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Sensitivity-Uncertainty Based Nuclear Criticality Safety Validation

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National Laboratory Professor, Nuclear Eng., UNM**



Abstract

Sensitivity-Uncertainty Based Nuclear Criticality Safety Validation

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Whisper is a statistical analysis package developed to support nuclear criticality safety validation. It uses the sensitivity profile data for an application as computed by MCNP6 along with covariance files for the nuclear data to determine a baseline upper-subcritical-limit for the application. Whisper and its associated benchmark files are developed and maintained as part of MCNP6, and will be distributed with all future releases of MCNP6.

Although sensitivity-uncertainty methods for NCS validation have been under development for 20 years, continuous-energy Monte Carlo codes such as MCNP could not determine the required adjoint-weighted tallies for sensitivity profiles. The recent introduction of the iterated fission probability method into MCNP led to the rapid development of sensitivity analysis capabilities for MCNP6 and the development of Whisper.

Sensitivity-uncertainty based methods represent the future for NCS validation – making full use of today's computer power to codify past approaches based largely on expert judgment. Validation results are defensible, auditable, and repeatable as needed with different assumptions and process models. The new methods can supplement, support, and extend traditional validation approaches.

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LANL PF4 Restart

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Sensitivity-Uncertainty Based Nuclear Criticality Safety Validation

Nuclear Criticality Safety

- **Background & Examples**

NCS Validation

- **Upper Subcritical Limits**
- **Traditional NCS Validation**

Sensitivity-Uncertainty Based NCS Validation

- **Overview**
- **Sensitivity Profiles, Covariance Data, Correlation Coefficients**
- **MCNP-Whisper Methodology**
 - Selection of benchmarks
 - Bias & bias uncertainty
 - USLs & validation
- **Examples**

Discussion

Nuclear Criticality Safety

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Examples of Experiments & Production

Nuclear Criticality Safety - Background

- **Why do we care about Validation?**
 - **Ensure what NCS determines to be subcritical is actually subcritical**
 - People make mistakes
 - Computer codes & nuclear data have approximations & errors
 - **Nuclear Criticality safety:**
 - Focus on avoiding worst-case combination of mistakes, uncertainties, approximations, errors, ...
 - Rigor & conservatism always
 - Never wishful thinking or "close enough"
 - **How can we be confident in assessing subcriticality?**
 - Verify that codes work as intended
 - Validate codes + data + methods against nature (experiments)
 - Be conservative, add extra margin for uncertainties & unknowns

Critical Experiments (1)

heu-met-therm-003

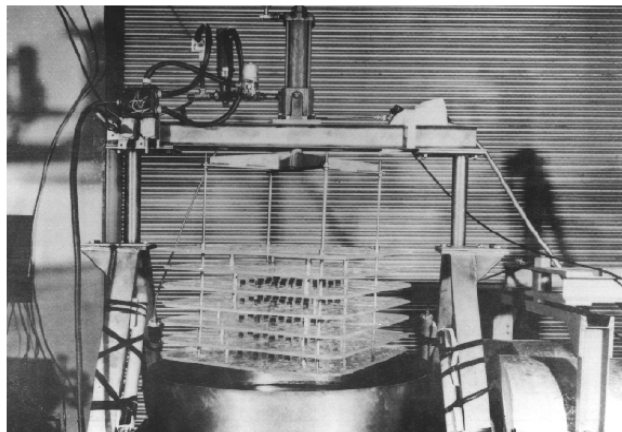
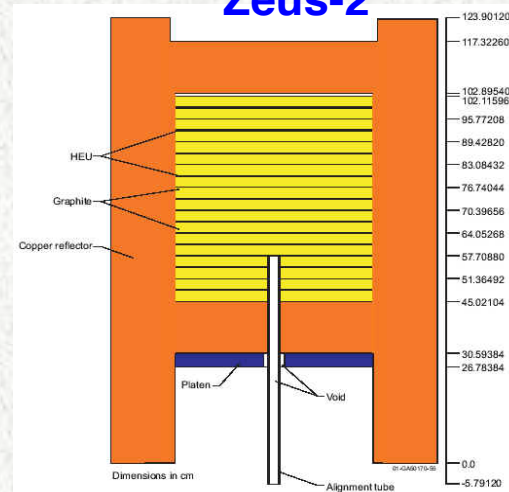
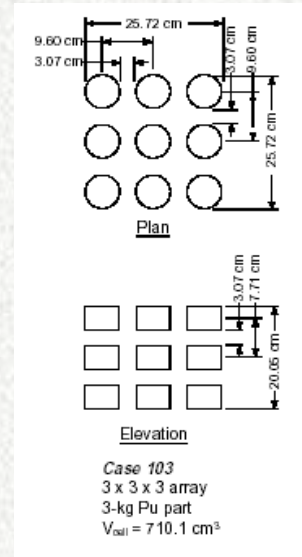


Figure 2. Array of 0.5-in. Cubes Prior to Immersion.

heu-met-inter-006-002 Zeus-2



pu-met-fast-003-00 3



ieu-comp-therm-002-003

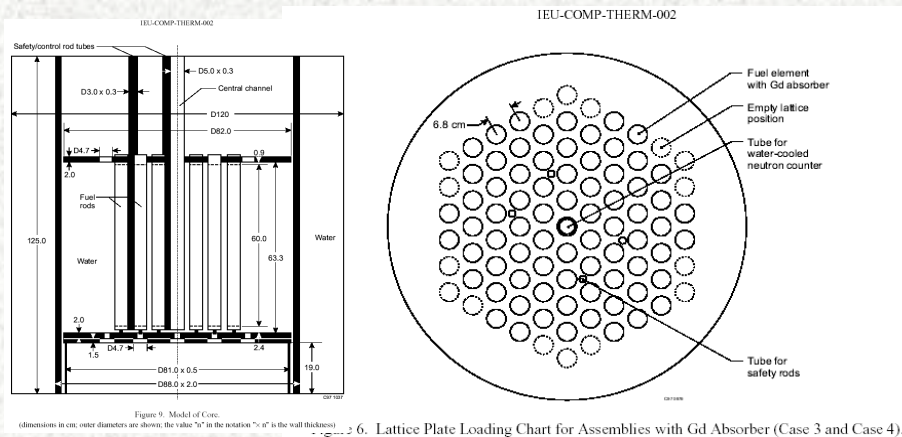
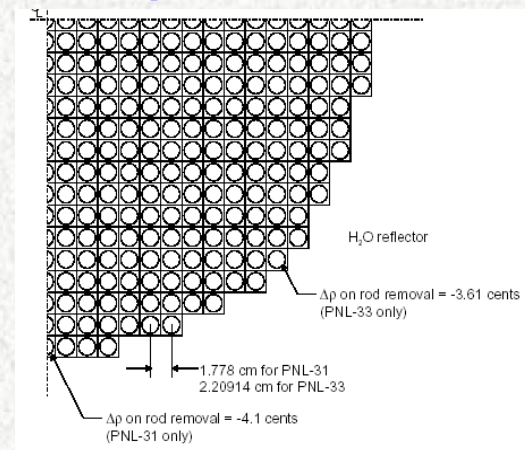


Figure 9. Model of Core.

(dimensions in cm; outer diameters are shown; the value "n" in the notation "n" is the wall thickness)

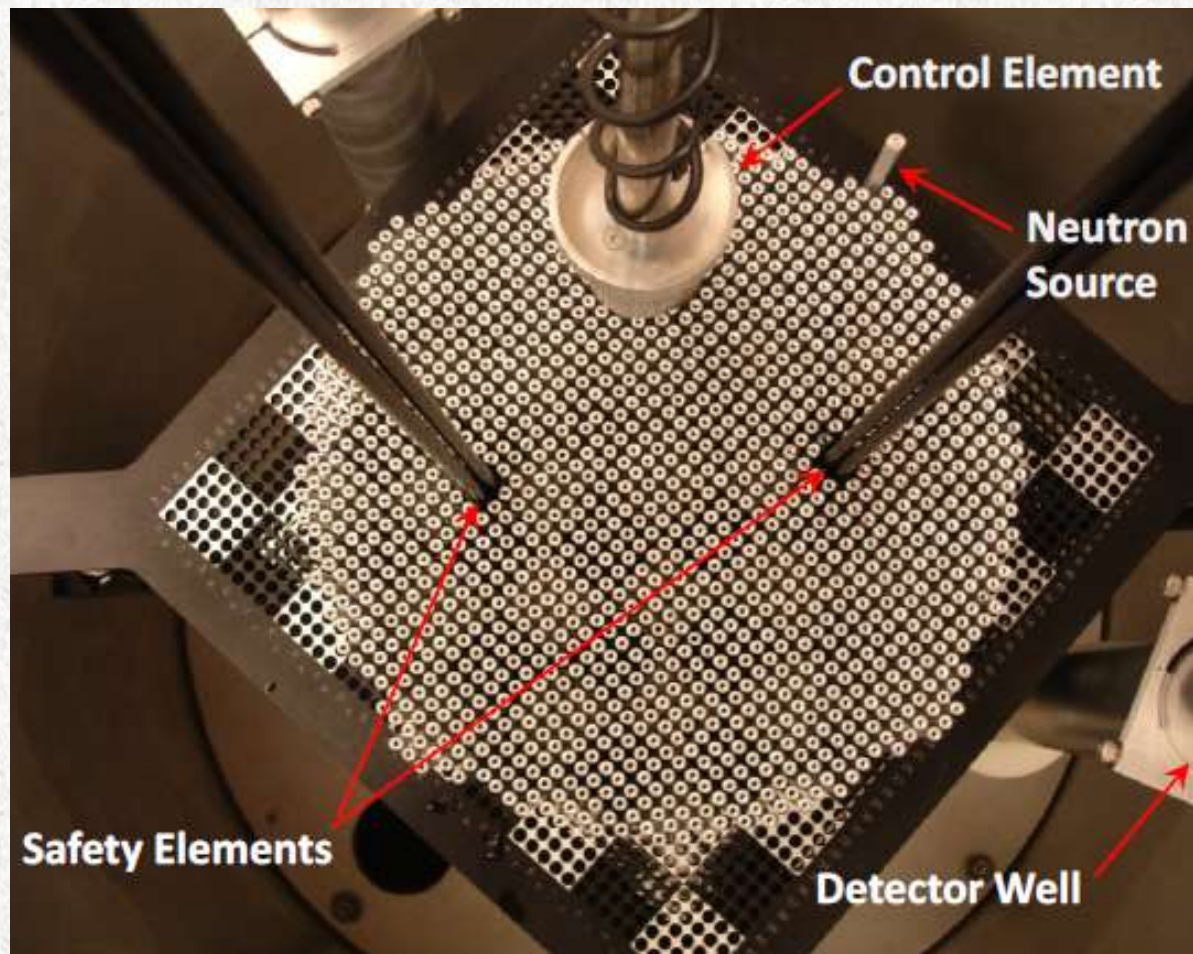
Figure 6. Lattice Plate Loading Chart for Assemblies with Gd Absorber (Case 3 and Case 4).

mix-comp-therm-002, PNL-33



Critical Experiments (3)

leu-comp-therm-080b



pu-met-fast-006

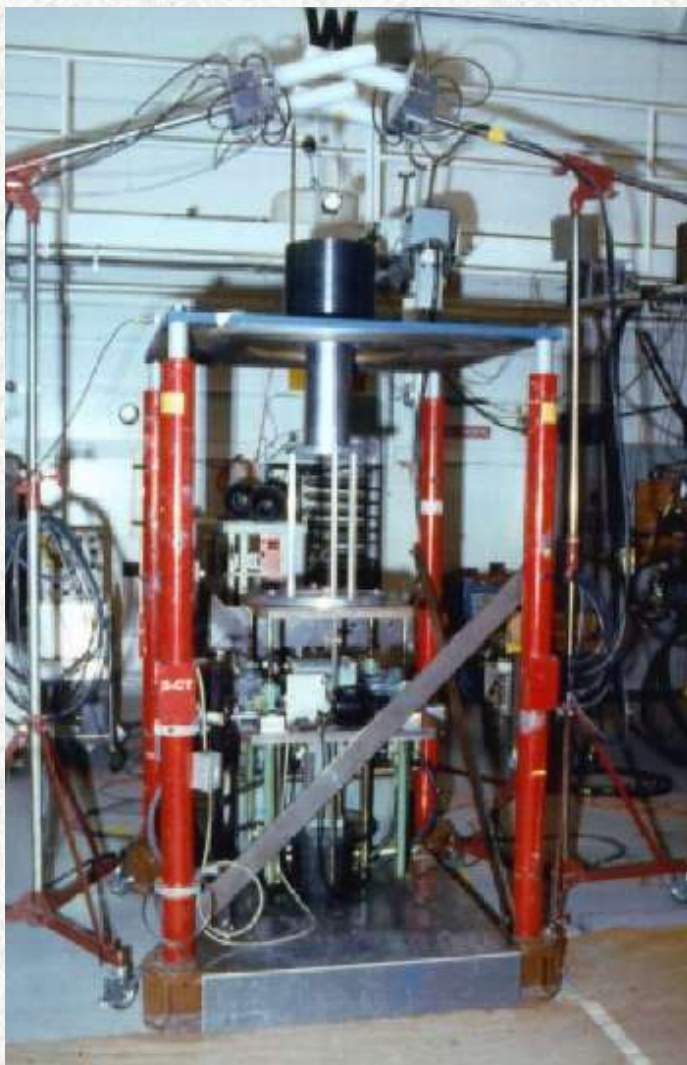


pu-sol-therm-030

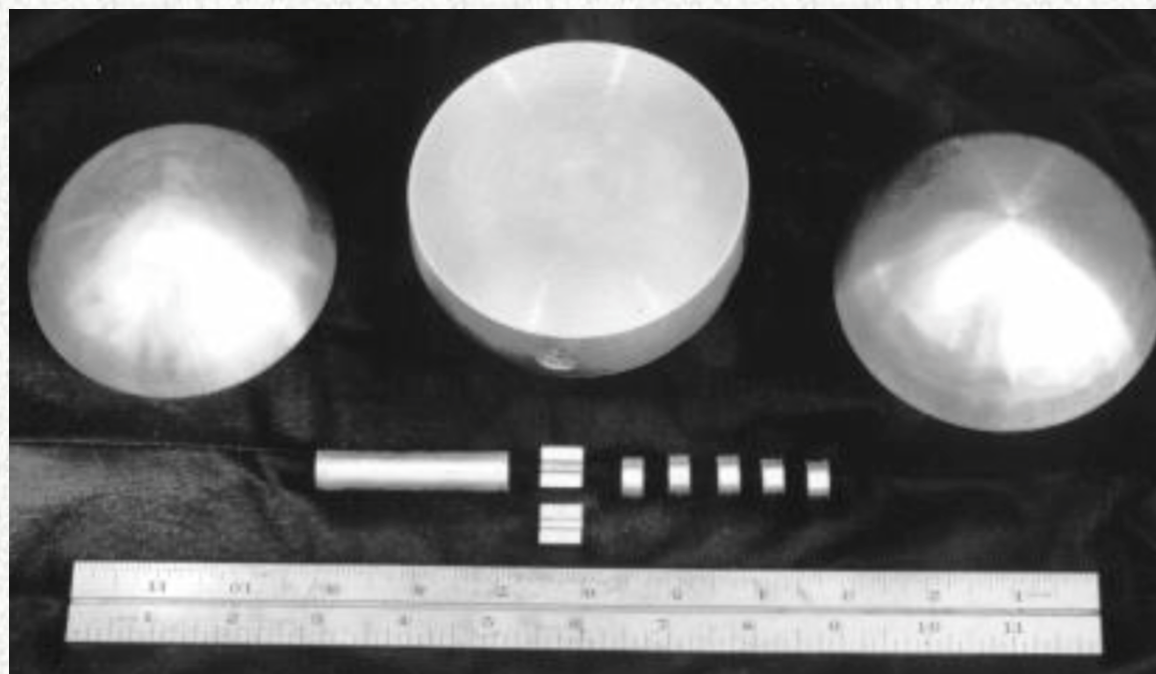


Critical Experiments (4)

pu-met-fast-044, THOR

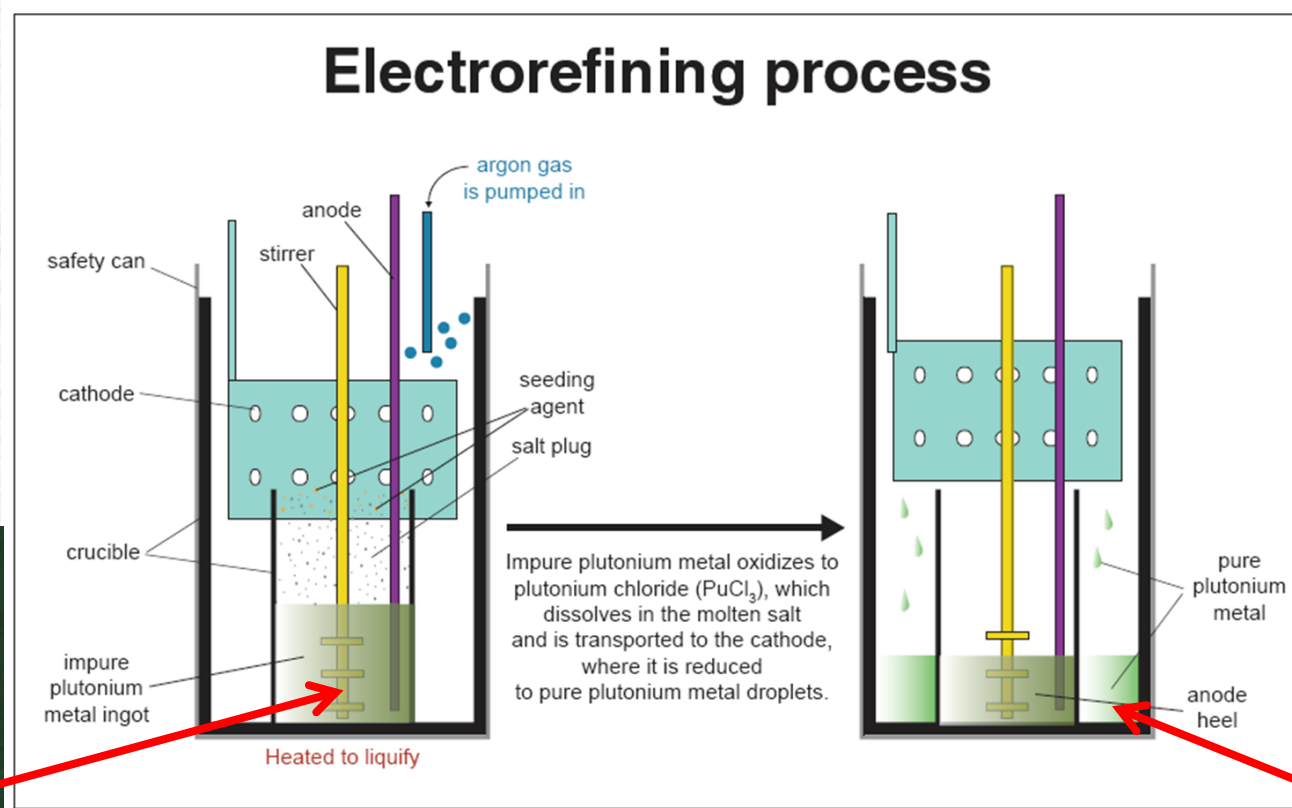


THOR components

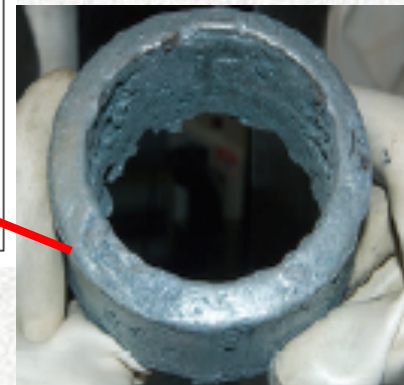


Pyrochemical Processing

- **Electrorefining is a batch plutonium metal purification process**
 - **Feed:** impure Pu metal ingot, up to 4500 g Pu
 - **Product:** highly purified Pu ring
 - **Waste:** salt, anode heel, crucible



Actinide Research Quarterly 3rd Quarter 2008



Nuclear Criticality Safety - Importance

- **Criticality Safety Evaluations**

- Must be performed before any operations or experiments involving fissile material
- CSEs must consider normal and all credible abnormal conditions
- Must conservatively account for:
Uncertainties & approximations in:
geometry, materials, isotopics, cross-sections, computer codes, etc.

- **CSEs must be performed for**

- Critical experiments performed at NCERC in Nevada
- Production operations at LANL Plutonium Facility (PF4)
 - Purification, glove box operations, machining, etc., etc.
- Production operations at Y-12, other DOE sites, fuel manufacturing facilities, enrichment plants, waste processing, etc.

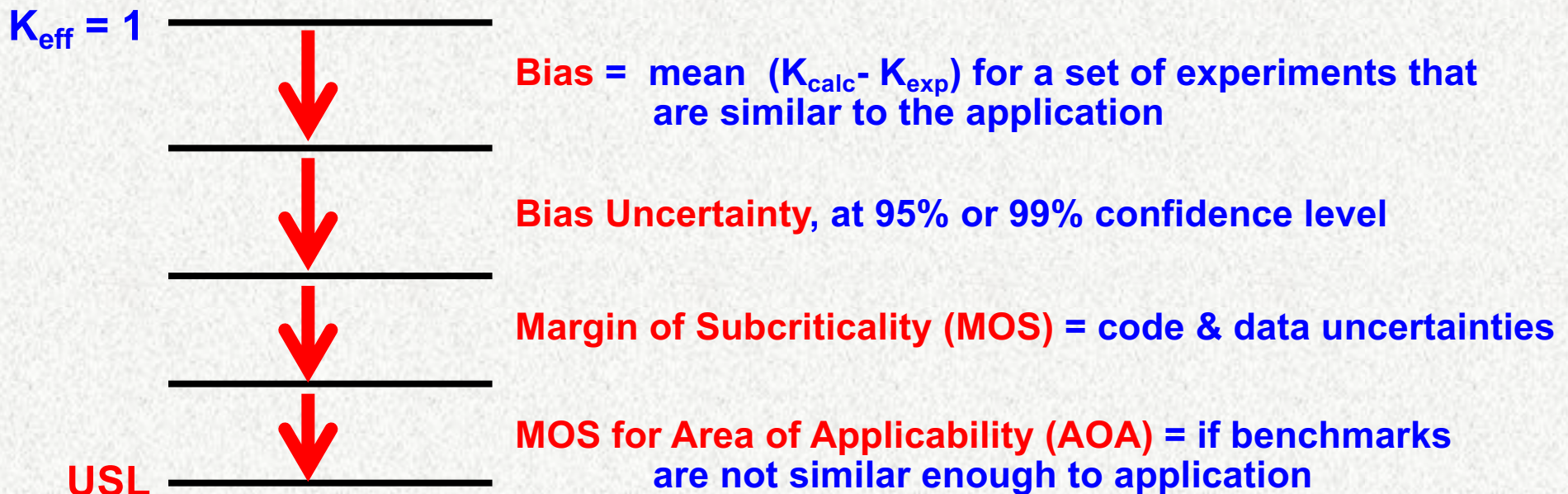
- **International Criticality Safety Benchmark Evaluation Project**

- The ICSBEP Handbook has peer-reviewed documentation for over 4,000 previous criticality safety experiments

Upper Subcritical Limits & Traditional Validation

Upper Subcritical Limit (USL)

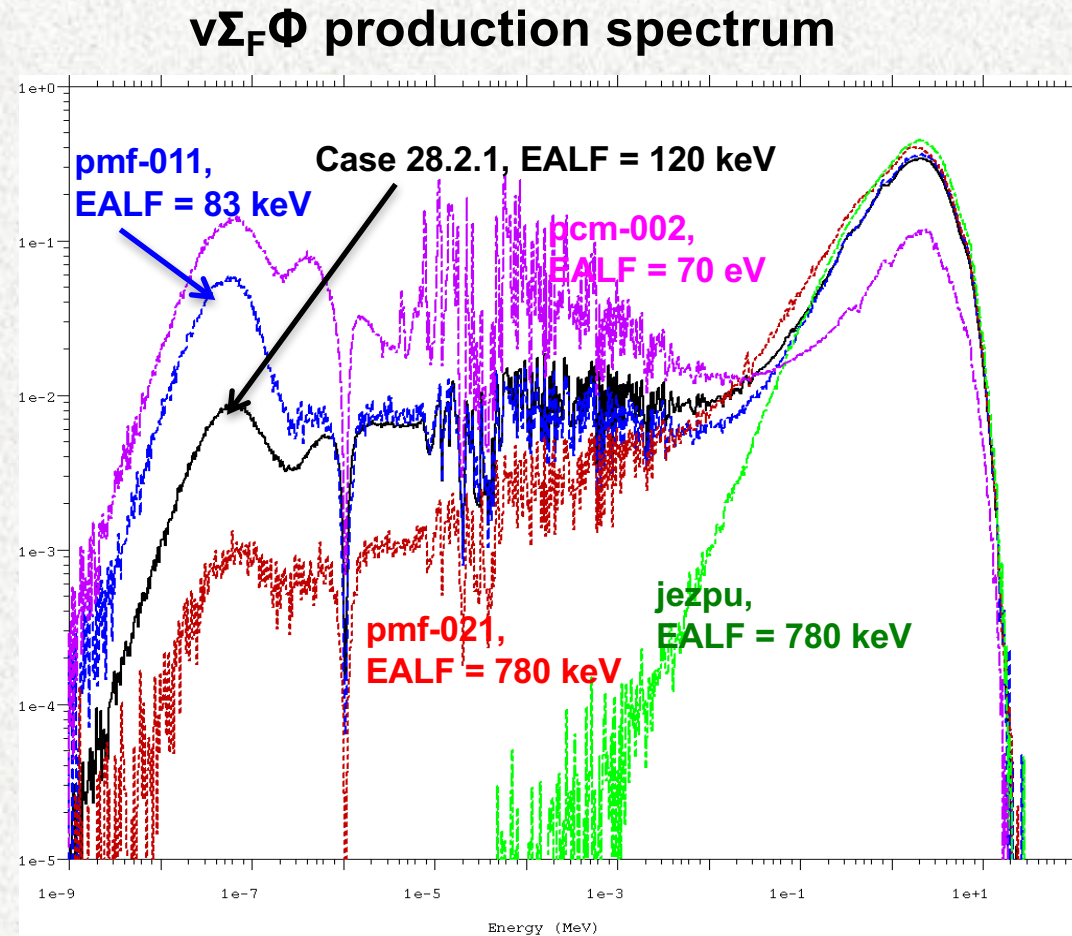
- **For an application:**
 - A calculated $K_{\text{eff}} < 1.0$ is NOT sufficient to ensure subcriticality
 - **Must conservatively account for**
 - Bias & uncertainties in the calculational method
 - Uncertainties in the physical model (eg, mass, isotopics, geometry, ...)



Must have: $K_{\text{calc}} + 2\sigma_{\text{calc}} < \text{USL}$

Selection of Benchmarks for Determining USL

- Nuclear Criticality Safety requires validation of computational methods
- Validation involves comparing calculation vs experiment for many benchmarks similar to the application of interest
- Neutron spectra are complex functions of geometry, materials, nuclear cross-sections, ...
- Simple metrics cannot capture the complexity of a fissile system
- **The figure shows neutron production spectra for 5 Pu systems:**
 - An application (Case 28)
 - 4 benchmarks for Pu systems
- **Which of the benchmarks are similar to the application?**
- In traditional NCS validation, the choice of benchmarks that were similar to an application was determined by **expert judgment**



Advances in NCS Validation

- During the past 20 years, a powerful set of tools has been developed based on sensitivity-uncertainty methods
 - From ORNL, the Scale system includes Keno, Tsunami, Tsurfer, & other tools
 - From LANL, the MCNP6 & Whisper tools are now available
 - Other tools have been developed by groups in England, France, Germany, Japan, S. Korea, China
- MCNP-WHISPER Methodology for NCS Validation
 - **MCNP** determines **sensitivity profiles** to characterize the neutronics of an application or benchmark, $S(\text{energy, reaction, isotope})$,
 $S = (dk/k) / (d\sigma/\sigma)$
 - **WHISPER** uses sensitivity profiles & data covariances to select similar benchmarks, determine bias, bias-uncertainty, & margin-of-subcriticality for setting the **Upper-Subcritical-Limit** (USL)

Comparison of Validation Approaches (Simplified)

	Traditional, Simple	Traditional, Enhanced	Sensitivity-Uncertainty Based
Benchmark Collection	Expert judgment 1 set to cover all applications	Expert judgment , Several subsets (metal, solutions, other)	Large collection with sensitivity profile data, Reject outliers, Estimate missing uncertainties
Selecting Benchmarks		Expert judgment , Select subset based on geometry & materials	Automatically select benchmarks with sensitivity profiles closest to application
Calculational Margin	Determine bias & bias uncertainty	Determine bias & bias uncertainty Possible trending within subset	Determine bias & bias uncertainty Automatically use weighting based on application-specific Ck values
Margin of Subcriticality	Expert judgment , Very large	Expert judgment , Large	Automatically determine margin for data uncertainty by GLLS, Code-expert judgment for code Expert judgment for additional MOS
Comment	Easy to use Highly dependent on expert judgment Requires large conservative MOS	More work if trending Very dependent on expert judgment Subsets & trending may permit smaller MOS	Computer-intensive, quantitative Less reliance on expert judgment Calculated estimate for most of MOS

Sensitivity-Uncertainty Based NCS Validation

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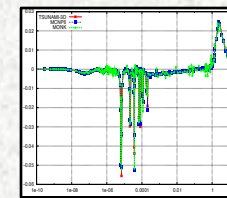
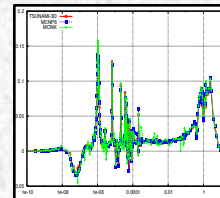
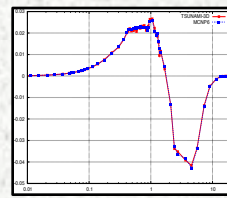
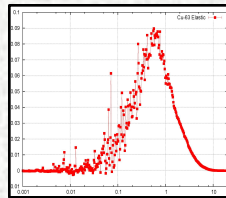
Overview

MCNP-Whisper Methodology for NCS Validation (1)

- The **sensitivity coefficient** is the ratio of relative change in k-effective to relative change in a system parameter:

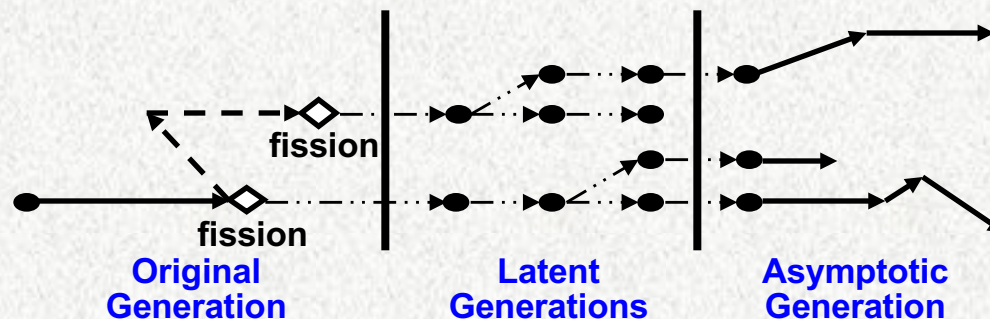
$$S_{k,x} = \frac{dk/k}{dx/x} = - \frac{\langle \psi^\dagger, (\Sigma_x - S_x - k^{-1}F_x) \psi \rangle}{\langle \psi^\dagger, k^{-1}F \psi \rangle}$$

- $S_{k,x}(E)$ is the **sensitivity profile**, that includes all isotopes, reactions, & energies for a system:

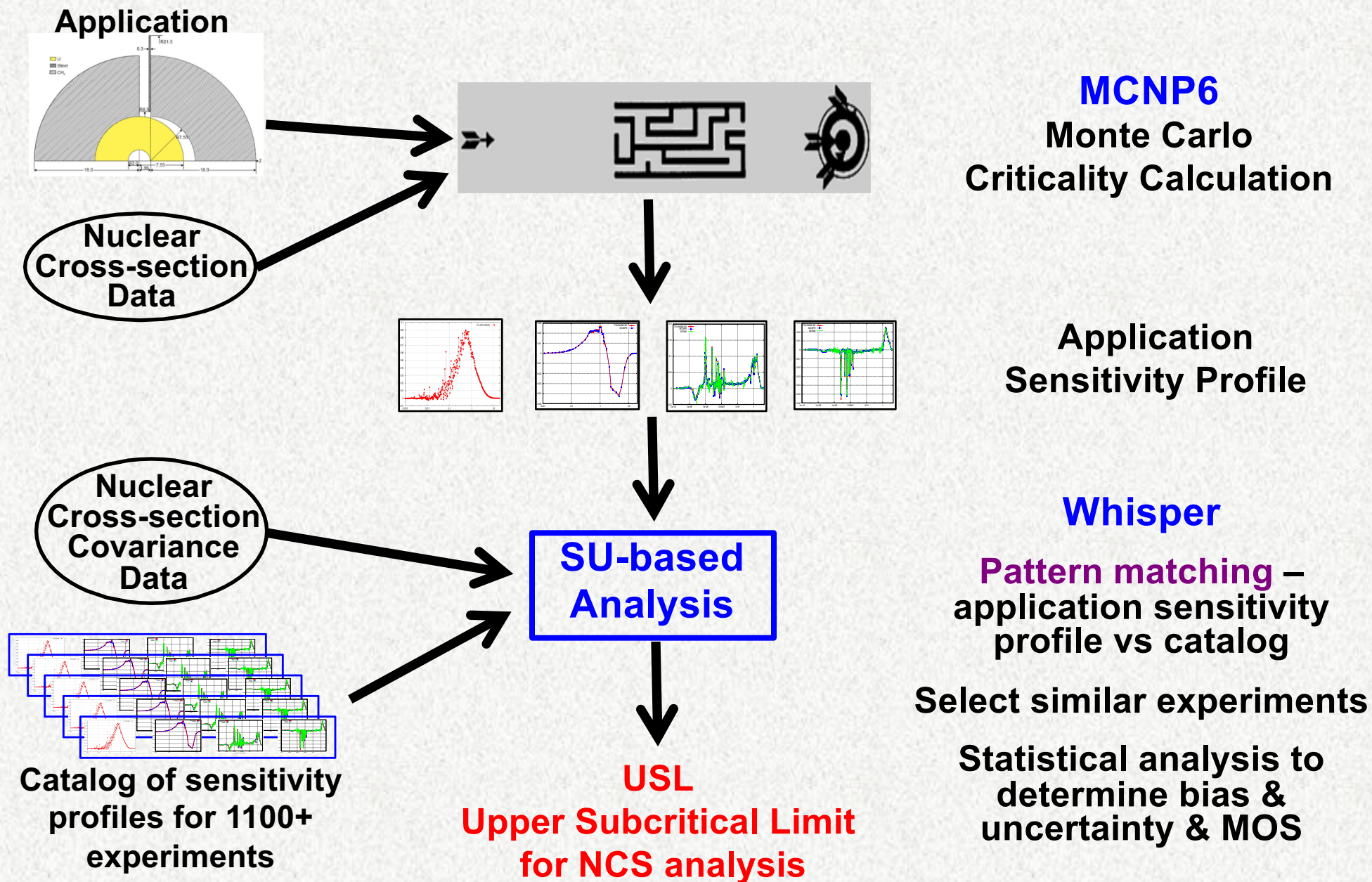


etc.

- MCNP6 & Scale/Tsunami Monte Carlo** can use the Iterated Fission Probability method to compute adjoint-weighted integrals for the sensitivity profiles
 - Tally scores are collected in original generation, adjoint-weighting is based on the progeny in the asymptotic generation



MCNP-Whisper Methodology for NCS Validation (2)



Sensitivity-Uncertainty Based NCS Validation

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Details:

Sensitivity Profiles

Nuclear Data Covariances

Correlation Coefficients

Sensitivity Profiles

- The sensitivity coefficient is defined as the ratio of relative change in k-effective to relative change in a system parameter:

$$S_{k,x} = \frac{dk / k}{dx / x}$$

- This may be expressed using perturbation theory:

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

- Includes both the forward & adjoint neutron fluxes.
- S = scatter operator, F = fission operator in integral transport eq
- x subscript implies that the perturbation is just for data x
- $S_{k,x}(E)$ is the sensitivity profile, a function of neutron energy

Sensitivity Profiles – Adjoint Weighting

- The adjoint transport equation:

$$\begin{aligned} -\mathbf{\Omega} \cdot \nabla \psi^\dagger(\mathbf{r}, \mathbf{\Omega}, E) + \Sigma_t \psi^\dagger(\mathbf{r}, \mathbf{\Omega}, E) = \\ \iint dE' d\mathbf{\Omega}' \Sigma_s(\mathbf{r}, \mathbf{\Omega}' \cdot \mathbf{\Omega}, E \rightarrow E') \psi^\dagger(\mathbf{r}, \mathbf{\Omega}', E') \\ + \frac{1}{k_{\text{eff}}} \iint dE' d\mathbf{\Omega}' \chi(E \rightarrow E') \nu \Sigma_f(\mathbf{r}, E) \psi^\dagger(\mathbf{r}, \mathbf{\Omega}', E') \end{aligned}$$

- Adjoint fundamental mode has physical meaning:

The importance at a location in phase space is proportional to the expected value of a measurement, caused by a neutron introduced into a critical system at that location, after infinitely many fission generations.

- Using the **Iterated Fission Probability** method, MCNP6 can compute adjoint-weighted integrals of any quantity.

Example – Need for Adjoint-Weighting

- MCNP can compute lifetimes (prompt removal times) with non-importance weighted tallies:

unweighted

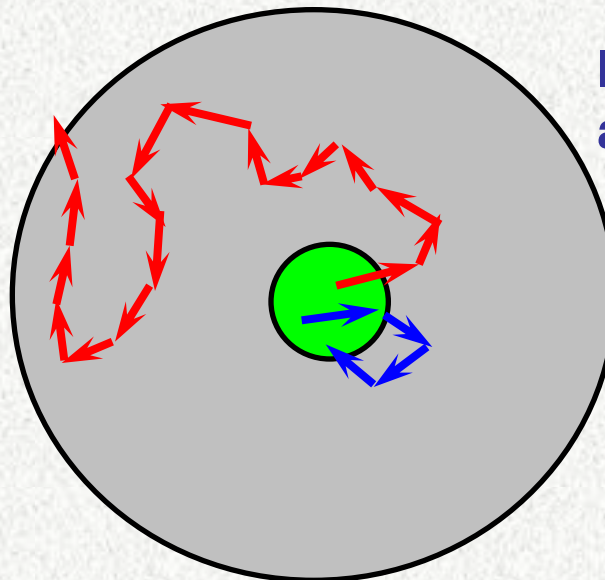
$$\Lambda_{rem} = \frac{\langle 1, 1/v \psi \rangle}{\langle 1, F\psi \rangle}$$

adjoint-weighted

$$\Lambda_{eff} = \frac{\langle \psi^\dagger, 1/v \psi \rangle}{\langle \psi^\dagger, F\psi \rangle}$$

- Example: Importance weighting is necessary in systems with thick reflectors. Unweighted lifetimes are often very much larger than effective lifetimes (adjoint-weighted)

Neutrons in the reflector unlikely to cause fission, not very important

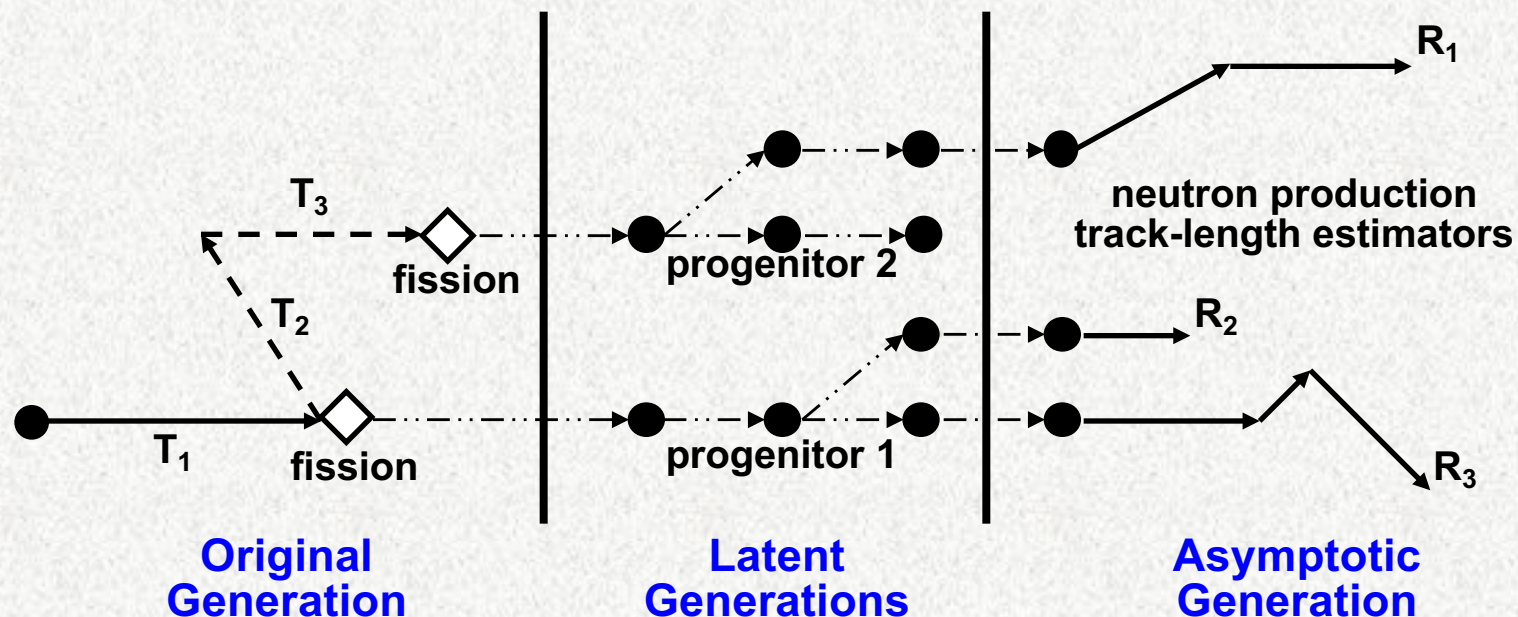


Important neutrons are often short-lived

Net Effect: Not weighting by importance overvalues long-lived neutrons, leading to lifetimes much too long.

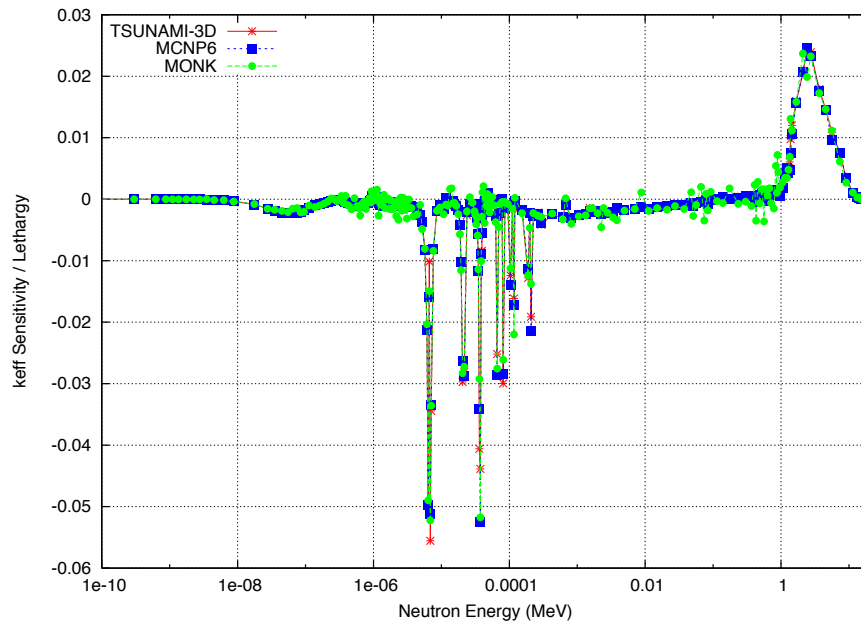
Sensitivity Profiles – Adjoint Weighting

- MCNP breaks active cycles into consecutive blocks:
 - Tally **scores** are collected in **original generation**, & progenitor neutrons tagged
 - All subsequent progeny within the **latent generations** remember their progenitor
 - **Importance** is the population of progeny from each progenitor in the **asymptotic generation**
 - **(Score)*(importance)** is tallied for adjoint-weighted results

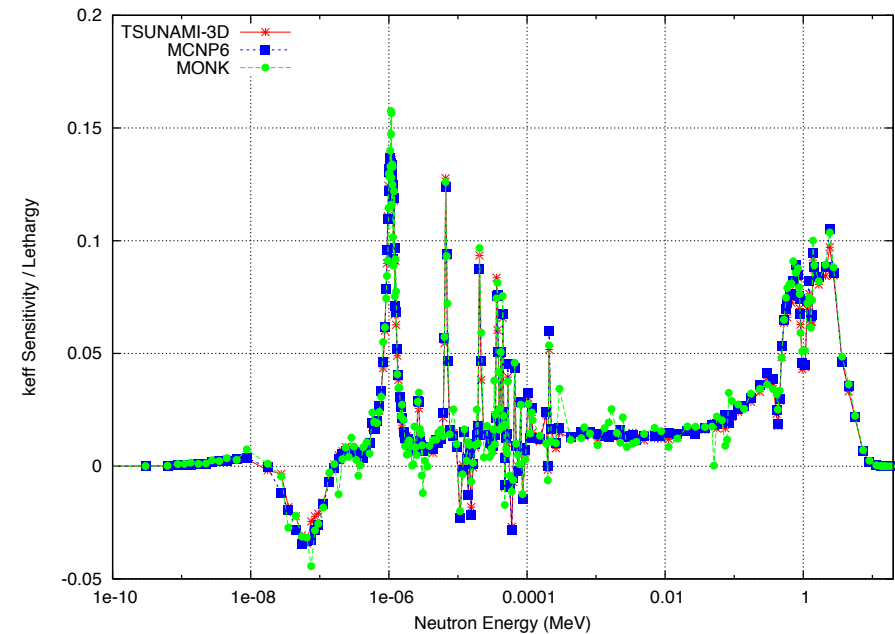


Sensitivity Profiles - Examples

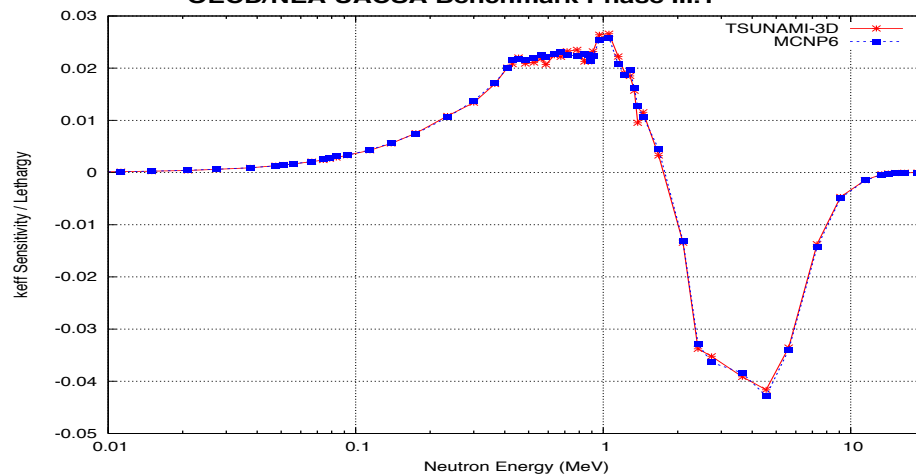
U-238: total cross-section sensitivity
OECD/NEA UACSA Benchmark Phase III.1



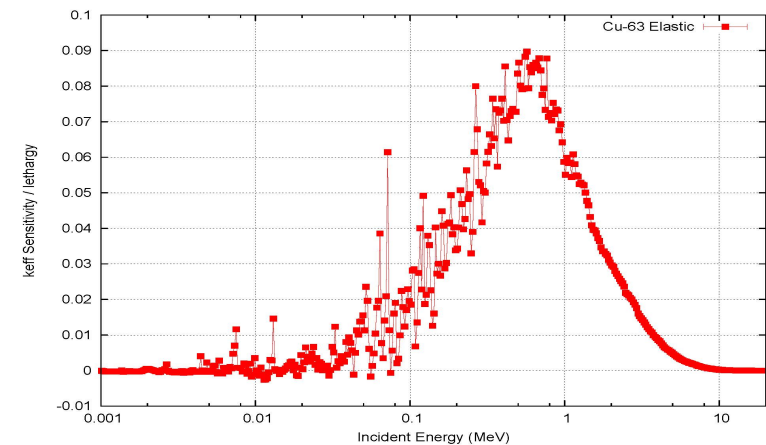
H-1: elastic scattering cross-section sensitivity
OECD/NEA UACSA Benchmark Phase III.1



Pu-239: fission $\chi(E)$ sensitivity
OECD/NEA UACSA Benchmark Phase III.1



Cu-63: Elastic Scattering Sensitivity
Copper-Reflected Zeus experiment:

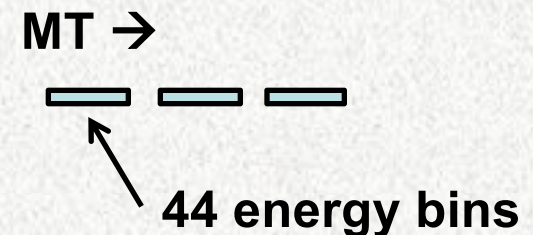


Sensitivity Profiles - Vectors

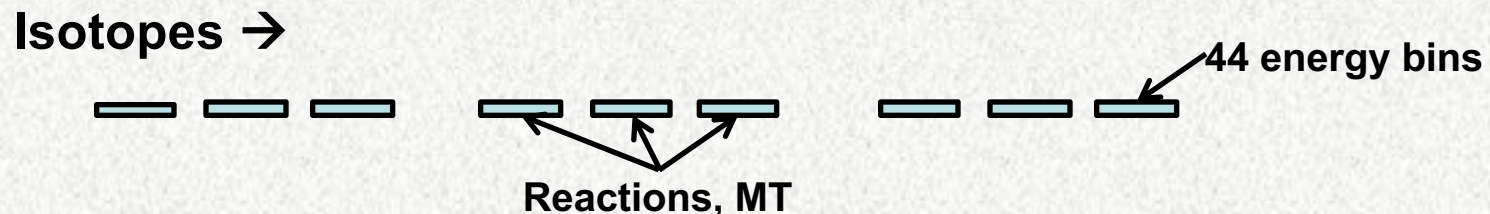
- For each **isotope**, the sensitivity coefficients for a specific problem are stored consistent with the layout of the covariance data
 - Recall that the sensitivity of K_{eff} to a particular reaction type & energy bin is:

$$S_{k,x} = \frac{\Delta k/k}{\Delta x/x} = \frac{x}{k} \frac{dk}{dx}$$

where x is the cross-section for a particular **isotope, reaction (MT), & energy bins**



- For a particular application **problem**, A , the sensitivity profiles for all isotopes are combined into one sensitivity vector S_A

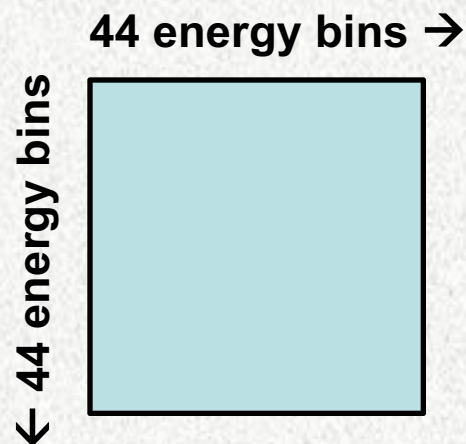


The sensitivity profile $S_A(E, MT, iso)$ completely characterizes the neutronics of an application

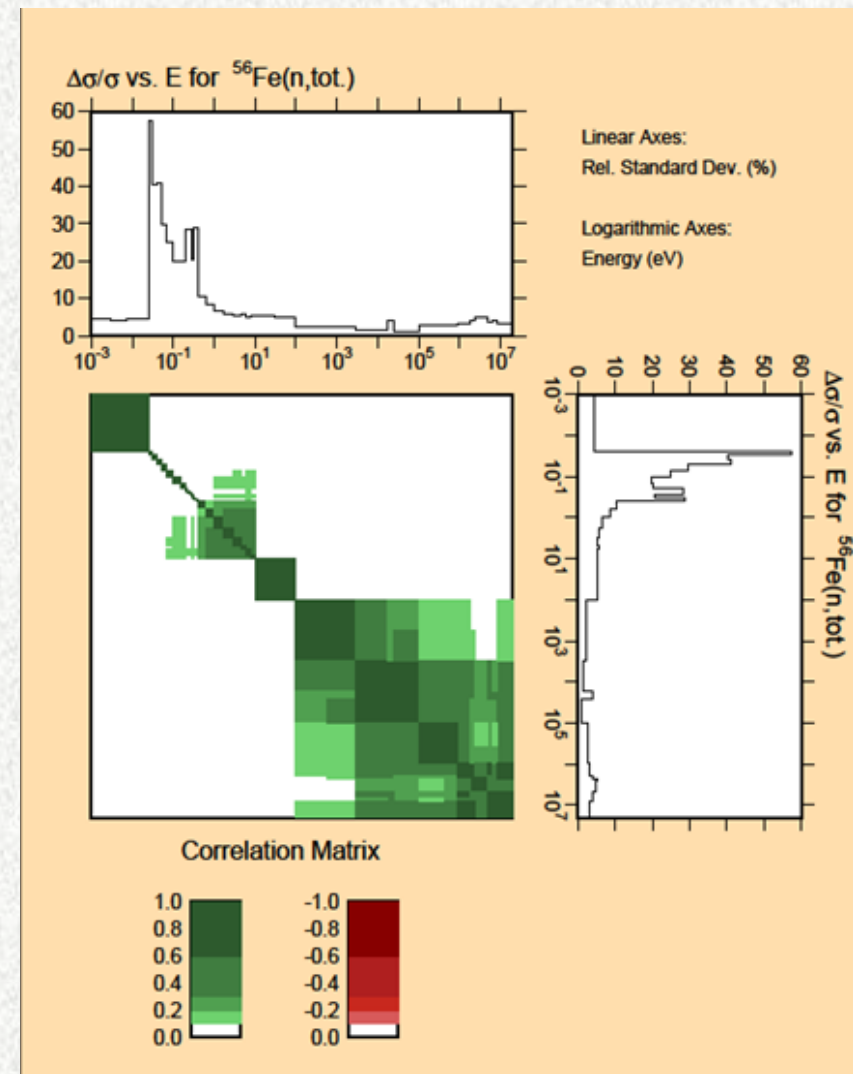
size of S_A = (44 E bins) x (12 reactions) x (number of isotopes)

Cross-section Covariance Data

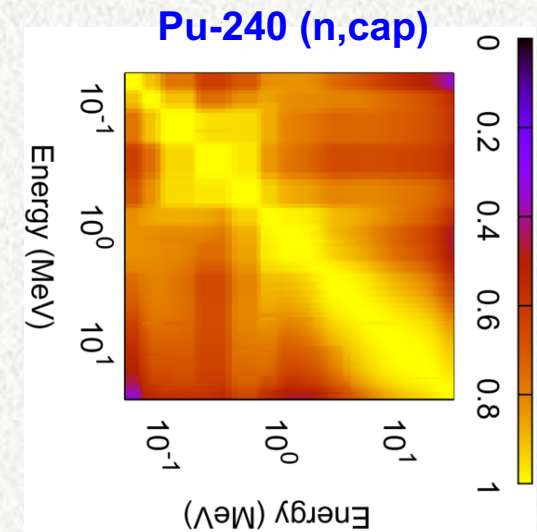
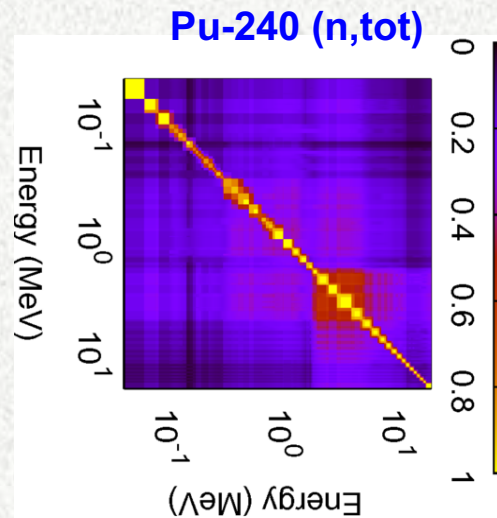
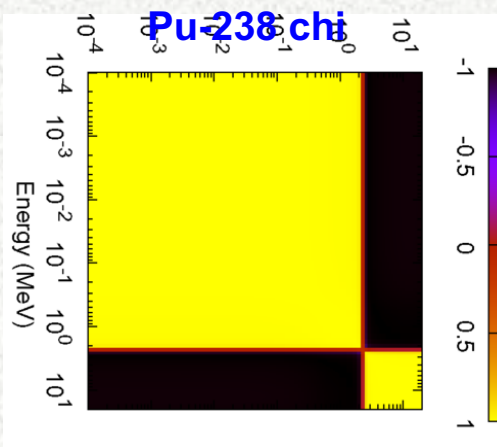
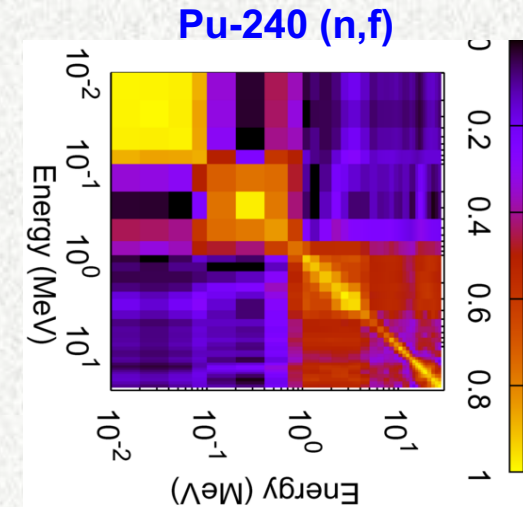
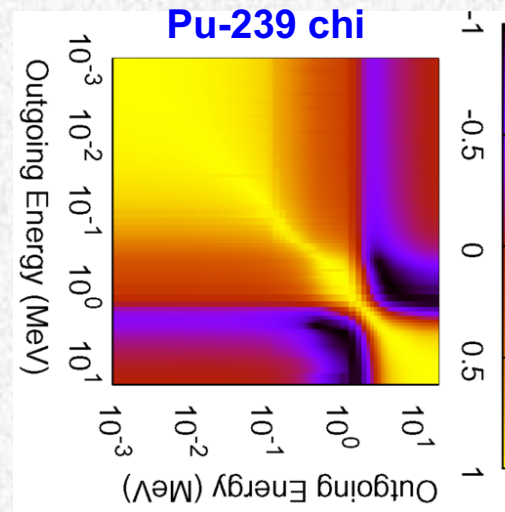
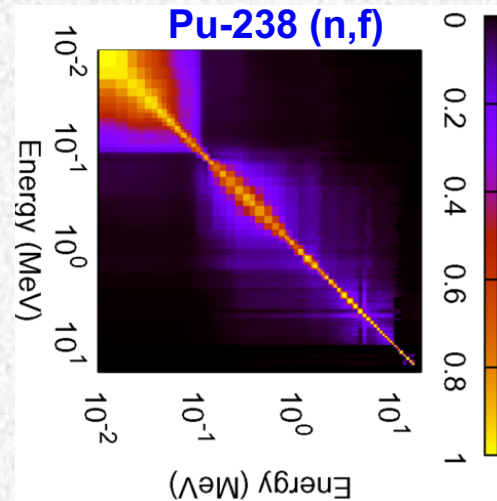
- For a particular isotope & particular reaction (MT), the nuclear data uncertainties are a $G \times G$ matrix, where G = number of energy groups = 44



- Each diagonal is the **variance** of the cross-section for a particular energy bin
- Off-diagonal elements are the **shared variance** between the data for pairs of energy bins



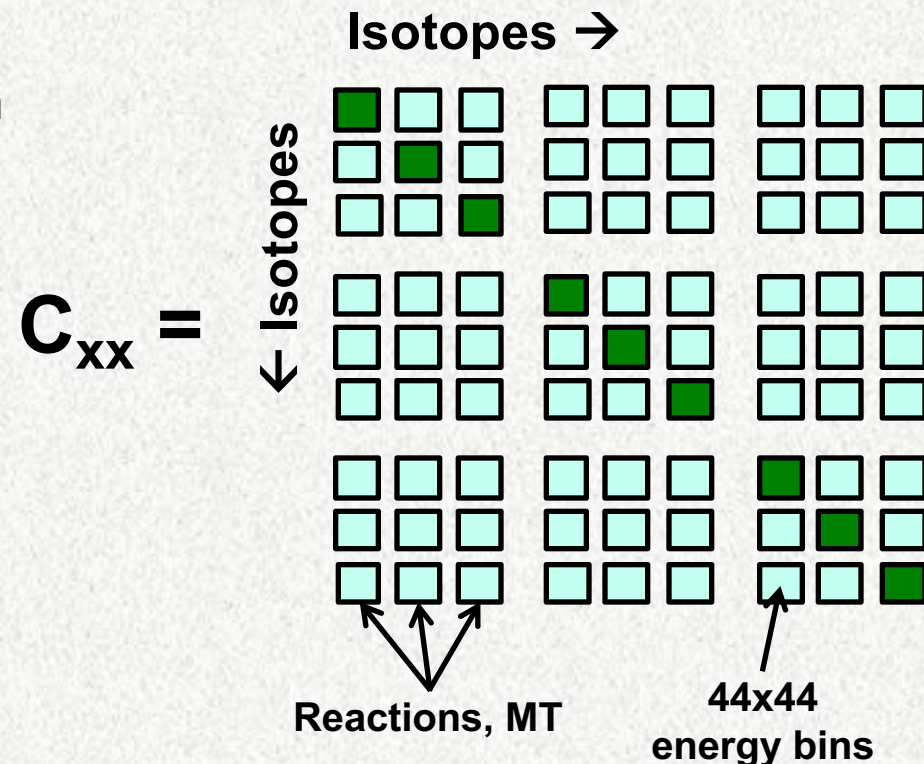
Cross-section Covariance Data



Cross-section Covariance Data

- The covariance matrices for all isotopes can be combined, including off-diagonal blocks that relate uncertainties in one iso-MT-E with a different iso-MT-E

- Each diagonal element of C_{xx} is the **variance** of the cross-section for a particular isotope, MT, & energy bin
- Off-diagonal elements of C_{xx} are the **shared variance** between pairs of Iso-MT-E & Iso'-MT'-E'
- Very sparse (lots of zeros), block-structured matrix
(Off-diagonal I-I' blocks would generally be zero)



$$\text{size of } C_{xx} = [(44 \text{ E bins}) \times (12 \text{ reactions}) \times (\text{number of isotopes})]^2 \sim (25k)^2$$

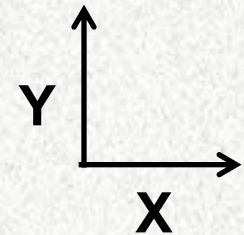
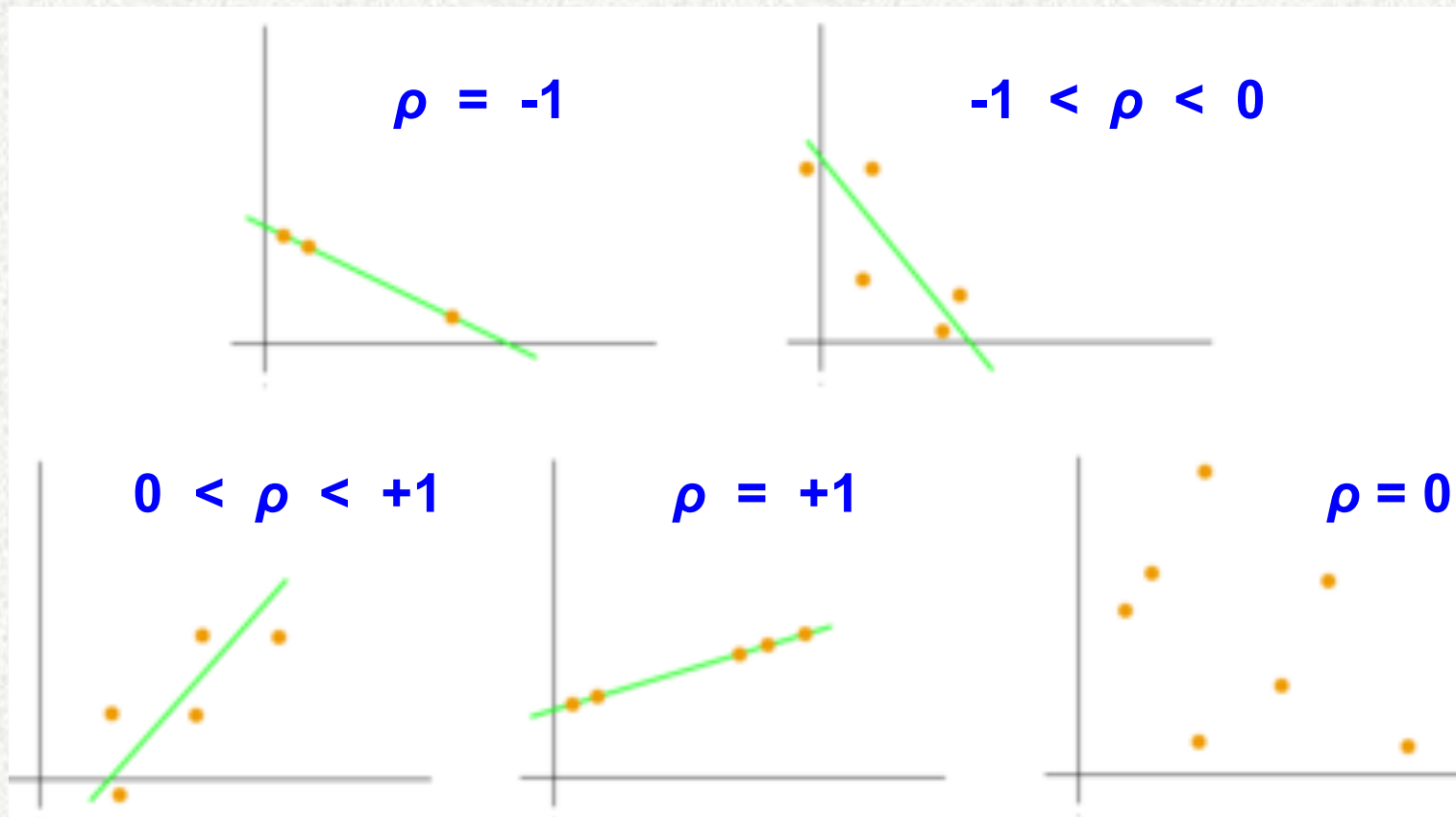
Correlation Coefficient

- Correlation coefficient

- Pearson product-moment correlation coefficient, r or ρ
- A measure of the linear correlation between variables X & Y

$\rho = +1$ total positive correlation

$\rho = -1$ total negative correlation



Variance in Keff & Correlation Between Problems

- Given: Application A, Sensitivity \mathbf{S}_A computed by MCNP
Benchmark B, Sensitivity \mathbf{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:

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

Sandwich Rule – Variance & Covariance

- Matrix-vector operations

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

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

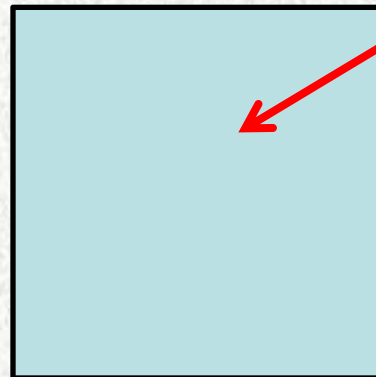
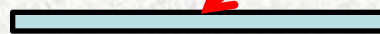
$$c_k(A, B) = \frac{Cov_k(A, B)}{\sqrt{Var_k(A)} \cdot \sqrt{Var_k(B)}}$$

Problem-dependent sensitivity vector, S .
Based on flux spectrum, adjoint spectrum, nuclear data, problem isotopes, geometry, temperature

Size = $G \times MT \times NI$

Nuclear Data Covariances

Size = $(G \times MT \times NI)^2$



= scalar

S^T

Sensitivity-Uncertainty Based NCS Validation

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MCNP-Whisper Methodology:
Selecting Benchmarks
Statistical Analysis
MOS Estimates

Whisper Methodology for Validation & USLs

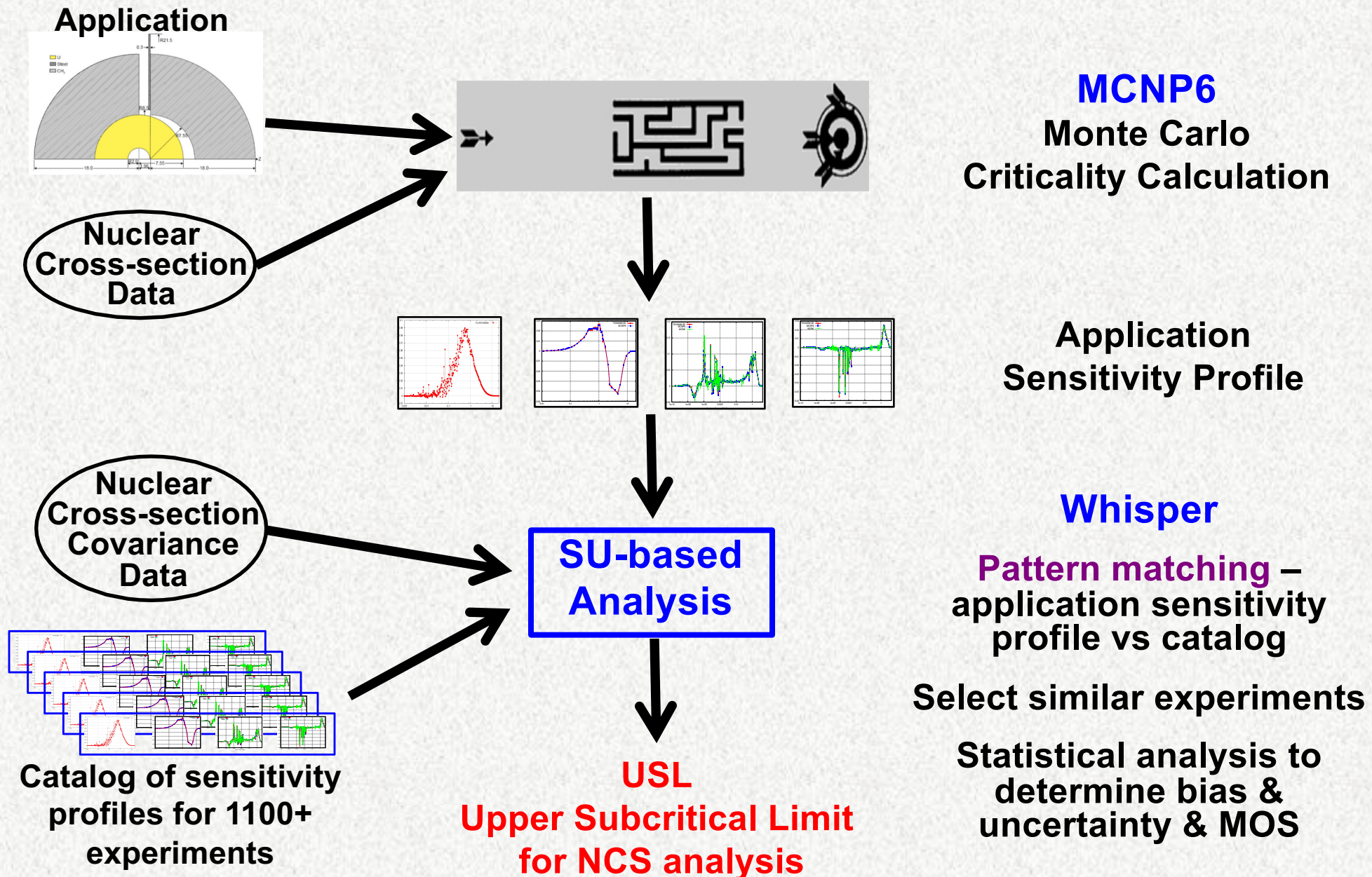
Whisper

- Statistical analysis code to determine baseline USLs
- Uses sensitivity profiles from continuous-energy MCNP6
- Uses covariance data for nuclear cross-sections

Sensitivity-Uncertainty NCS Validation Using MCNP6-Whisper

- ➊ Run MCNP6 for an Application, & get Application sensitivity profile, S_A
- ➋ Run Whisper:
 - ➊ Automated, physics-based selection of benchmarks that are neutronically similar to the application, ranked & weighted
 - Compute $C_k(i)$ for Application S_A vs. Benchmark sensitivities $S_{B(i)}$
 - Select most-similar benchmarks, based on highest $C_k(i)$ correlations
 - ➋ Bias + bias uncertainty from Extreme Value Theory
 - Statistical analysis – Extreme Value Theory, using Benchmarks selected
 - ➌ Margin for nuclear data uncertainty estimated by GLLS method
 - Use benchmark sensitivities & cross-section covariance data to estimate the MOS for nuclear data uncertainties

MCNP-Whisper Methodology for NCS Validation (2)



Upper Subcritical Limit

- To consider a simulated system subcritical, the computed keff must be less than the Upper Subcritical Limit (USL):

$$K_{\text{calc}} + 2\sigma_{K_{\text{calc}}} < \text{USL}$$

$$\text{USL} = 1 + (\text{Bias}) - (\text{Bias uncertainty}) - \text{MOS}$$

$$\text{MOS} = \text{MOS}_{\text{data}} + \text{MOS}_{\text{code}} + \text{MOS}_{\text{application}}$$

- The bias and bias uncertainty are at some confidence level, typically 95% or 99%.
 - These confidence intervals may be derived from a normal distribution, but the normality of the bias data must be justified.
 - Alternatively, the confidence intervals can be set using non-parametric methods.

Sensitivity-Uncertainty Based NCS Validation

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Examples:

Pu cylinder with water reflector

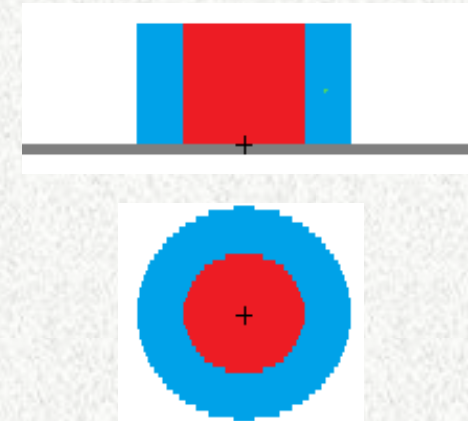
Pu sphere with thick Ta reflector

Examples

Pu cylinder with water reflector

- 4.5 kg Pu-239 right-circular cylinder
- Pu density = 19.86 g/cm^3
- Reflected radially with 1 inch of water
- Reflected on the bottom with $\frac{1}{4}$ inch steel
- Height-to-diameter (H/D) = 1.0

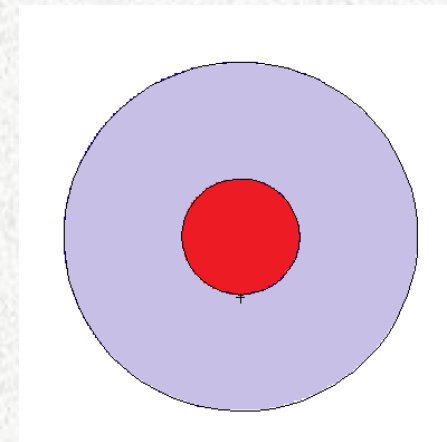
Note: Lots of benchmarks similar to this



Pu sphere with thick Ta reflector

- 4.5 kg Pu-239 sphere
- Pu density = 19.8 g/cm^3
- Reflected radially with Ta
- Ta-reflector thickness = 30. cm

Note: No benchmarks similar to this



Example: Pu cylinder, H/D=1, water reflector

Calculating application nuclear data uncertainties ...

application	adjusted	prior
pu-hd-1.0	0.00075	0.01385

Calculating upper subcritical limits ...

application	calc margin	data unc (1-sigma)	baseline USL	k(calc) > USL
pu-hd-1.0	0.01443	0.00075	0.97863	-0.14353

Benchmark population = 43
Population weight = 25.30973
Maximum similarity = 0.99691

Bias = 0.00850
Bias uncertainty = 0.00593
Nuc Data uncert margin = 0.00075
Software/method margin = 0.00500
Non-coverage penalty = 0.00000

For this application, 43 of the 1101 benchmarks were selected as neutronically similar & sufficient for valid statistical analysis

Benchmark rankings shown below

benchmark	ck	weight
pu-met-fast-036-001.i	0.9969	1.0000
pu-met-fast-024-001.i	0.9966	0.9916
pu-met-fast-022-001.i	0.9948	0.9386
pu-met-fast-023-001.i	0.9931	0.8887
pu-met-fast-044-005.i	0.9931	0.8870
.		
mix-met-fast-007-022.i	0.9724	0.2824
mix-met-fast-007-023.i	0.9693	0.1915
pu-met-fast-045-005.i	0.9670	0.1240
pu-met-fast-003-103.i	0.9662	0.1021
mix-met-fast-001-001.i	0.9650	0.0664

Excellent c_k 's
In range .96 - .99

Traditional validation
gave USL = 0.970

Example: Pu sphere with Thick Ta Reflector

Calculating application nuclear data uncertainties ...

application	adjusted	prior
pu-ta-30	0.01387	0.03005

application	margin	(1-sigma)	USL	> USL
pu-ta-30	0.01679	0.01387	0.94215	0.02222

Benchmark population = 114
Population weight = 59.05861
Maximum similarity = 0.65942

Bias = 0.00903
Bias uncertainty = 0.00776
Nuc Data uncert margin = 0.01387
Software/method margin = 0.00500
Non-coverage penalty = 0.00000

For this application, 114 of the 1101 benchmarks were selected as neutronically similar & sufficient for valid statistical analysis

Benchmark rankings shown below

benchmark	ck	weight
pu-met-fast-045-006.i	0.6594	1.0000
pu-met-fast-045-004.i	0.6590	0.9991
pu-met-fast-045-003.i	0.6562	0.9939
pu-met-fast-045-002.i	0.6496	0.9813
pu-met-fast-045-007.i	0.6452	0.9728
pu-met-fast-045-001.i	0.6412	0.9652
pu-met-fast-045-005.i	0.5667	0.8225
pu-met-fast-023-001.i	0.4420	0.5836
.		
pu-comp-mixed-002-008.i	0.1824	0.0863
pu-comp-mixed-002-009.i	0.1778	0.0775
pu-comp-inter-001-001.i	0.1375	0.0003

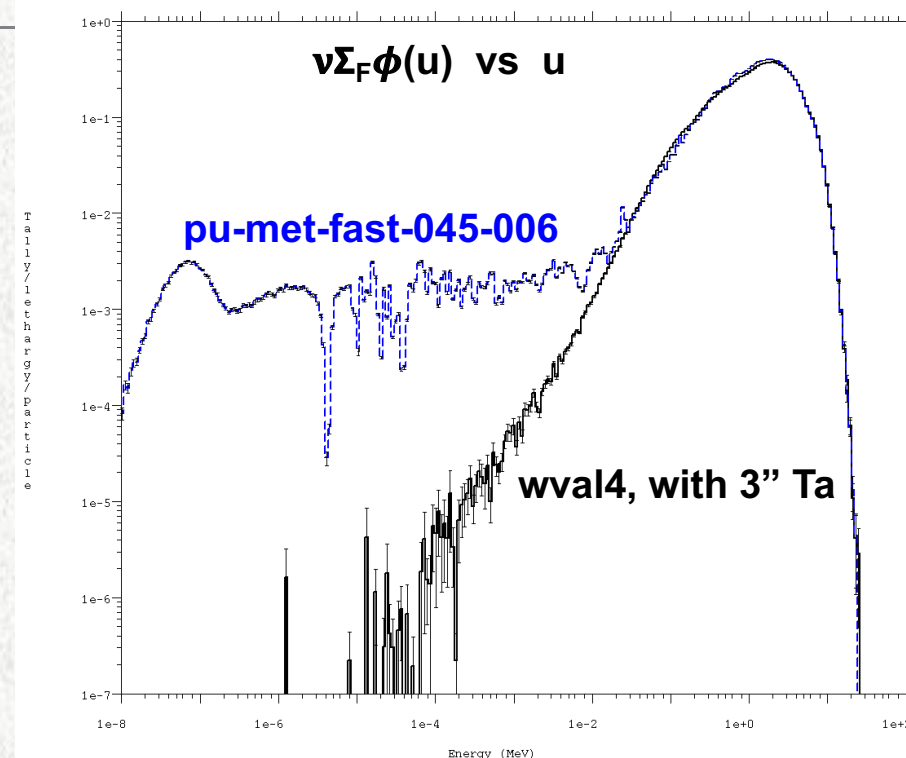
Very poor c_k 's,
Max is only 0.65

Traditional validation
gave USL = 0.970

Pu with Thick Ta Reflector - Comments

- None of the benchmarks appear to have the same neutronics as the application
 - Largest C_k in the Whisper example output is 0.659 – very low
 - Guidance for maximum C_k :

$0.95 < C_k$	→ great
$0.90 < C_k < 0.95$	→ good
$0.80 < C_k < 0.90$	→ fair
$C_k < 0.80$	→ questionable
- If all C_k 's are low, there is a need to expand the benchmark suite, add similar benchmarks
- If no similar benchmarks, need extra analysis, analyst judgment, & extra margin



- The current benchmark suite for Whisper was focused on main needs for LANL validation
- Few benchmarks with Ta, none with thick Ta reflectors
- Need to find more benchmarks with Ta reflector & add to Whisper suite, if Ta-reflected applications are expected

Sensitivity-Uncertainty Based NCS Validation

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Conclusions

Conclusions & Discussion (1)

Whisper? Who cares?

- **Sensitivity/Uncertainty methods for validation have been under development for > 18 yrs at ORNL (Broadhead, Rearden, Perfetti, ...)**
- **Kiedrowski & Brown developed MCNP iterated fission probability, adjoint weighted tallies, & S/U capabilities, 2008-2013. Whisper in 2014.**
- **There are now 2 US calculational paths for S/U based validation:**
 - **SCALE/Tsunami**
 - **MCNP/Whisper**
- **International effort for comparisons being planned**
 - **LANL, ORNL, IRSN**
- **S/U based validation methods can supplement, support, & extend traditional validation methods**

Conclusions & Discussion (2)

- **Traditional validation methods are 40+ years old; S-U methods are new. Should not argue for exclusive use of either**
- **Traditional & S-U methods complement each other, & provide greater assurance for setting USLs**
 - **Traditional methods provide a check on S-U methods**
 - **S-U approach to automated benchmark selection is quantitative, physics-based, & repeatable. Provides a check on traditional.**
 - **Traditional methods use MOS of 2-5%. Quantitative, physics-based, repeatable MOS from S-U usually smaller**
- **The next 5 years or so should be a transition period, where both traditional & S-U methods should be used**
- **In today's environment of audits, reviews, & "justify everything", it is prudent to use both traditional & S-U methods for validation**

Questions ?