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Title: Application of Covariance Data in Nuclear Criticality

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Application of Covariance Data in Nuclear Criticality

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Abstract

The DOE/NNSA Nuclear Criticality Safety Program (NCSP) has funded the development of a sensitivity/uncertainty capability for criticality safety methods development at LANL. Updates are given on the continuous-energy sensitivity capability in MCNP and other related efforts. Efforts on the development of the capability for processing of covariance data by NJOY are summarized. The application of these techniques and the development of new software infrastructure to support validation for Pu operations at LANL is discussed.

Introduction

- Motivation
- MCNP Sensitivity Capability
- Application at LANL
- Update on NJOY-MCNP S/U Capability

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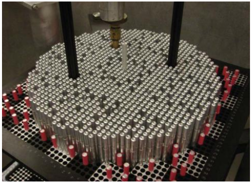
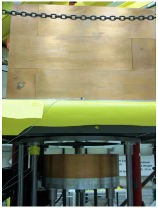
Motivation

- Sensitivity/uncertainty analysis allows us to quantify how well (or poorly) software predicts criticality.








Motivation

- The uncertainty in the effective multiplication (or any response) can be predicted to a first-order Taylor series approximation with the sandwich rule:

$$\sigma_k^2 = \mathbf{SCS}^T \qquad (1)$$

- **S** is a vector of sensitivity coefficients (involves derivatives) for the system computed by simulation package.
- **C** is a (relative) covariance matrix for the nuclear data.

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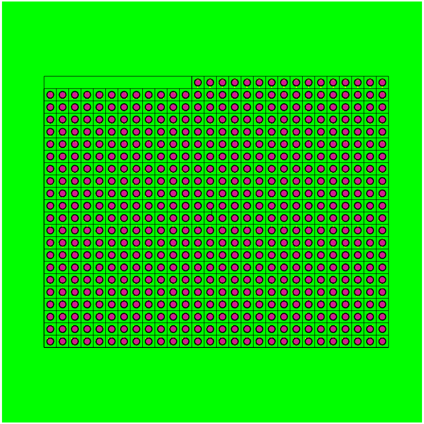
MCNP6.1 Sensitivity Capability

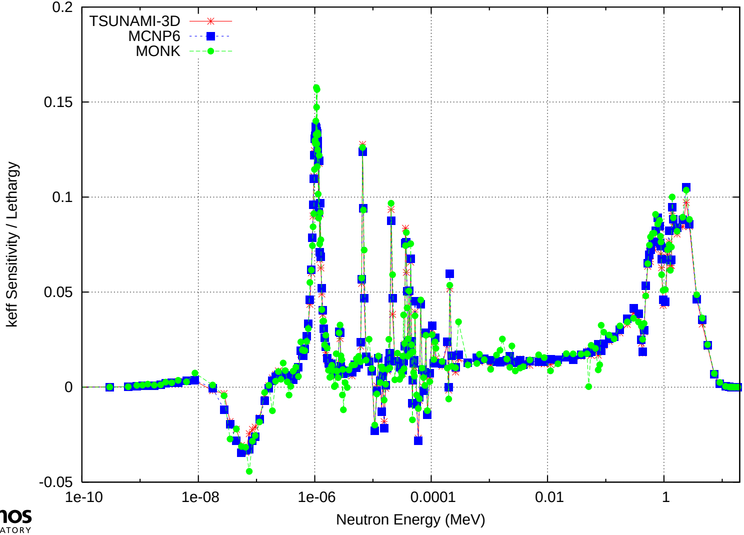
- Continuous-energy k sensitivity coefficient capability is available today in MCNP6.1 (released summer 2013).
- Uses adjoint weighting methodology (similar to TSUNAMI) with Iterated Fission Probability method.
  - Benchmarked with analytic solutions, direct perturbations, and comparisons with TSUNAMI.
- Robust method with minimal user involvement.
  - Define the isotopes, reactions, and energy grid, run, and get results.
- Journal paper describing methodology published in Nuclear Science and Engineering (July 2013).

Results: MOX Lattice Benchmark

- Array of mixed-oxide (MOX) fuel pins submerged in water.
- ENDF/B-VII.0 data used.
- $k = 0.99899 \pm 0.00012$



MOX Lattice: H-1 Elastic + $S(\alpha, \beta)$



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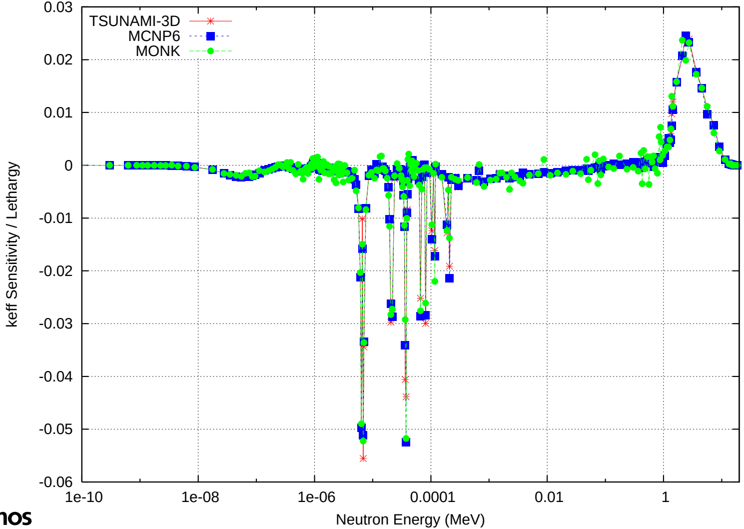
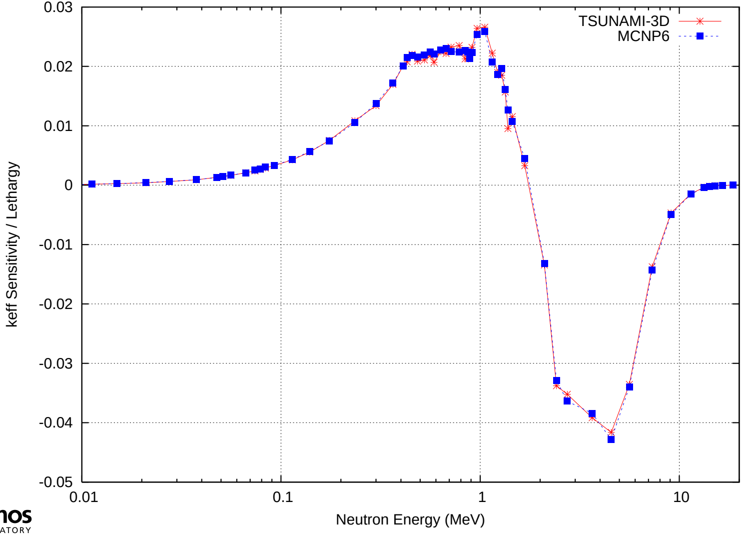
MOX Lattice: U-238 Total



MOX Lattice: Pu-239 Fission-χ (Normalized)



New Capability: Legendre Moment Sensitivities

- Often the scattering distributions and uncertainties are given as Legendre moments.
- Can express renormalized sensitivity coefficient $\hat{S}_{k,f}(\mu)$ as Legendre moment sensitivity $\hat{S}_{k,f,\ell}$.
- Given a defined cosine grid with N bins with index i, the ℓth Legendre moment sensitivity is

$$\hat{S}_{k,f,\ell} = \frac{2\ell + 1}{2} f_\ell \sum_{i=0}^{N-1} \left(\mu_{i+1} - \mu_i\right) \frac{P_\ell(\mu_{i+1/2})}{F_{i+1/2}} \hat{S}_{k,f,i+1/2}$$

- Presented at NCSD Topical (Sep. 2013) and ANS Winter Meeting (Nov. 2013).

Legendre Moment Sensitivities

- The linearly anisotropic (P_1) component of elastic scattering may have a significant effect on k.
- Higher orders of scattering are typically not important, and neither is anisotropy of inelastic scattering.
- For fast systems with significant leakage, core and reflector materials are often significant and should be included in nuclear data adjustments.
- For thermal systems, scattering distributions matter less.
- **Next step: convolve covariance data.**

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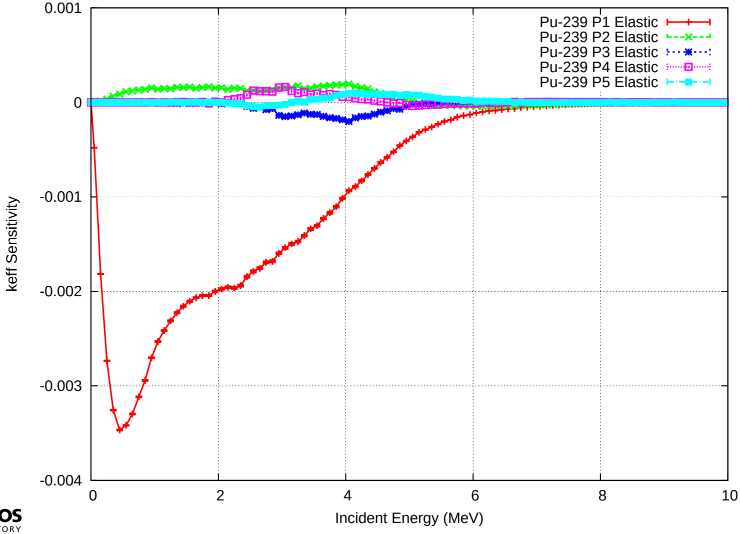
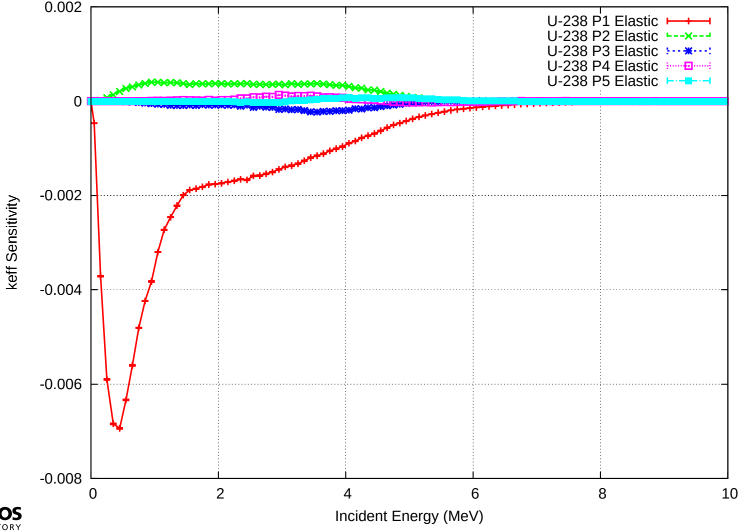
Jezebel ^{239}Pu Elastic Moment Sensitivity



Flattop (HEU) ^{238}U Elastic Moment Sensitivity



Application at LANL

- LANL Pu operations currently halted.
- One issue identified by reviews is the validation for MCNP criticality safety calculations.
  - Requires compliance with ANSI/ANS-8.1 and 8.24.
  - My opinion: Previous effort was a very good start, but not sufficient.
- Goal is to develop a robust computational tool set to assist with validation that fits within their MCNP-centric workflow.
- Based on the ORNL sensitivity/uncertainty methodologies.

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Sensitivity/Uncertainty Methodology

- Use sensitivity coefficients and covariance data as similarity parameter c_k to identify benchmarks relevant to a set of computational models.
- Uses MCNP6.1 sensitivity coefficient capability, ENDF/VII.1 nuclear data, and ORNL 44-group covariance libraries that have been processed into LANL format.
- Search benchmark suite to develop weighting factors for calculational margin computation.
  - NCS validation suite has been expanded to over 1000 benchmarks covering a broad set of areas.
- Hope is to distribute these capabilities outside LANL and possibly as a library for MCNP that integrates validation as part of the k calculation.

Expanded Validation Suite

- Current NCS benchmark set (1095 cases) from ICSBEP:

	Fast	Inter	Therm	Mixed	Total
Pu	54	1	158	34	247
HEU	251	5	122	8	386
IEU	12	0	1	0	12
LEU	0	0	209	0	209
Mix	35	1	36	1	73
U233	10	33	115	0	158
Spec	10	0	0	0	10

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Selection of Benchmarks

- Compute the c_k of process and benchmarks.
- Find maximum c_k, use to determine total “weight” required for validation:

$$w_{req} = A + B(1 - c_{k,max}).$$

- $A = 25$, $B = 100$. Need more benchmarks for lower $c_{k,max}$.
- Reduce acceptance $c_{k,acc}$ until total weight of included benchmarks reaches w_{req}.
- Weight for a benchmark is

$$w = \frac{c_k - c_{k,acc}}{c_{k,max} - c_{k,acc}}.$$

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Calculational Margin Methodology

- Uses extreme value theory to find probability that worst case bias in k is < 0.99.
- Including more benchmarks only increases the calculational margin; fail safe.
- Cumulative density function for bias in k for a benchmark j:

$$F_j(x) = (1 - w_j) + \frac{w_j}{2}\left[1 + erf\left(\frac{x - \beta_j}{\sqrt{2\sigma_j^2}}\right)\right].$$

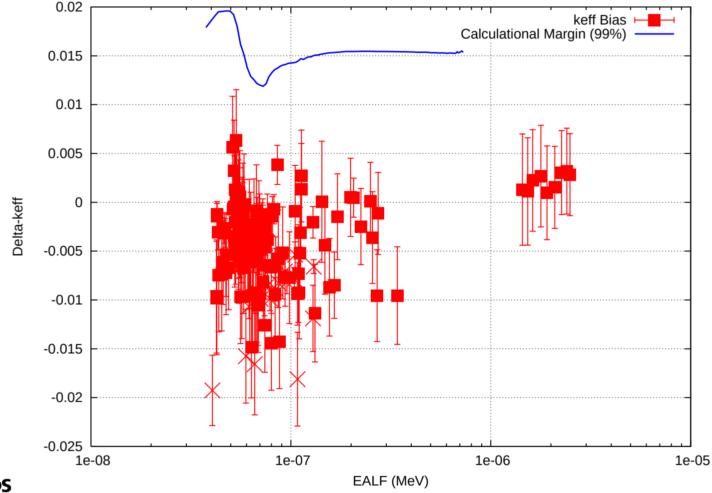
- Cumulative density function for worst case bias:

$$F(x) = \prod_{j=1}^{N} F_j(x).$$

Margin of Subcriticality

- Make recommendation for starting point for NCS analyst.
- Margin for unknown and undetected software errors in MCNP6.1: 0.005.
- Margin for variability in cross section data uses residual nuclear data uncertainty (99% confidence level assuming Normal distribution) in k obtained from with GLLS technique (TSURFER methodology) with rejection of outliers.
- Additional margin may be required for analyst to ensure subcriticality.

Pu Metal-Water Mix Results



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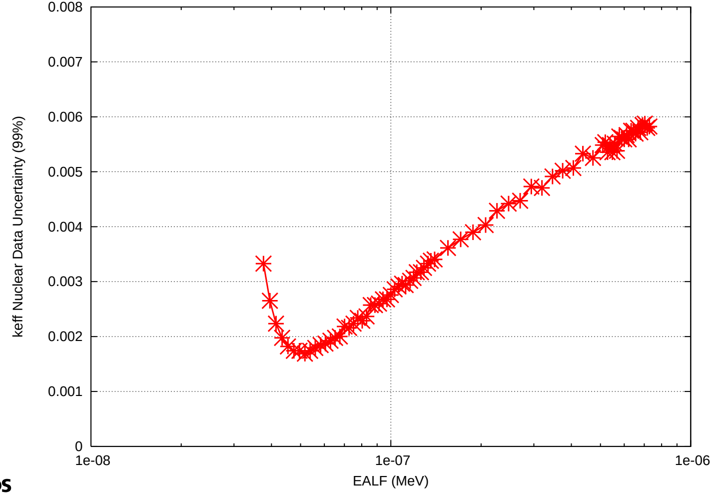
Pu Metal-Water Mix Results



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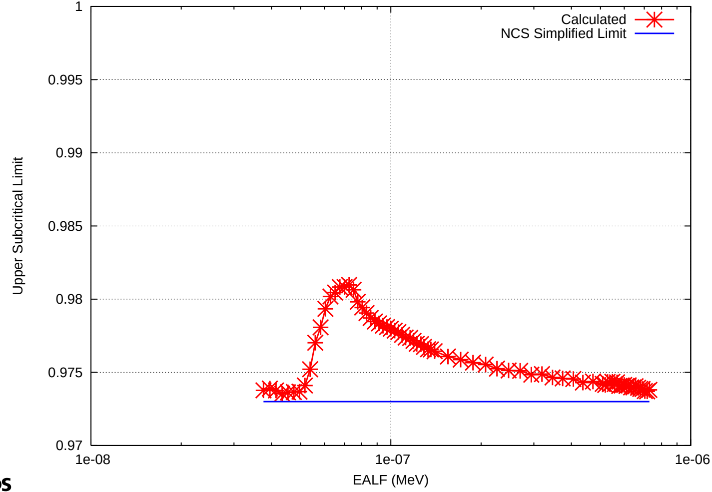

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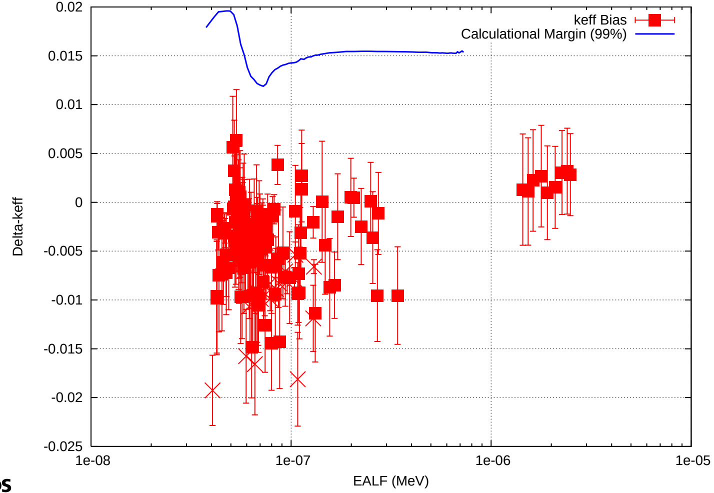
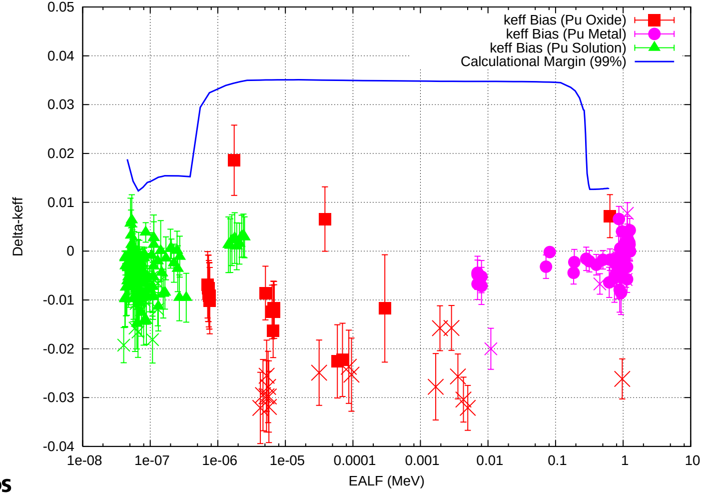
Pu Metal-Water Mix Results



Pu Oxide-Water Mix Results



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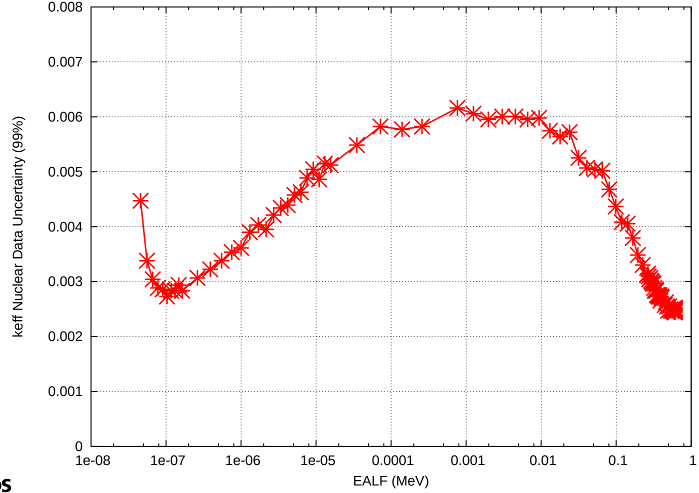
Pu Oxide-Water Mix Results



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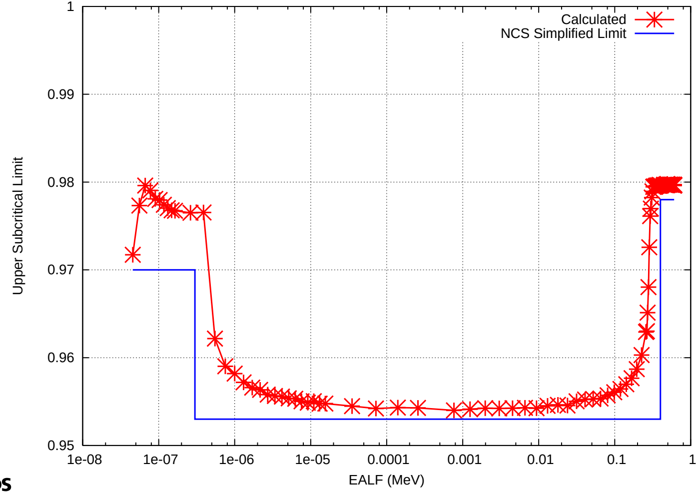

Uncertainty/Covariance Project

- Develop a capability in the MCNP framework that automates uncertainty quantification of nuclear data.
  - Beginning of calculation, query covariance data and automatically create sensitivity profiles.
  - Run criticality calculation normally and compute k and $S_{k,x}$ for all data.
  - At end of calculation, read covariance data and compute uncertainty in k using “sandwich rule”:

$$(\delta k)^2 = \mathbf{SCS}^T.$$

- Goal is to have covariances processed by NJOY.

Uncertainty/Covariance Project

- Studied two formats:
  - Compressed upper triangular or full matrix.
  - Principal eigenvectors.
- Principal eigenvector method requires less storage, but savings may not be large enough in many cases to justify the cost.
- Issues identified in NJOY for processing covariance data. Being worked on.

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Uncertainty/Covariance Project

- Prototype version of MCNP6 developed that automatically computes uncertainty in k.
- Uses covariance data generated from NJOY that is processed externally.
- Preliminary results presented at NCSD Topical (Sep. 2013).
- Identifies what I believe are inconsistencies in ENDF/B-VII.1 covariance data.

Preliminary Uncertainty Results

- Covariance data generated with ENDF/B-VII.1 for ^{1}H , ^{16}O , ^{235}U , ^{238}U , and ^{239}Pu .
- No thermal scattering law covariances included.
- Benchmarks:
  - Bare-HEU Sphere (Lady Godiva)
  - Reflected-HEU Sphere (Flattop)
  - Uranium-Hydride Experiment
  - Light-Water Moderated LEU Lattice
  - Bare-Pu Sphere (Jezebel)
  - Reflected-Pu Sphere (Flattop)
  - Light-Water Moderated MOX Lattice
  - Pu Solution (Light-Water)

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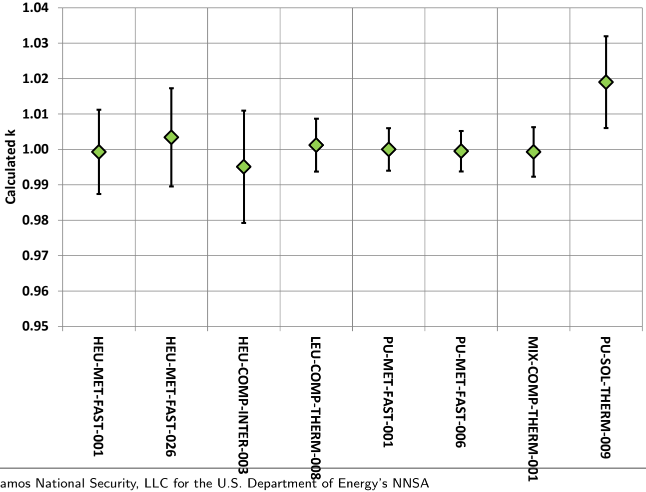
Preliminary Uncertainty Results

- MCNP calculated *k* with nuclear data uncertainty:



Summary

- MCNP currently supports generation of continuous-energy sensitivity coefficients.
- Immediate LANL needs in Pu operations has spurred the development of external capabilities for validation using S/U methodologies funded by NCSP and developed by ORNL.
  - **Covariance data employed for validation for PF-4.**
- Development of uncertainty quantification capabilities in or with MCNP proceeding.

Acknowledgments

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Questions?