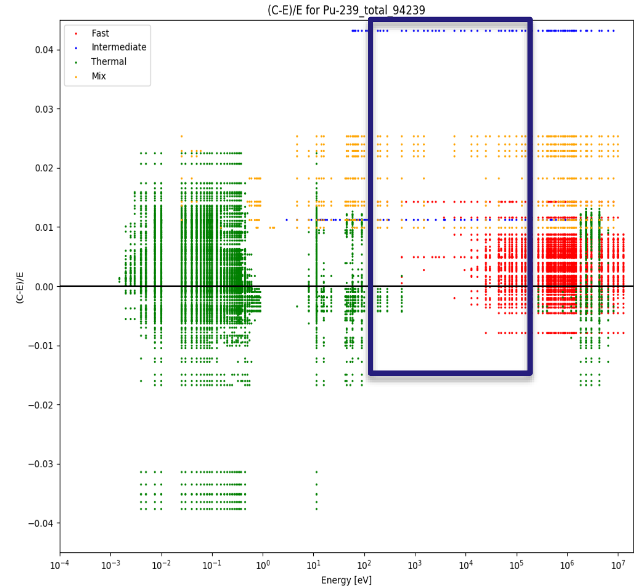
Acknowledgements

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

BACKUPS

Gap Analysis – Method 2 – Heatmaps





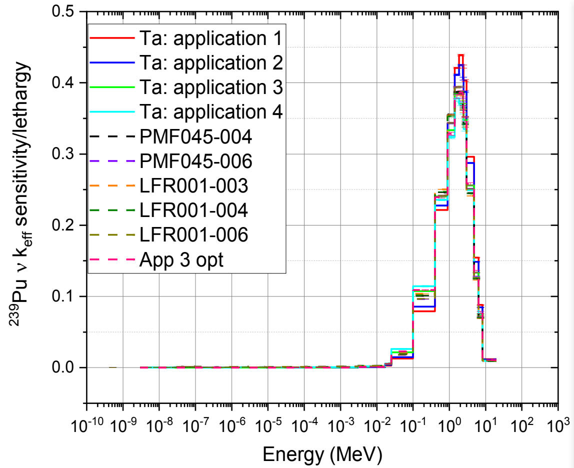
- ^{239}Pu has an average C/E well above 1 from ~100 eV to 100 keV

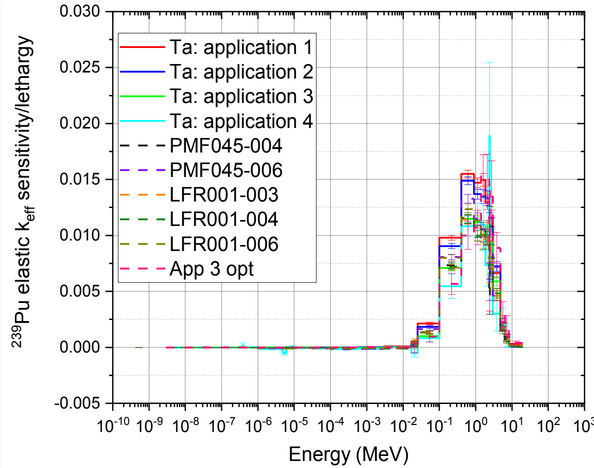
- In that energy region, nearly all benchmarks have a (C-E)/E above 0.
- Interestingly, all intermediate or mixed spectrum benchmarks are above 0.
- Might be worth reviewing these benchmarks and making new intermediate ^{239}Pu benchmarks.

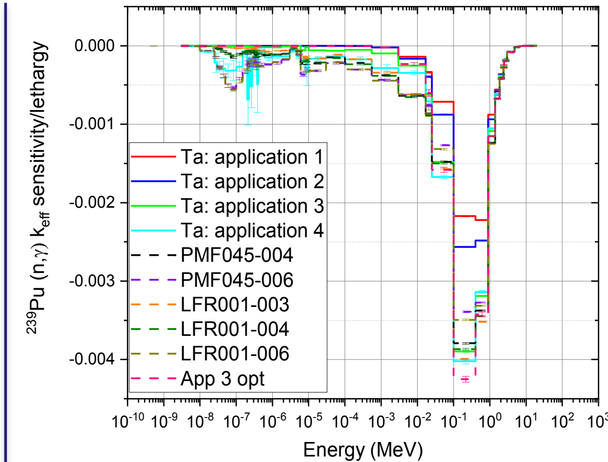
Caveats

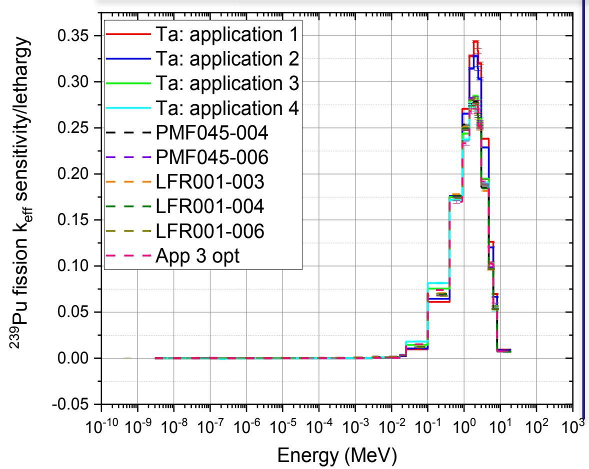
- Covariance library for MCNP / Whisper is old – based on a 44-group library released with SCALE 6.1 that pre-dated ENDF/B-VII.1.
- Evaluated covariance data continues to need improvement.
- Some historical benchmarks have major deficiencies.

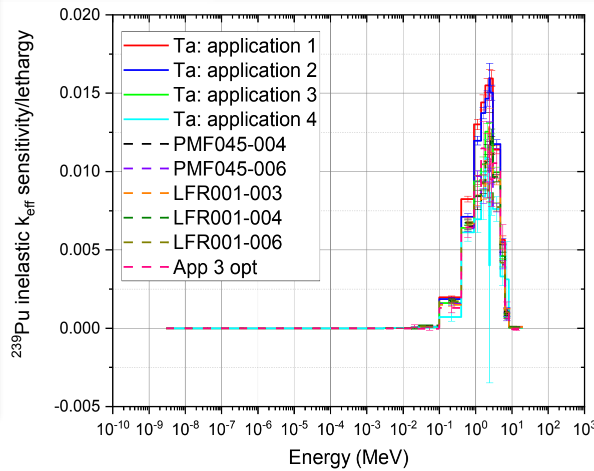
PF-4 Applications: Plutonium Casting (Tantalum)







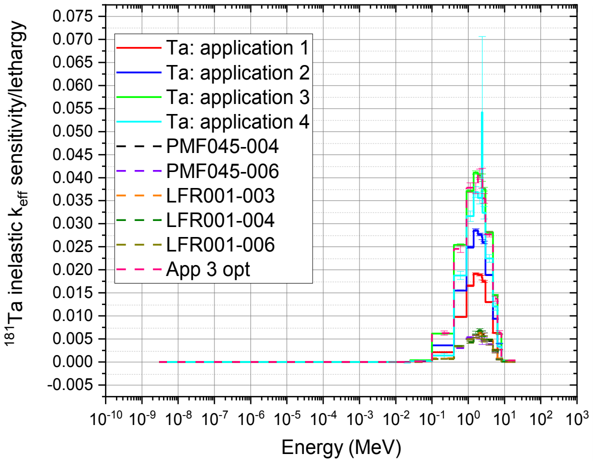


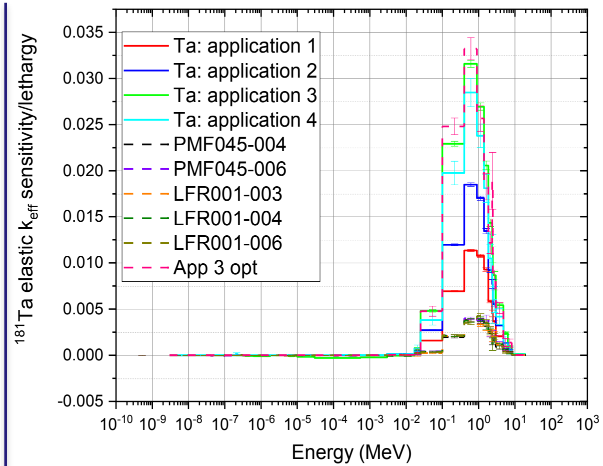


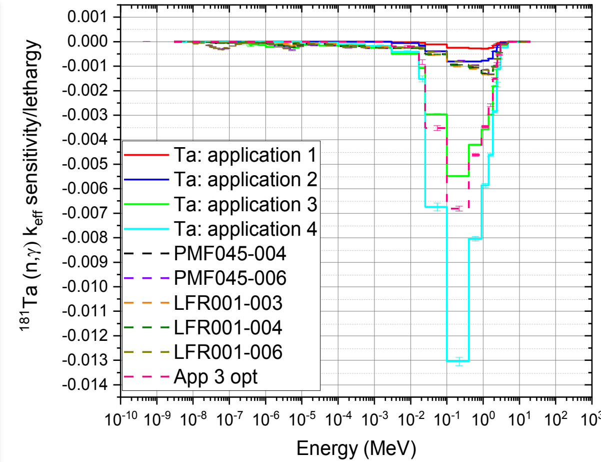
Solid lines are Ta applications. Dashed lines are benchmarks.

Dashed pink line is the optimization which should be compared to the Ta: application 3 (in green).

PF-4 Applications: Plutonium Casting (Tantalum)





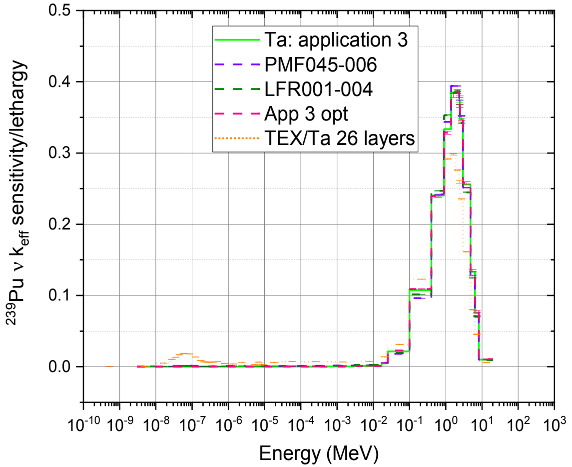


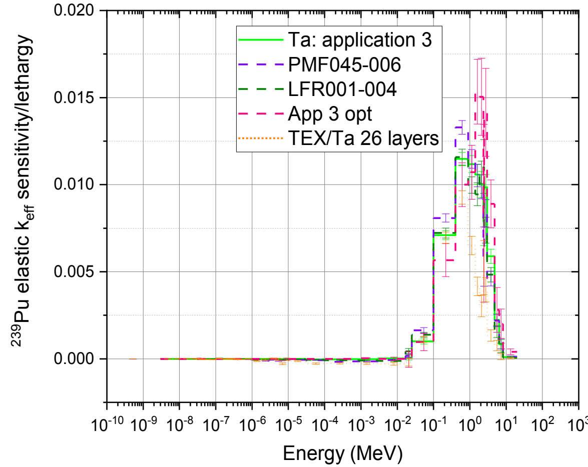
The four Ta applications have varying Ta sensitivities.

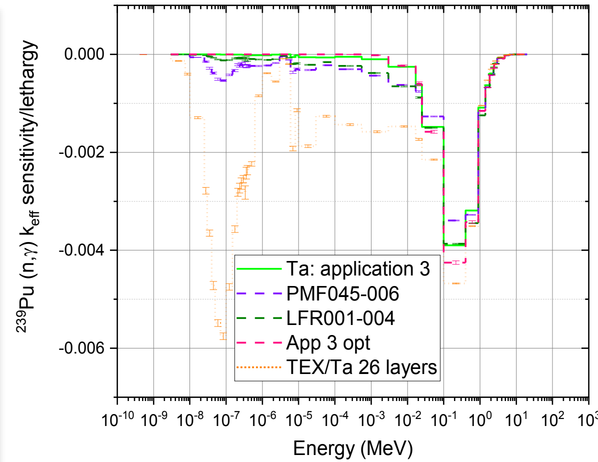
The applications with high Ta sensitivities are greater than any existing benchmarks.

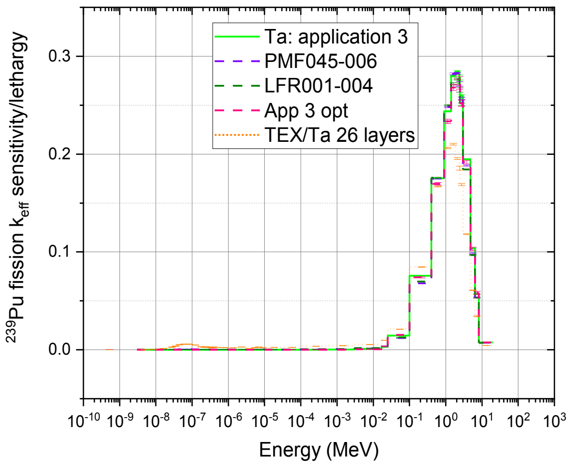
Dashed pink line is the optimization which should be compared to the Ta: application 3 (in green).

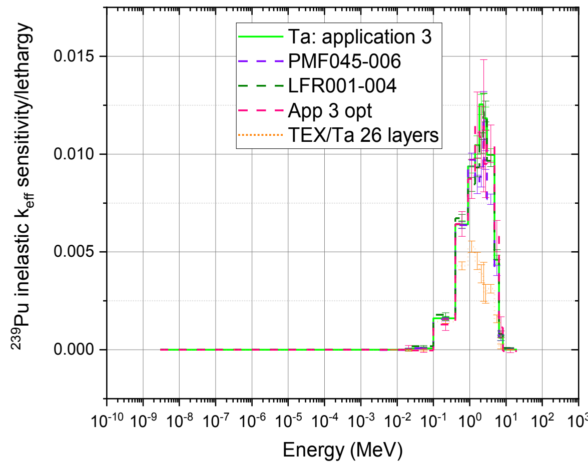
PF-4 Applications: Plutonium Casting (Tantalum)





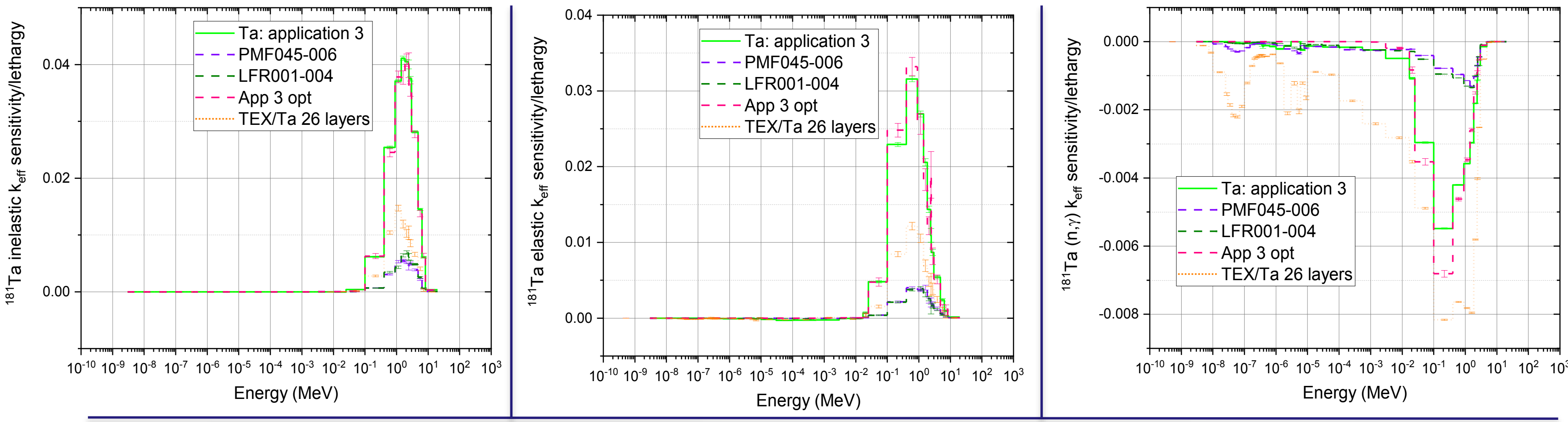






- Solid line is the aliquot casting Ta application.
- Dashed lines include the highest c_k including 1000+ ICSBEP and IRPhEP configurations.
- Dotted line is the TEX configuration with the highest c_k.
- App 3 opt is the optimization result for the aliquot casting application.

PF-4 Applications: 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.