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Title: Lecture Notes on Criticality Safety Validation Using MCNP & Whisper

Author(s): Brown, Forrest B.
Rising, Michael Evan
Alwin, Jennifer Louise

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Lecture Notes on Criticality Safety Validation Using MCNP & Whisper

Forrest Brown, Michael Rising, Jennifer Alwin

Monte Carlo Codes Group, XCP-3
Los Alamos National Laboratory
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Contents

Lecture Notes on Criticality Safety Validation Using MCNP & Whisper

Whisper – Summary

Whisper - Software for Sensitivity-Uncertainty-Based Nuclear Criticality Safety Validation

Whisper is computational software designed to assist the nuclear criticality safety (NCS) analyst with validation studies with the Monte Carlo radiation transport package MCNP. Standard approaches to validation rely on the selection of benchmarks based upon expert judgment. Whisper uses sensitivity/uncertainty (S/U) methods to select relevant benchmarks to a particular application or area of applicability (AOA), or set of applications being analyzed. Using these benchmarks, Whisper computes a calculational margin from an extreme value distribution. In NCS, a margin of subcriticality (MOS) that accounts for unknowns about the analysis. Typically, this MOS is some prescribed number by institutional requirements and/or derived from expert judgment, encompassing many aspects of criticality safety. Whisper will attempt to quantify the margin from two sources of potential unknowns, errors in the software and uncertainties in nuclear data. The Whisper-derived calculational margin and MOS may be used to set a baseline upper subcritical limit (USL) for a particular AOA, and additional margin may be applied by the NCS analyst as appropriate to ensure subcriticality for a specific application in the AOA.

Whisper provides a benchmark library containing over 1,100 MCNP input files spanning a large set of fissionable isotopes, forms (metal, oxide, solution), geometries, spectral characteristics, etc. Along with the benchmark library are scripts that may be used to add new benchmarks to the set; this documentation provides instructions for doing so. If the user desires, Whisper may analyze benchmarks using a generalized linear least squares (GLLS) fitting based on nuclear data covariances and identify those of lower quality. These may, at the discretion of the NCS analyst and their institution, be excluded from the validation to prevent contamination of potentially low quality data. Whisper provides a set of recommended benchmarks to be optionally excluded.

Whisper also provides two sets of 44-group covariance data. The first set is the same data that is distributed with SCALE 6.1 in a format that Whisper can parse. The second set is an adjusted nuclear data library based upon a GLLS fitting of the benchmarks following rejection. Whisper uses the latter to quantify the effect of nuclear data uncertainties within the MOS. Whisper also has the option to perform a nuclear covariance data adjustment to produce a custom adjusted covariance library for a different set of benchmarks.

Background: These lecture notes were prepared during 2015-2016 for educational & technical interchanges between the Monte Carlo Codes Group (XCP-3) and Criticality Safety Analysts in the Nuclear Criticality Division at LANL.

Acknowledgements: Thanks to the XCP & NCS Division Leaders for promoting and supporting the XCP3-NCS interchange sessions. Thanks to the DOE Nuclear Criticality Safety Program for its long-term support for developing advanced MCNP6 capabilities, including the iterated fission probability, adjoint-weighted tallies, sensitivity/uncertainty features, and Whisper statistical analysis. Thanks to the LANL PF4-Restart program for supporting some of the LANL-specific portions of this work, including direct support for assisting the NCS criticality safety analysts.

Whisper Validation - Comments

Whisper? Who cares?

- Sensitivity/Uncertainty methods for validation have been under development for > 18 years 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 calculational paths for S/U based validation:
  - SCALE/Tsunami/Tsurfer ORNL
  - MCNP/Whisper LANL
- International effort for comparisons being planned
  - LANL, ORNL, IRSN
- S/U based validation methods can supplement, support, & extend traditional validation methods, provide greater assurance for setting USLs

- The next 5 years or so should be a transition period, where both traditional & S/U methods should be used
  - 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 selection
  - Traditional methods use $MOS_{data+code}$ of 2-5%.
    Quantitative, physics-based, repeatable $MOS_{data+code}$ from S/U usually smaller

Validation

Background

Some facts:

- **Computer codes have approximations & errors**
- **Nuclear data have approximations & errors**

How can we ever design anything?

- **Verify that codes work as intended**
- **Validate codes + data + methods against nature (experiments)**
- **Reactor design:**
  - Calibrate codes & methods to nominal, but do 1000s or over/under calculations
- **Criticality safety:**
  - Focus on avoiding worst-case combination of mistakes, uncertainties, errors, ...
  - Rigor & conservatism always; never wishful thinking or "close enough"

DOE & ANS Standards for Criticality Safety

- 10 CFR 830 Subpart A, Quality Assurance
- 10 CFR 830 Subpart B, Nuclear Safety Management

- DOE O 414.1C, Quality Assurance
- DOE G 414.1-4, Safety Software Guide for use with 10 CFR 830 Subpart A, Quality Assurance Requirements
- DOE G 421.1-2, Implementation Guide for Use in Developing Documented Safety Analyses to Meet Subpart B of 10 CFR 830
- DOE O 420.1C, Facility Safety

- DOE-STD-3007-2007, Guidelines for Preparing Criticality Safety Evaluations at DOE Nonreactor Nuclear Facilities
- DOE STD 1134-99 Review Guide for Criticality Safety Evaluations
- DOE-STD-1158-2010, Self-Assessment Standard for DOE Contractor Criticality Safety Programs
- DOE-STD-3009-94, Change Notice 3, Preparation Guide for U.S. Department of Energy Nonreactor Nuclear Facility Safety Analysis
- DOE-STD-1186-2004, Specific Administrative Controls
- DOE-STD-1027-92, Change Notice 1, Hazard Categorization and Accident Analysis Techniques for Compliance with DOE Order 5480.23, Nuclear Safety Analysis Reports

- **ANSI/ANS-8.1-2014, Nuclear Criticality Safety in Operations with Fissionable Materials Outside Reactors**
- ANSI/ANS-8.3-2003, Criticality Accident Alarm System
- ANSI/ANS-8.5-1996(R2007), Use of Borosilcate-Glass Raschig Rings as a Neutron Absorber in Solutions of Fissile Material
- ANSI/ANS 8.7-1998(R2012), Nuclear Criticality Safety in the Storage of Fissile Materials
- ANSI/ANS-8.10-2005, Criteria for Nuclear Criticality Safety Controls in Operations with Shielding and Confinement
- ANSI/ANS 8.14-2004, Use of Soluble Neutron Absorbers in Nuclear Facilities Outside Reactors
- ANSI/ANS 8.17-2004, Criticality Safety Criteria for the Handling, Storage, and Transportation of LWR Fuel Outside Reactors
- ANSI/ANS-8.19-2014, Administrative Practices for Nuclear Criticality Safety
- ANSI/ANS 8.20-1991(R2005), Nuclear Criticality Safety Training
- ANSI/ANS-8.21-1995(R2001), Use of Fixed Neutron Absorbers in Nuclear Facilities Outside Reactors
- ANSI/ANS-8.23-2007, Nuclear Criticality Accident Emergency Planning and Response
- **ANSI/ANS 8.24-2007, Validation of Neutron Transport Methods for Nuclear Criticality Safety Calculations**
- ANSI/ANS 8.26-2007, Criticality Safety Engineer Training and Qualification Program

Validation: Definitions (1)

- **From ANSI/ANS-8.24-2007, Validation of Neutron Transport Methods for Nuclear Criticality Safety Calculations:**
  - **Verification:** The process of confirming that the *computer code system* correctly performs numerical calculations.
  - **Validation:** The process of quantifying (e.g., establishing the appropriate **bias** and **bias uncertainty**) the suitability of the computer code system for use in nuclear criticality safety analyses.
  - **Computer code system:** A calculational method, computer hardware, and computer software (including the operating system).
  - **Calculational Method:** The mathematical procedures, equations, approximations, assumptions, and associated numerical parameters (e.g., cross sections) that yield the calculated results.

Validation: Definitions (2)

- **From ANSI/ANS-8.24-2007, Validation of Neutron Transport Methods for Nuclear Criticality Safety Calculations:**
  - **Bias:** The systematic difference between calculated results and experimental data.
  - **Bias Uncertainty:** The uncertainty that accounts for the combined effects of uncertainties in the experimental benchmarks, the calculational models of the benchmarks, and the calculational method.
  - **Calculational Margin:** An allowance for bias and bias uncertainty plus considerations of uncertainties related to interpolation, extrapolation, and trending.
  - **Margin of Subcriticality:** An allowance beyond the calculational margin to ensure subcriticality.
  - **Validation Applicability:** A domain, which could be beyond the bounds of the benchmark applicability, within which the margins derived from validation of the calculational method have been applied.

Excerpts from ANSI/ANS - 8.24-2007

5.1 Appropriate system or process parameters that correlate the experiments to the system or process under consideration shall be identified. .....

5.2 Normal and credible abnormal conditions for the system or process shall be identified when determining the appropriate parameters and their range of values.

5.4 Selected benchmarks should encompass the appropriate parameter values spanning the range of normal and credible abnormal conditions anticipated for the system or process to which the validation will be applied.

7.2 The validation applicability should not be so large that a subset of the data with a high degree of similarity to the system or process would produce an upper subcritical limit that is lower than that determined for the entire set. This criterion is recommended to ensure that a subset of data that is closely related to the system or process is not nonconservatively masked by benchmarks that do not match the system as well.

8.1 The validation activity shall be documented with sufficient detail to allow for independent technical review.

8.1.5 The margin of subcriticality and its basis shall be documented.

8.2 An independent technical review of the validation shall be performed. The independent technical review should include, but is not limited to, the following:

(1) a review of the benchmark applicability;

(2) a review of the input files and output files to ensure accurate modeling and adequate convergence;

(3) a review of the methodology, and its use, for determining bias, bias uncertainty, and margins;

(4) concurrence with the validation applicability.

Overview of Validation Methods

- **Identify the range of applications to be considered**
  - Fissile material, geometry, reflection, moderation, etc.
  - Metrics to help characterize neutronics – EALF, % fast/thermal fissions, H/U or H/Pu for solutions, etc.
- **Select a set of experimental benchmarks from ICSBEP Handbook that are neutronically similar to the applications**
  - Must select sufficient number for valid statistical analysis
  - Analyze the set of benchmarks with Monte Carlo
- **Statistical analysis**
  - Determine bias & bias uncertainty for the set of benchmarks
  - For conservatism, usually set positive biases to zero & only consider negative biases for individual benchmarks
- **Estimate additional margin of subcriticality (MOS)**
  - Extra margin to account for nuclear data uncertainty
  - Extra margin to account for unknown code errors
  - Extra margin if applications not similar enough to benchmark set

Upper Subcritical Limit

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

$$K_{calc} < USL$$

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

Note: Bias = calculated – experiment,

For conservatism:

- positive biases are normally set to zero
- only negative biases are considered

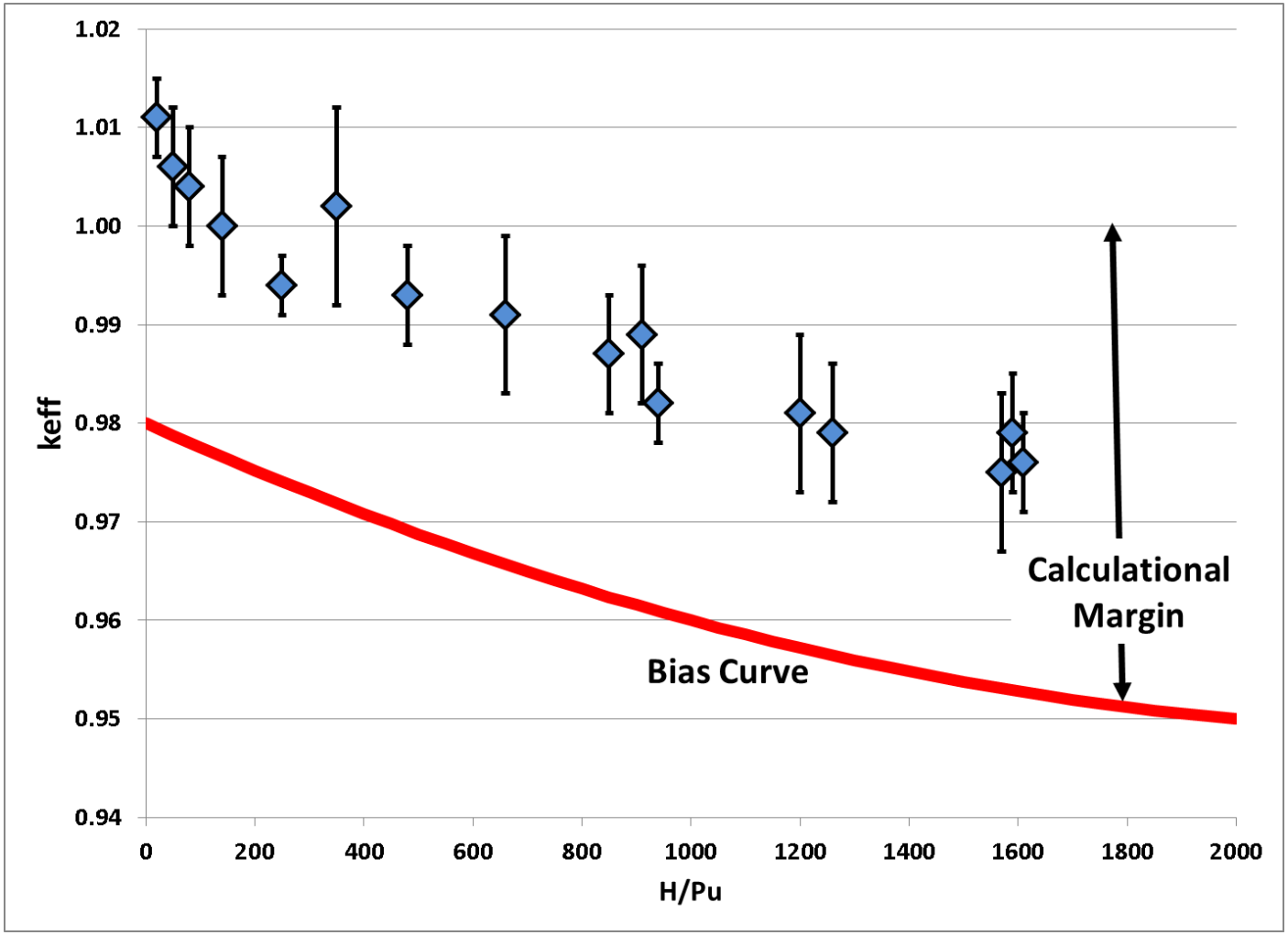
- **Bias & bias uncertainty are at some confidence level, typically 95% or 99%.**
  - **If these confidence intervals are derived from a normal distribution, the normality of the bias data must be justified.**
  - **Alternatively, the confidence intervals can be set using non-parametric methods.**

Calculational Margin

- **The calculational margin is the sum of the bias and the bias uncertainty.**
  - **Bias:** represents the systematic difference between calculation and benchmark experiments.
  - **Bias uncertainty:** relates to uncertainties in the experimental benchmarks and the calculations.
  - Bias & bias uncertainty are routine calculations, for a given application & set of benchmarks
  - Bias & bias uncertainty are only credible when the application & chosen benchmarks are neutronically similar
  - Often quoted as 95/95 confidence, meaning that the calculation margin bounds 95% of the benchmark deviations at the 95% confidence level (assuming normality).
  - May trend calculational margin based upon physical parameters.

Calculational Margin Example

- **Hypothetical bias curve**
  - **Selected experiments with Pu metal and water mixtures**



Margin of Subcriticality

- **To establish a Margin of Subcriticality (MOS) need to consider the process, validation, codes, data, etc. holistically.**
  - **Confidence in the codes and data.**
    - More mature codes that are widely used have greater confidence than newer ones.
    - Deterministic methods require additional margin beyond Monte Carlo because of numerical issues (e.g., ray effects, discretization errors, self-shielding approximations, etc.).
  - **Adequacy of the validation**
    - Unlikely to find a benchmark experiment that is exactly like the model being simulated.
    - Based on trending analysis of physical parameters and/or sensitivity and uncertainty studies, can quantify "similarity".
    - Sparsity of benchmark data, extrapolations, and wide interpolations necessitate larger margins.

- **Major contributors**
  - **Margin for uncertainties in nuclear cross-section data**
  - **Margin for unknown errors in codes**
  - **Additional margin to consider the limitations of describing process conditions based upon sensitivity studies, operating experience, administrative limits, etc.**

Comparison of Validation Approaches (Simplified)

Monte Carlo Codes
XCP-3, LANL

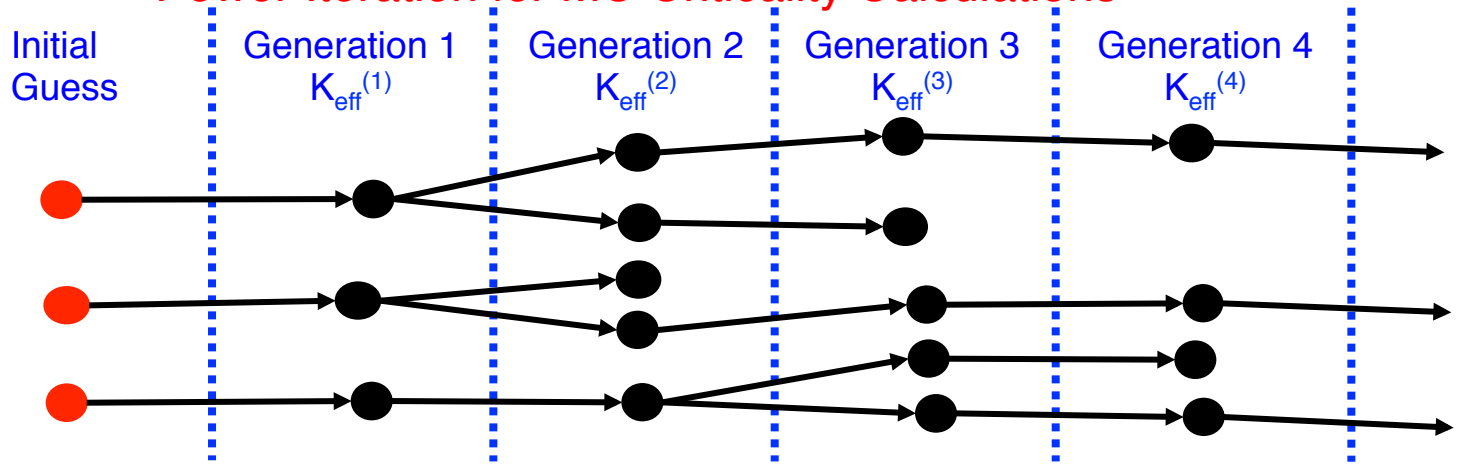
	Traditional, Simple	Traditional, Enhanced	S/U-Based Method
Benchmark Collection	Expert judgment, 1 set, Geometry & materials cover applications	Expert judgment, Several subsets (metal, solutions, other)	Large collection with sensitivity profile data, Reject outliers, Estimate missing uncertainties
Selecting 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 similarities
Margin of Subcriticality	Expert judgment, Very large	Expert judgment, Large	Automatically determine specific margin for data uncertainty by GLLS, Code-expert judgment for code, Expert judgment for additional
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

Best Practices for Monte Carlo Criticality Calculations

- Monte Carlo Criticality Calculations
  - Methodology & Concerns
  - Convergence
  - Bias
  - Statistics
- Best Practices
  - Discussion
  - Conclusions

Methodology & Concerns

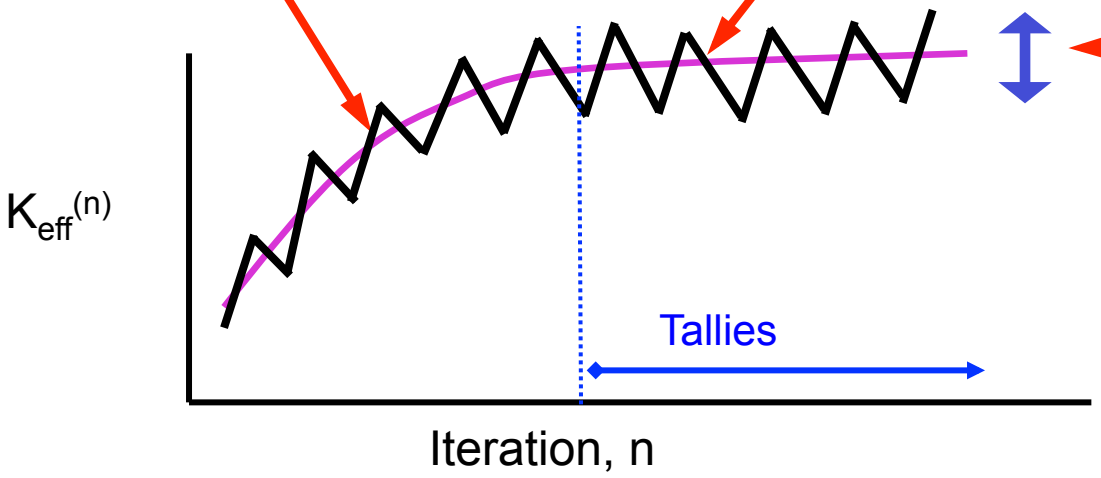
Power Iteration for MC Criticality Calculations



Convergence of K_{eff} & fission distribution

Bias in average K_{eff} & tallies

Bias in statistics for tallies



Monte Carlo
Deterministic (S_n)

Convergence

- **Monte Carlo codes use power iteration to solve for K_{eff} & Ψ for eigenvalue problems**
- **Power iteration convergence is well-understood:**

n = cycle number, k_0,u_0 - fundamental, k_1,u_1 - 1st higher mode

$$\Psi^{(n)}(\vec{r}) = \vec{u}_0(\vec{r}) + a_1 \cdot \rho^n \cdot \vec{u}_1(\vec{r}) + \ldots$$

$$k_{eff}^{(n)} = k_0 \cdot \left[1 - \rho^{n-1}(1-\rho) \cdot g_1 + \ldots\right]$$

  - **First-harmonic source errors die out as ρ^n, $\rho = k_1 / k_0 < 1$**
  - **First-harmonic K_{eff} errors die out as $\rho^{n-1}(1-\rho)$**
  - **Source converges slower than K_{eff}**

- **Most codes only provide tools for assessing K_{eff} convergence.**

➜ **MCNP also looks at Shannon entropy of the source distribution, H_{src}.**

Bias in K_{eff} & Tallies

- **Power iteration is used for Monte Carlo K_{eff} calculations**
  - **For one cycle (iteration):**
    - **M_0** neutrons start
    - **M_1** neutrons produced, $E[\ \mathbf{M_1}\ ] = K_{eff} \cdot \mathbf{M_0}$
  - **At end of each cycle, must renormalize by factor $\mathbf{M_0 / M_1}$**
  - **Dividing by stochastic quantity (M_1) introduces bias in K_{eff} & tallies**
- **Bias in Keff, due to renormalization**

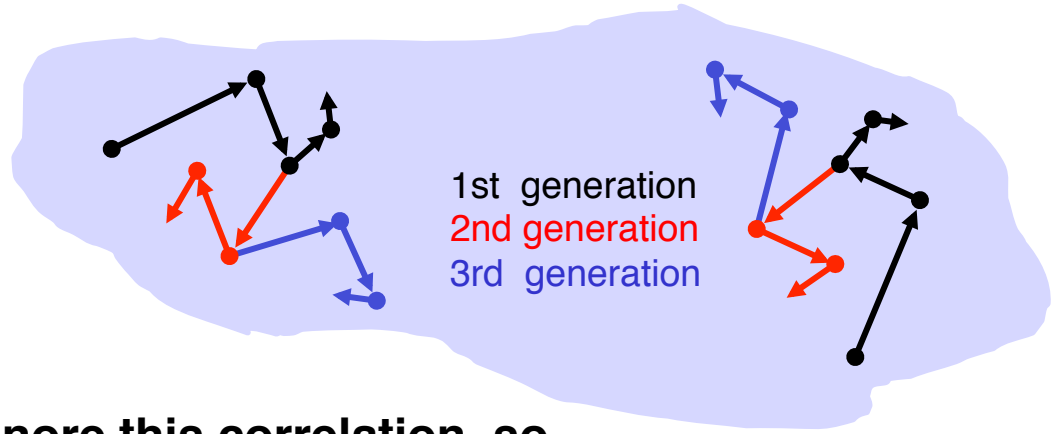
$$\text{Bias in } K_{eff} \propto \frac{1}{M}$$

M = neutrons / cycle

  - **Power & other tally distributions are also biased, produces "tilt"**

Bias in Statistics

- **MC eigenvalue calculations are solved by power iteration**
  - **Tallies for one generation are spatially correlated with tallies in successive generations**
  - **The correlation is positive**



  - **MCNP & other MC codes ignore this correlation, so computed statistics are smaller than the real statistics**
  - **Errors in statistics are small/negligible for K_{eff}, may be significant for local tallies (eg, fission distribution)**
  - **Running more cycles or more neutrons/cycle does not reduce the underprediction bias in statistics**
  - **(True σ^2) > (computed σ^2), since correlations are positive**

$$\frac{\text{True } \sigma^2_{\bar{x}}}{\text{Computed } \sigma^2_{\bar{x}}} = \frac{\sigma^2_{\bar{x}}}{\tilde{\sigma}^2_{\bar{x}}} \approx 1 + 2 \cdot \left(\begin{array}{c} \text{sum of lag-i correlation} \\ \text{coeff's between tallies} \end{array} \right)$$

Best Practices – MC Crit Calcs - Summary

- **To avoid bias in K_{eff} & tally distributions:**
  - **Use 10K or more neutrons/cycle (maybe 100K+ for large system)**
  - **Always check convergence of both K_{eff} & H_{src}**
  - **Discard sufficient initial cycles**

- **To help with convergence & coverage:**
  - **Take advantage of problem symmetry, if possible**
  - **Use good initial source guess, cover fissionable regions -- points in each fissile region, or volume source for large systems**

- **Run at least a few 100 active cycles to allow codes to compute reliable statistics**

- **Statistics on tallies from codes are underestimated, often by 2-5x; possibly make multiple independent runs**
  [note: statistics on k_{eff} are OK, not underestimated]

Other Suggestions

For serious work, my work-flow includes the actions below:

- **In MCNP input files, include a summary of { date, names, changes }**
- **Confirm that calculations used correct versions of code, data, scripts**
- **Always look at geometry with MCNP plotter**
- **Always check convergence plots for Keff & Hsrc**
- **Always check output file (not screen) for lost particles**
- **Check details if any unusual warnings appear**
- **Record for each run:**
  - Name, date, computer, input/output file names
  - keff ± σ (combined col/trk/abs only)
  - EALF, ANECF, % fast/intermed/thermal fissions
  - For solutions, H/Pu^{239} or H/U^{235}
  - Any issues?

If I'm in a hurry & skip some of the above, I usually end up paying big-time later on – having to repeat work to resolve errors or confusion

References

Previous discussion of details concerning bias, convergence, & statistics and "Best Practices" presented at

- 2008 - PHYSOR Monte Carlo workshop
- 2009 - M&C Monte Carlo workshop
- 2009 - Paper at NCSD topical meeting (best paper award)
- 2010 - PHYSOR Monte Carlo Workshop
- 2008 – present – MCNP Criticality Classes

Presentations available at mcnp.lanl.gov

Monte Carlo Methods

F. B. Brown, "Fundamentals of Monte Carlo Particle Transport," LA-UR-05-4983, available at mcnp.lanl.gov (2005).

Monte Carlo k-effective Calculations

F.B. Brown, "Review of Best Practices for Monte Carlo Criticality Calculations", ANS NCSD-2009, Richland, WA, Sept 13-17 (2009).

G.E. Whitesides, "Difficulty in Computing the k-effective of the World," *Trans. Am. Nucl. Soc.,* 14, No. 2, 680 (1971).

J. Lieberoth, "A Monte Carlo Technique to Solve the Static Eigenvalue Problem of the Boltzmann Transport Equation," *Nukleonik* 11,213 (1968).

M. R. Mendelson, "Monte Carlo Criticality Calculations for Thermal Reactors," *Nucl. Sci Eng.* 32, 319-331 (1968).

H. Rief and H. Kschwendt, "Reactor Analysis by Monte Carlo," *Nucl. Sci. Eng.*, 30, 395 (1967).

W. Goad and R. Johnston, "A Monte Carlo Method for Criticality Problems," *Nucl. Sci. Eng.* 5, 371-375 (1959).

J Yang & Y. Naito, "The Sandwich Method for Determining Source Convergence in Monte Carlo Calculations", *Proc. 7th Int. Conf. Nuclear Criticality Safety, ICNC2003, Tokai-mura, Iburaki, Japan, Oct 20-24, 2003*, JAERI-Conf 2003-019, 352 (2003).

References

Shannon entropy & convergence

T. Ueki & F.B. Brown, "Stationarity and Source Convergence in Monte Carlo Criticality Calculations", ANS Topical Meeting on Mathematics & Computation, Gatlinburg, TN April 6-11, 2003 [also, LA-UR-02-6228] (September, 2002).

T. Ueki & F.B. Brown, "Stationarity Modeling and Informatics-Based Diagnostics in Monte Carlo Criticality Calculations", *Nucl. Sci. Eng.* 149, 38-50 [also LA-UR-03-8343] (2005).

F.B. Brown, "On the Use of Shannon Entropy of the Fission Distribution for Assessing Convergence of Monte Carlo Criticality Calculations", proceedings PHYSOR-2006, Vancouver, British Columbia, Canada [also LA-UR-06-3737 and LA-UR-06-6294] (Sept 2006).

R.N. Blomquist, et al., "Source Convergence in Criticality Safety Analysis, Phase I: Results of Four Test Problems," OECD Nuclear Energy Agency, OECD NEA No. 5431 (2006).

R.N. Blomquist, et al., "NEA Expert Group on Source Convergence Phase II: Guidance for Criticality Calculations", 8th International International Conference on Criticality Safety, St. Petersburg, Russia, May 28 – June 1, 2007 (May 2007).

Bias in Keff & Tallies

E.M. Gelbard and R.E. Prael, "Monte carlo Work at Argonne National Laboratory", in Proc. NEACRP Meeting of a Monte Carlo Study Group, ANL-75-2, Argonne National Laboratory, Argonne, IL (1974).

R. C. Gast and N. R. Candelore, "Monte Carlo Eigenfunction Strategies and Uncertainties," in Proc. NEACRP Meeting of a Monte Carlo Study Group, ANL-75-2, Argonne National Laboratory, Argonne, IL (1974).

R. J. Brissenden & A. R. Garlick, "Biases in the Estimation of Keff and Its Error by Monte Carlo Methods," Ann. Nucl. Energy, 13, 2, 63-83 (1986)

T Ueki, "Intergenerational Correlation in Monte Carlo K-Eigenvalue Calculations", Nucl. Sci. Eng. 141, 101-110 (2002)

L.V. Maiorov, "Estimates of the Bias in the Results of Monte Carlo Calculations of Reactors and Storage Sites for Nuclear Fuel", *Atomic Energy*, Vol 99, No 4, 681-693 (2005).

Correlation & Bias in Uncertainties

T Ueki, "Intergenerational Correlation in Monte Carlo K-Eigenvalue Calculations", Nucl. Sci. Eng. 141, 101-110 (2002)

T. Ueki and F. B. Brown, "Autoregressive Fitting for Monte Carlo K-effective Confidence Intervals," Trans. Am. Nucl. Soc., 86, 210 (2002).

T. Ueki, "Time Series Modeling and MacMillan's Formula for Monte Carlo Iterated-Source Methods," Trans. Am. Nucl. Soc., 90, 449 (2004).

T. Ueki & B. R. Nease, "Times Series Analysis of Monte Carlo Fission Sources - II: Confidence Interval Estimation", Nucl. Sci. Eng., 153, 184-191 (2006).

D. B. MacMillan, "Monte Carlo Confidence Limits for Iterated-Source Calculations," Nucl. Sci. Eng., 50, 73 (1973).

E.M. Gelbard and R.E. Prael, "Monte carlo Work at Argonne National Laboratory", in Proc. NEACRP Meeting of a Monte Carlo Study Group, ANL-75-2, Argonne National Laboratory, Argonne, IL (1974).

R. J. Brissenden & A. R. Garlick, "Biases in the Estimation of Keff and Its Error by Monte Carlo Methods," Ann. Nucl. Energy, 13, 2, 63-83 (1986)

E. M. Gelbard and R. E. Prael, "Computation of Standard Deviations in Eigenvalue Calculations," Prog. Nucl. Energy, 24, 237 (1990).

Neutron Spectra

- Neutron slowing down theory
- Lethargy
- Neutron spectra
- Resonance absorption
- Spectral indicators
- Examples

- **Consider the transport equation for:**
  - Infinite medium of hydrogen
  - Steady source at energy E_S
  - Isotropic elastic scatter
  - Scattering nuclides are stationary, no upscattering occurs
  - No absorption

$$\cancel{\Omega \cdot \nabla \phi(E)} + \Sigma_T(E)\phi(E) = \int_E^{E_S} dE' \Sigma_S(E' \rightarrow E)\phi(E') + S \cdot \delta(E - E_S)$$

- **For hydrogen at rest (E >> kT)** $\Sigma_S(E' \rightarrow E) = \dfrac{\Sigma_S(E')}{E'}$

- **Slowing down in hydrogen at rest:**

$$\Sigma_S(E)\phi(E) = \int_E^{E_S} dE' \frac{\Sigma_S(E')}{E'}\phi(E') + S \cdot \delta(E - E_S)$$

- **Solution**

$$\phi(E) = \frac{S}{\Sigma_S(E) \cdot E} + \frac{S}{\Sigma_S(E)}\delta(E - E_S)$$

- **For theory, visualization, understanding, it is useful to change variables from energy (E) to lethargy (u)**

$$u = \ln\frac{E_0}{E}, \quad \text{where } E_0 \text{ is large, eg 20 MeV}$$

$$du = -\frac{dE}{E}, \quad E = E_0 e^{-u}$$

$$\phi(u) = \left|\frac{dE}{du}\right| \phi(E) = E \cdot \phi(E)$$

  - **As energy decreases, lethargy increases**

- **Consider slowing down flux in hydrogen, $E<E_S$**

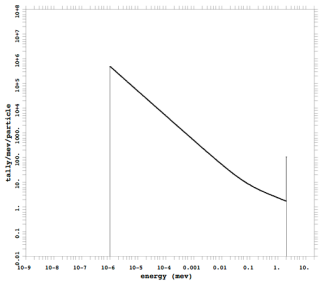
$$\phi(E) = \frac{S}{\Sigma_S(E)\cdot E} \sim \frac{1}{E}$$

$$\phi(u) = \frac{S}{\Sigma_S(u)} \sim \text{constant}$$

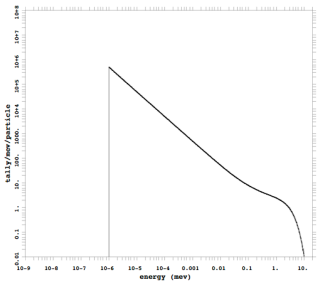
Flux Spectra for Neutron Slowing Down & Criticality

Monte Carlo Codes
XCP-3, LANL

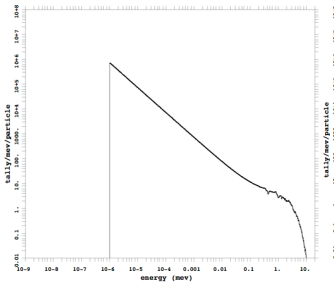
loglog plots of ϕ(E) vs E



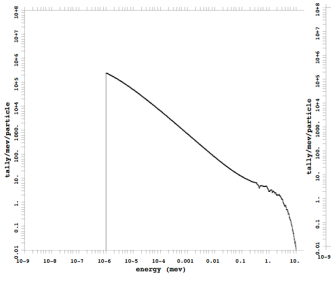
2 MeV neutrons
hydrogen



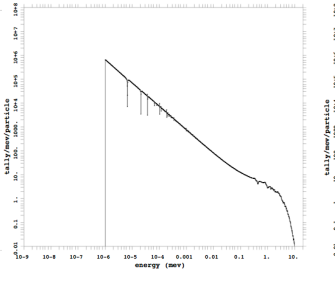
fission neutrons
hydrogen



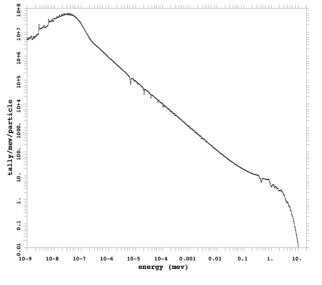
fission neutrons
water



fission neutrons
water + B^{10}

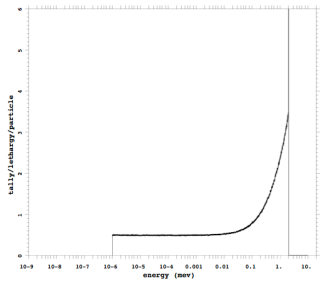


fission neutrons
water + U^{238}

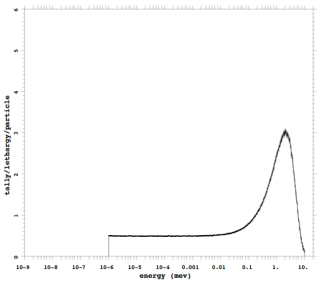


Fuel Pin
Unit Cell

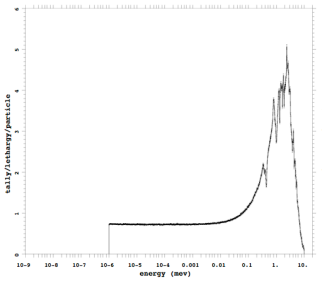
loglin plots of ϕ(u) vs u



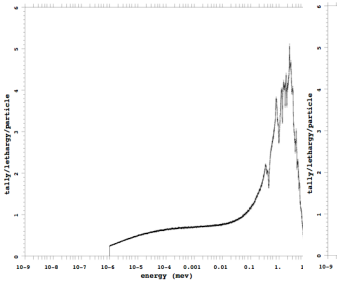
2 MeV neutrons
hydrogen



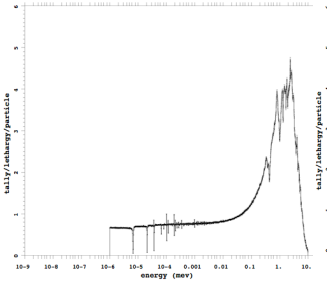
fission neutrons
hydrogen



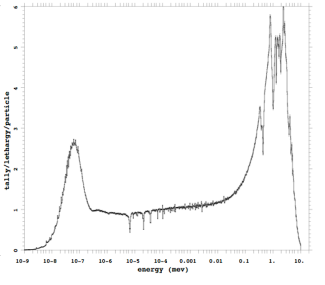
fission neutrons
water



fission neutrons
water + B^{10}



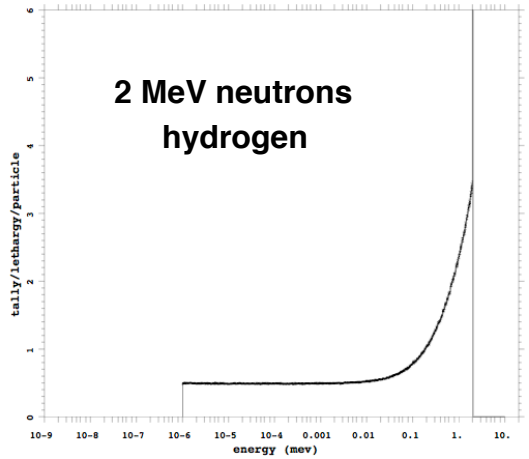
fission neutrons
water + U^{238}

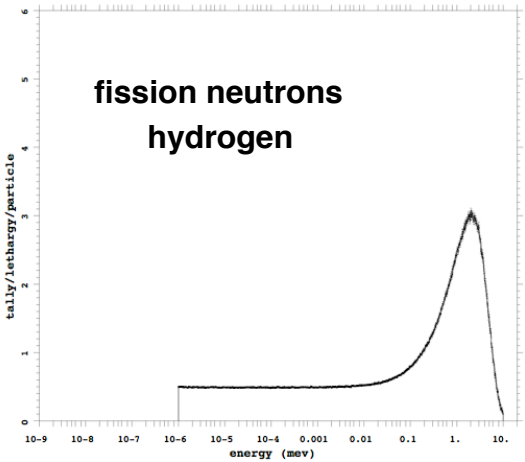


Fuel Pin
Unit Cell

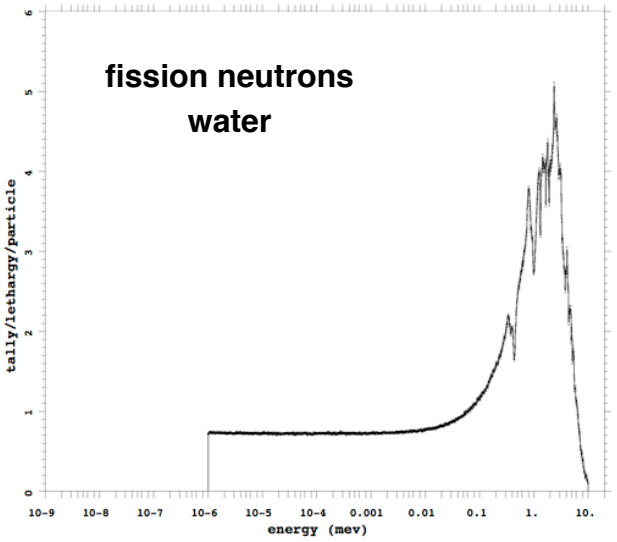
Flux Spectra for Neutron Slowing Down

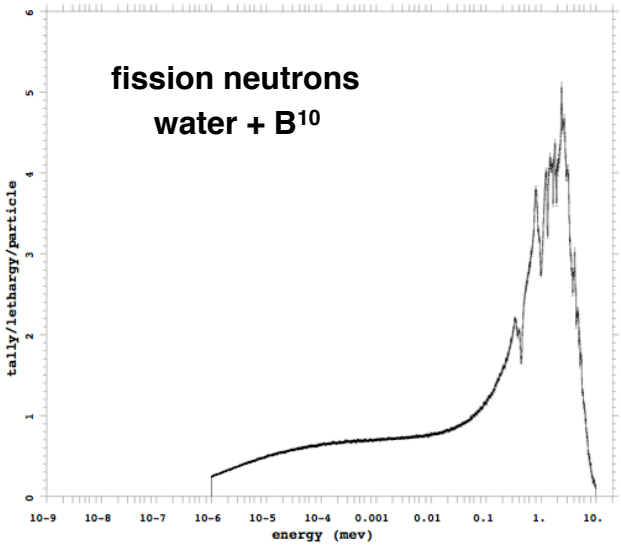
Monte Carlo Codes
XCP-3, LANL

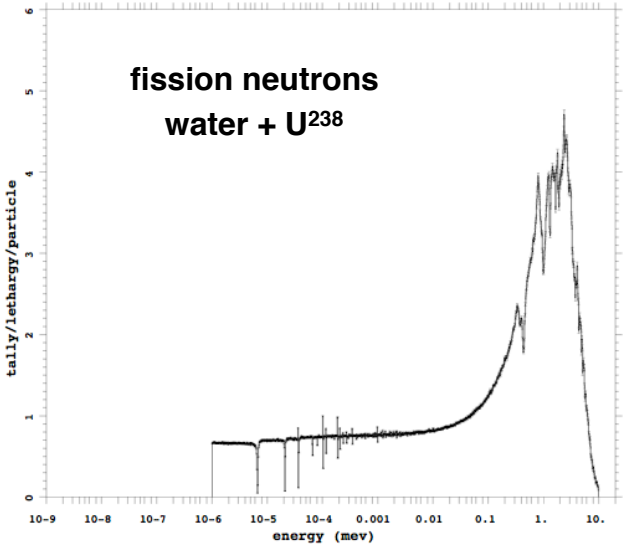




loglin plots of ϕ(u) vs u

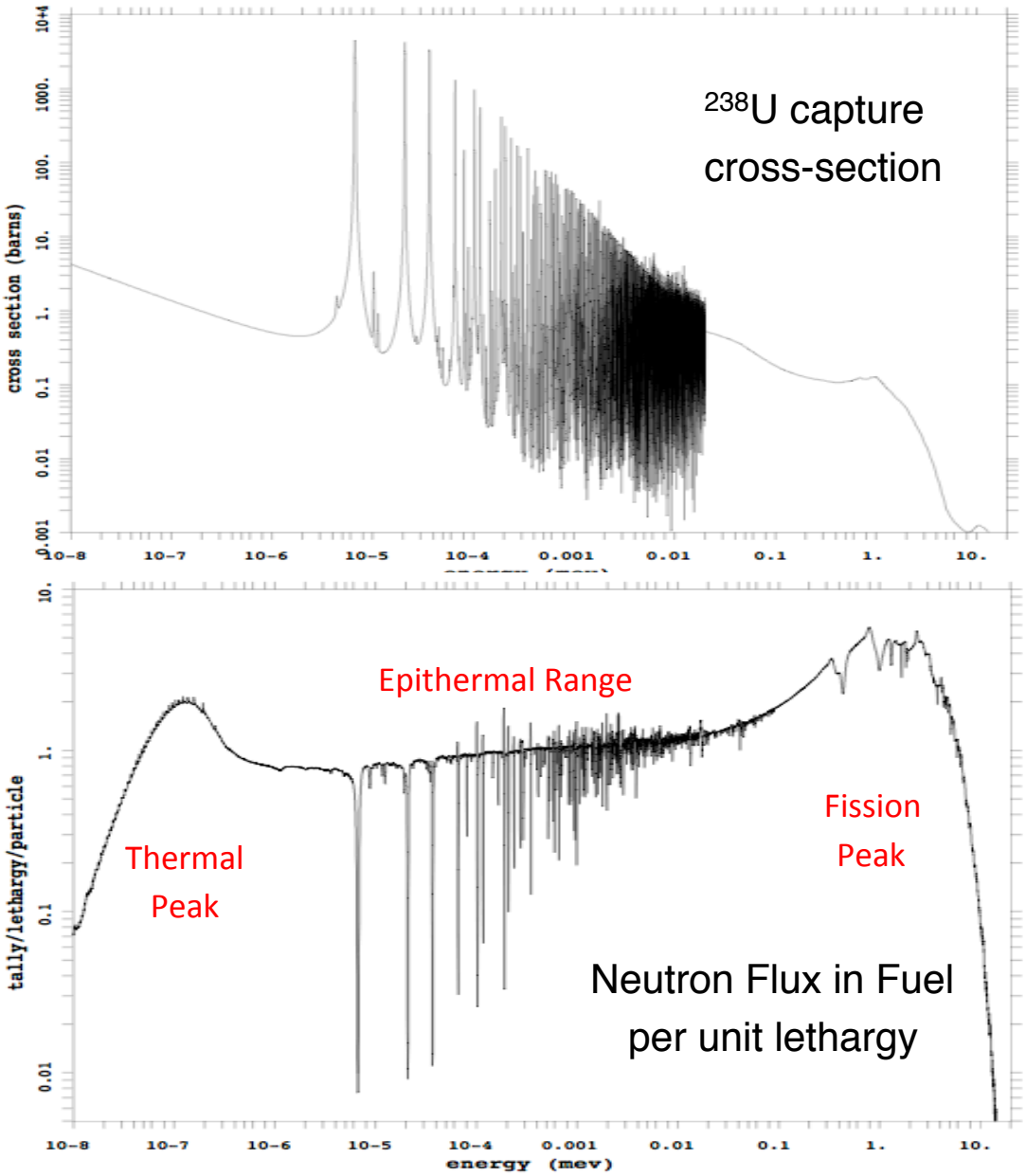






UO_2 Fuel Pin

Monte Carlo Codes
XCP-3, LANL



UO_2 Fuel Pin

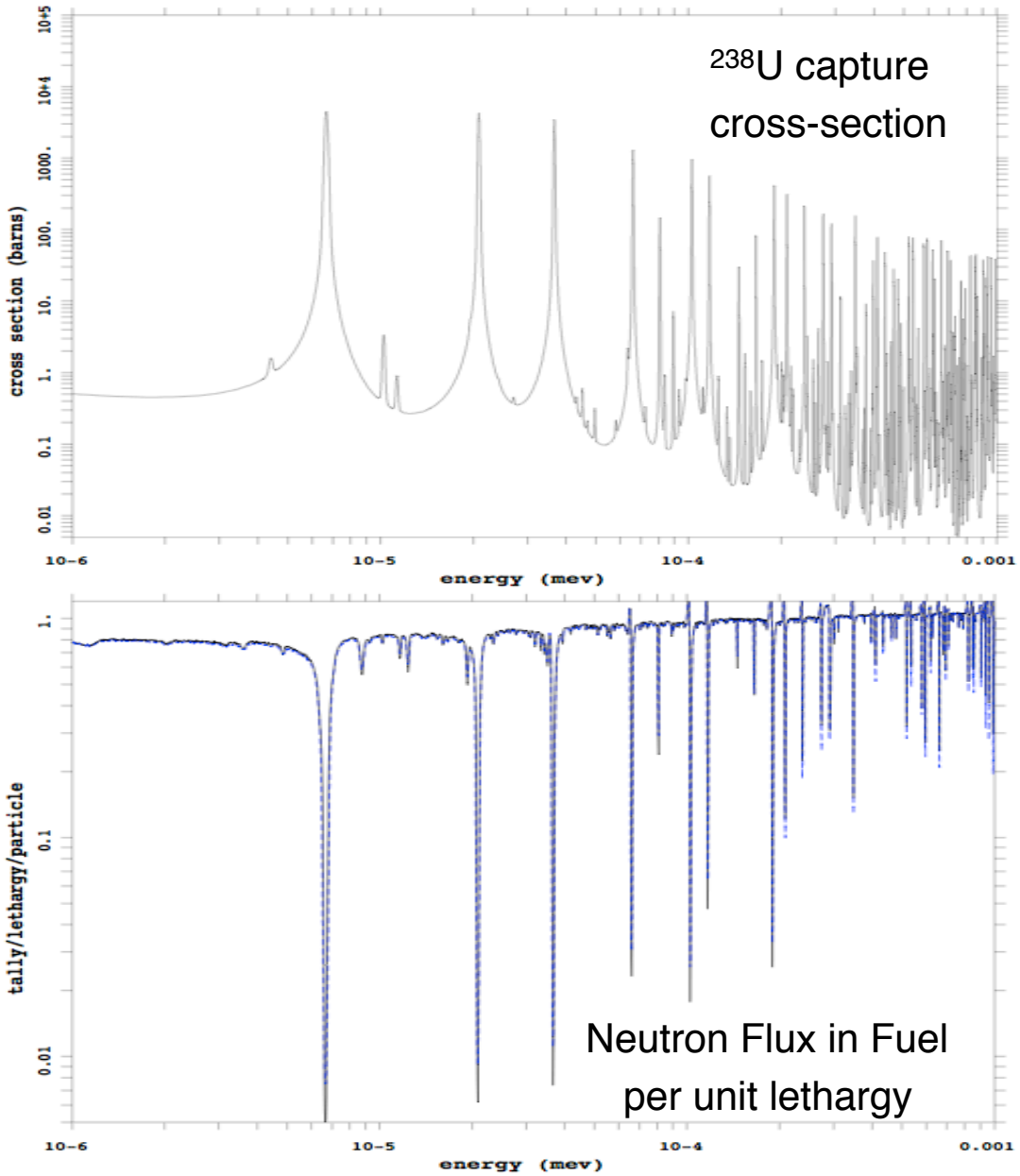
3.1% Enriched

293.6 ^{o}K

.01 eV – 20 MeV

- Neutrons born in MeV range from fission
- Most fissions caused by thermal neutrons
- **1/3 of neutron losses are due to ^{238}U capture in epithermal energy range during slowing down**

UO_2 Fuel Pin



UO_2 Fuel Pin

3.1% Enriched

293.6 ^{o}K

Detail for
1 eV – 1 KeV

1/3 of neutron losses are due to ^{238}U capture at epithermal energies during slowing down

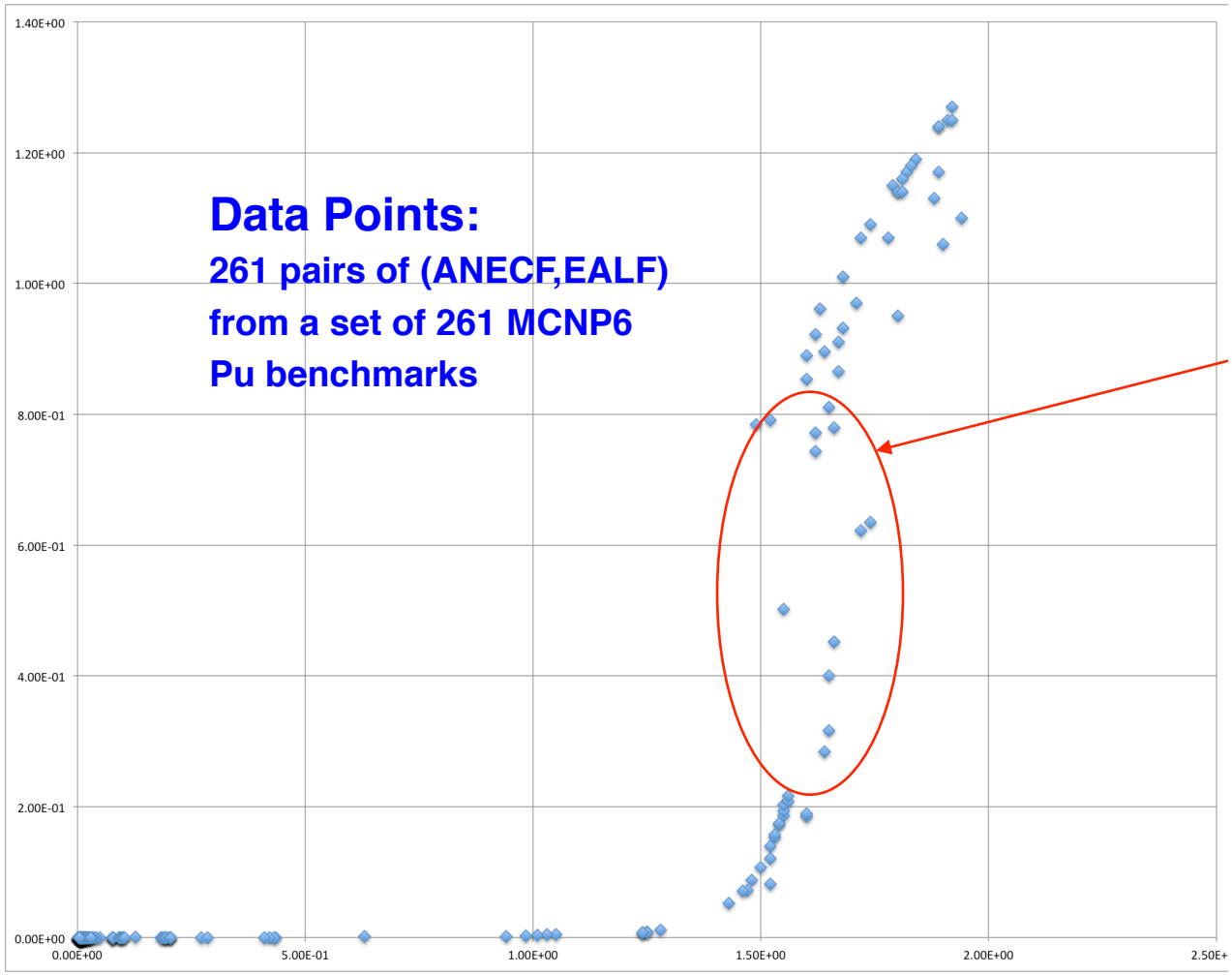
Characterizing the Neutron Spectrum

- The neutron spectrum – Φ(E) or Φ(u) – is a complex function of geometry, materials, isotopes, reflectors, temperature, cross-sections, …
- Many different spectral index parameters can be used to characterize the spectrum
  - EALF – energy corresponding to the average lethargy of neutrons causing fission
  - ANECF – average energy of neutrons causing fission
  - Above thermal leakage fraction
  - H/Pu ^{239} or H/U^{235} ratios, for solutions
  - Fraction of fissions caused by fast (E > 100 keV), intermediate (1 eV < E < 100 keV), and thermal (E < 1 eV) neutrons
  - ^{238}U(n,f)/^{235}U(n,f), ^{237}Np(n,f)/^{235}U(n,f), other ratios
  - etc.
- These parameters are useful for comparing different reactors or benchmark experiments, in looking for trends in code or cross-section accuracy
- Spectrum hardness is often characterized by one of these parameters
- No single parameter tells the whole story

EALF vs ANECF

ANECF = average neutron energy causing fission

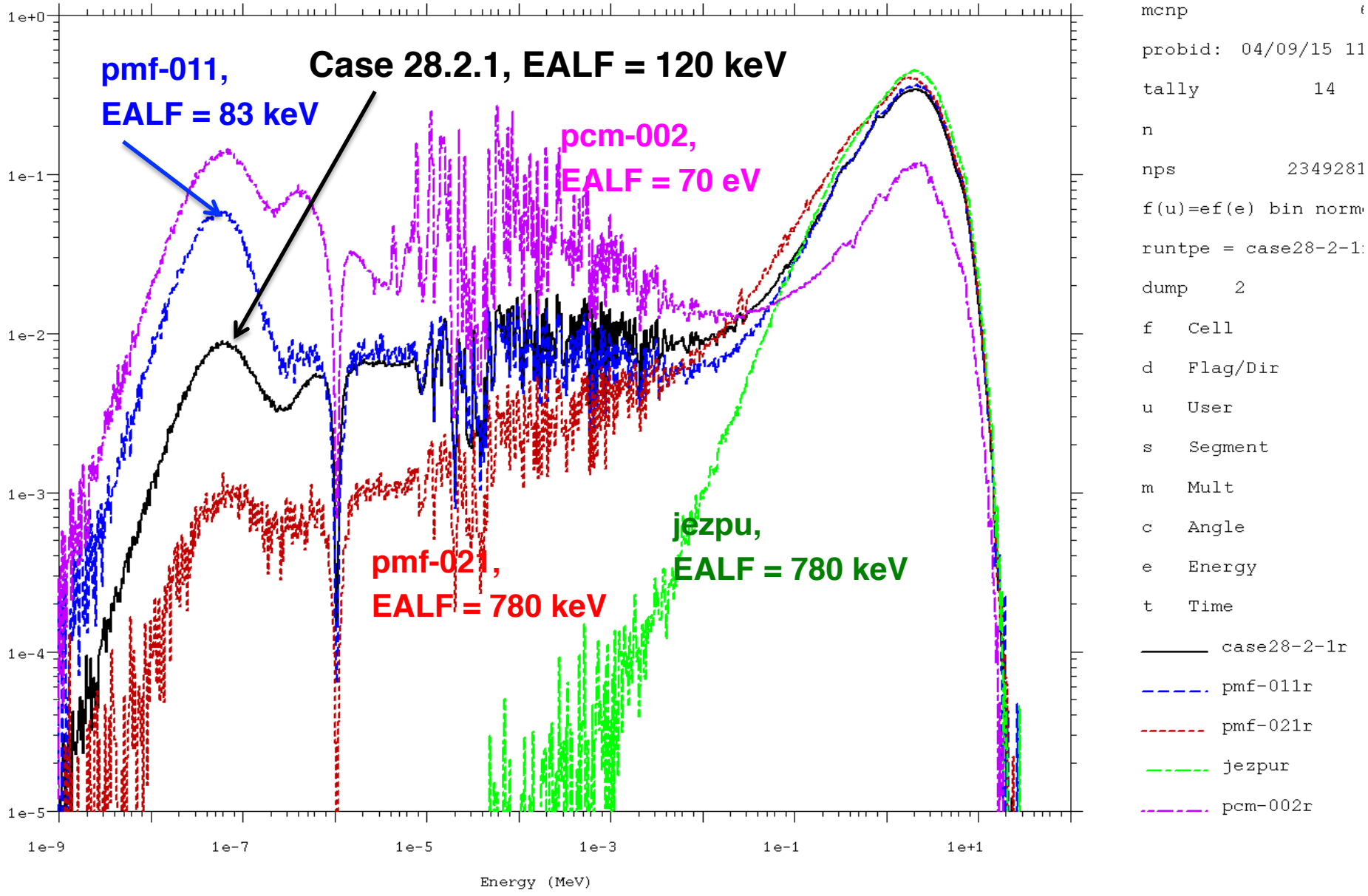
EALF = energy of the average neutron lethargy causing fission



Sparse EALF coverage,
dense ANECF coverage

Pu Systems – $\nu\Sigma_F\Phi$ production & spectrum hardness

Monte Carlo Codes
XCP-3, LANL



S(α,β) Thermal Neutron Scattering Data

Thermal Scattering – S(α,β) Data

- **At low energies (E < 9 eV), neutron scattering interactions are influenced by chemical binding, temperature, molecular effects, …**
  - Important for light nuclei (moderators)
  - MCNP libraries include thermal scattering laws, **S(α,β) libraries**, for water, heavy water, polyethylene, methane, benzene, graphite, beryllium, zirc-hydride, etc.
  - Include thermal scattering law(s) for every moderator nuclide in any problem where neutrons reach energies of 9 eV or less, using an **MTn** card
- **SAB2002**
  - ENDF/B-VI-based S(α,β) data, released in 2002
  - Data for 15 combinations of nuclides and materials
  - Typical temperature ranges are from 294 K to 1200 K, in increments of 200
  - Data typically tabulated at 16 angles and 64 energies for each temperature
  - Data are provided at ~ 20 K for a limited number of nuclides
- **ENDF70SAB (discrete), ENDF71SaB (continuous)**
  - ENDF/B-VII - based S(α,β) data, ca. 2008
  - Many more nuclide - material combinations:
    al27, be, be-o, benz, dortho, dpara, fe56, grph, h-zr, hortho, hpara, hwtr, lmeth, lwtr, o-be, o2-u, poly, smeth, u-o2, zr-h
  - Many more temperatures, data every 50 K or 100 K
  - See **Listing of Available ACE Data Tables, LA-UR-13-21822**

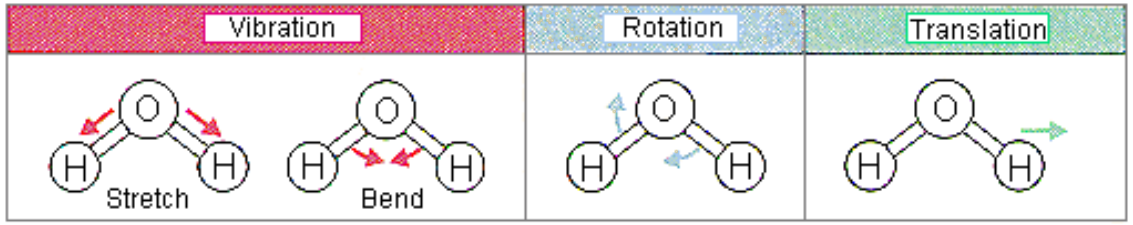
Neutron S(a,b) Thermal Scattering Libraries

Monte Carlo Codes
XCP-3, LANL

ENDF/B-V	ENDF/B-VI	ENDF/B-VII.0	ENDF/B-VII.1		
tmccs	sab2002	endf70sab	ENDF71SaB		
discrete	discrete	discrete	continuous		
be	be	al27	al27		
benz	benz	be	be	be-o	be/o
beo	beo	be/o	benz		
grph	dortho	benz	dortho		
h/zr	dpara	dortho	dpara		
hwtr	grph	dpara	fe56		
lwtr	h/zr	fe56	grph		
poly	hortho	grph	h-zr	h/zr	
zr/h	hpara	h/zr	hortho		
	hwtr	hortho	hpara		
	lmeth	hpara	hwtr		
	lwtr	hwtr	lmeth		
	poly	lmeth	lwtr		
	smeth	lwtr	o-be	o/be	
	zr/h	o/be	o2-u	o2/u	
		o2/u	poly		
		poly	sio2		
		smeth	smeth		
		u/o2	u-o2	u/o2	
		zr/h	zr-h	zr/h	

Thermal Neutron Scattering

- **Moderator materials contain light isotopes (H, D, He, Be, Li, C)**
  - **Water, heavy water, poly, concrete, etc.**
  - **Fast neutrons colliding with moderator lose lots of energy**
  - **Systems with moderator material:**
    - Large thermal neutron flux
    - Fission cross-sections are very large at thermal energies
    - Significant fraction of fissions caused by thermal neutrons (maybe all!)
- **Thermal neutron physics** 1×10^{-5} **eV** $<$ **E** $<$ **9 eV**
  - **Neutron energy comparable to chemical binding effects, gives rise to incoherent inelastic scatter**



  - **Neutron wavelength comparable to atomic spacing**
    - In solids, may need **coherent elastic scatter** (Bragg) from crystals
    - In liquids & gases, may need **incoherent elastic scatter**

S(α,β) Thermal Neutron Scattering Data

- **S(α,β) data is used to model the physics for**
  - **Inelastic scatter (chemical binding, temperature, etc.)**
  - **Elastic scatter for some solids & liquids**
- **S(α,β) data is contained in special ACE files for MCNP**

α and β are dimensionless quantities representing:

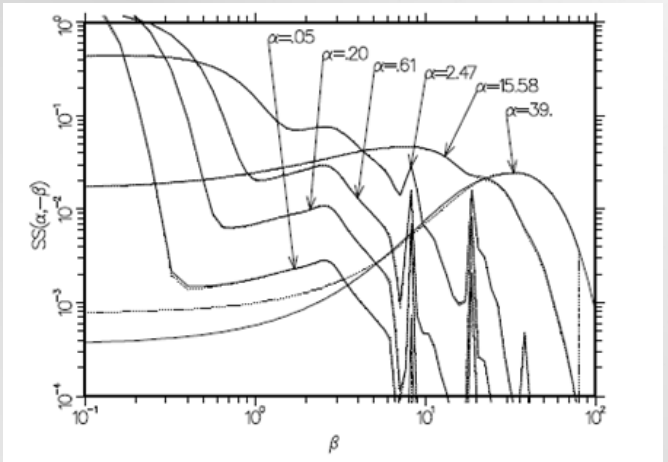
α: momentum transfer

$$\alpha = \frac{E + E' - 2\mu\sqrt{EE'}}{A_0 kT}$$

β: energy transfer

$$\beta = \frac{E' - E}{kT}$$

$$\sigma(E \to E', \mu, T) = \frac{\sigma_b}{2kT}\sqrt{\frac{E'}{E}}e^{-\beta/2}S(\alpha, \beta, T)$$



where:

E, E': pre- and post-collision energy
μ: cosine of the scattering angle
σ_b: bound atom scattering cross section
k: Boltzmann constant
T: temperature
S(α,β,T): symmetric form of the scattering law

S(α,β) Thermal Neutron Scattering Data

- **When to NOT use S(α,β) data:**
  - **Fast & intermediate systems, % thermal fissions small (< 10% ?)**
  - **Whenever no significant amount of moderator material**
    - Very thin coatings, very thin reflectors, paint, varnish, trace impurities
  - **Heavy isotopes - U, Zr, Fe, Al (anything heavier than O^{16})**
- **When to use S(α,β) data:**
  - **Thermal systems, significant % fissions from thermal neutrons**
  - **Solutions, sizable reflectors, concrete, hands, ….**
  - **Suggested:**
    - light water: **lwtr**
    - heavy water: **hwtr**
    - polyethylene: **poly**
    - concrete: **lwtr** (for H in concrete)
    - zirc-hydride: **h-zr**
    - oil **benz**
    - Be metal: **be** (for thermal systems)
    - Be oxide: **be-o** (for thermal systems)
    - Graphite: **grph**

Things to consider:

- **Always used for thermal systems:** lwtr, hwtr, grph, poly, h-zr
- **Some S(α,β) datasets are only rarely used:** be-o, be, sio2, benz
- **Some S(α,β) datasets are almost never used:** u-o2, o2-u, zr-h, o-be
- **Some S(α,β) datasets were developed for specific research & experimental use (eg, ultra-cold neutron scatter experiments):** hortho, dortho, hpara, dpara, lmeth, smeth, al27, fe56
- **Cement:** $2\,Ca_3\,Si\,O_5 + 7\,H_2O \rightarrow 3(CaO)\cdot 2(SiO_2)\cdot 4(H_2O)(gel) + 3Ca(OH)_2$
  Usually just use lwtr (for H)

S(α,β) - Examples

- **Reactor fuel pin, 3.1% enriched UO2, with clad & water**
  - using lwtr (for H in water) k = 1.44853 +- 0.00005
  - using lwtr + o2-u (for O in UO2) k = 1.44853 +- 0.00005

  Can ignore S(a,b) for O, must include for H

- **pu-met-fast-018-001**
  - using S(a,b) for be: k = 0.99944 +- 0.00005
  - no S(a,b) k = 0.99942 +- 0.00005

  For fast spectrum systems, S(a,b) makes no difference

- **pu-comp-mixed-001-001**
  - using S(a,b) for lwtr, sio2, fe56: k = 1.02464 +- 0.00008
  - using S(a,b) for lwtr, sio2 only: k = 1.02463 +- 0.00008
  - using S(a,b) for lwtr only: k = 1.02458 +- 0.00008

- **pu-met-fast-041-001**
  - not using S(a,b) k = 1.00573 +- 0.00007
  - using S(a,b) for lwtr k = 1.00582 +- 0.00005

  0 % thermal fissions .....

Nuclear Data Sensitivities

Introduction & Objectives

- **MCNP can produce sensitivity profiles to determine which data most impacts criticality.**

- **Learning Objectives:**
  - **Understand the meaning of a sensitivity coefficient**
  - **Comprehend the techniques used by MCNP to estimate those tallies**
  - **Use the KSEN card to generate both energy-integrated and energy-resolved sensitivity profiles for specific reactions**
  - **Understand sensitivity output file information**

Motivation (1)

- Nuclear cross sections are a major driver for criticality, and their uncertainties usually the largest source of bias in calculations.

- Knowing which data most impacts criticality is useful for:
  - Critical experiment design
  - Uncertainty quantification and bias assessment
  - Code validation
  - Nuclear data adjustment and qualification
- Validation requires selecting benchmarks that are appropriate for the process being analyzed.
  - One method of picking appropriate benchmarks is to find the ones where the system multiplication is impacted by the same nuclear data.
  - For example, if the process k_{eff} is very sensitive to thermal plutonium capture, you should find benchmarks where the same is true.
- Critical experiment design
  - Often experiments are performed to address some defined nuclear data need.
  - Nuclear data sensitivities can determine if the as-designed experiment meets that need.

Sensitivity Coefficient

- **For criticality problems, often want to know:**
  - **How sensitive is Keff to uncertainty in some parameter ?**

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

$$S_{R,x} = \frac{\Delta R / R}{\Delta x / x}$$

- **Here, the response is the system multiplication k and the parameter x is some nuclear data (cross section).**

- **For a very small change in system parameter x:**

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

- This may be expressed using perturbation theory:

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

- This includes both the forward and adjoint neutron fluxes.
- The boldface S and F are shorthand for scattering and fission integrals of the transport equation.
- The x subscript implies that the quantity is just for data x.

Adjoint Transport Equation

- **The adjoint transport equation:**

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

- **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.

- **The iterated fission probability method is based on this concept, & can be used to determine adjoint or importance weighting for Monte Carlo tallies**

Example – Need for Adjoint-Weighting

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

unweighted

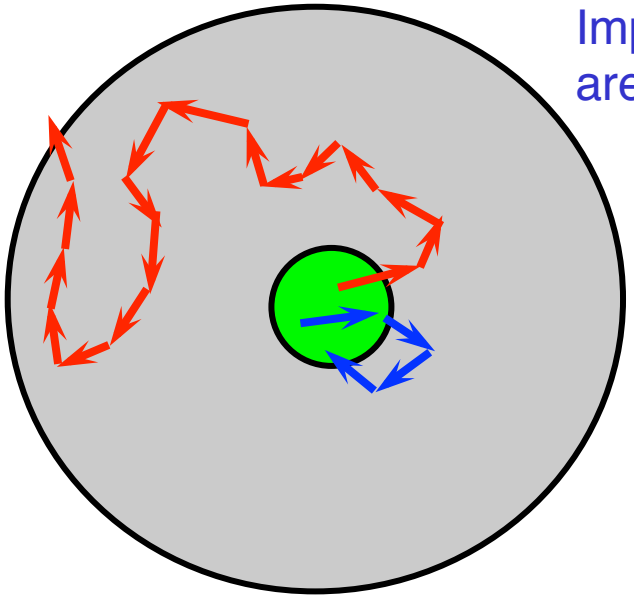
$$\Lambda_{rem} = \frac{\left\langle 1, \frac{1}{v}\psi \right\rangle}{\left\langle 1, F\psi \right\rangle}$$

adjoint-weighted

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

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

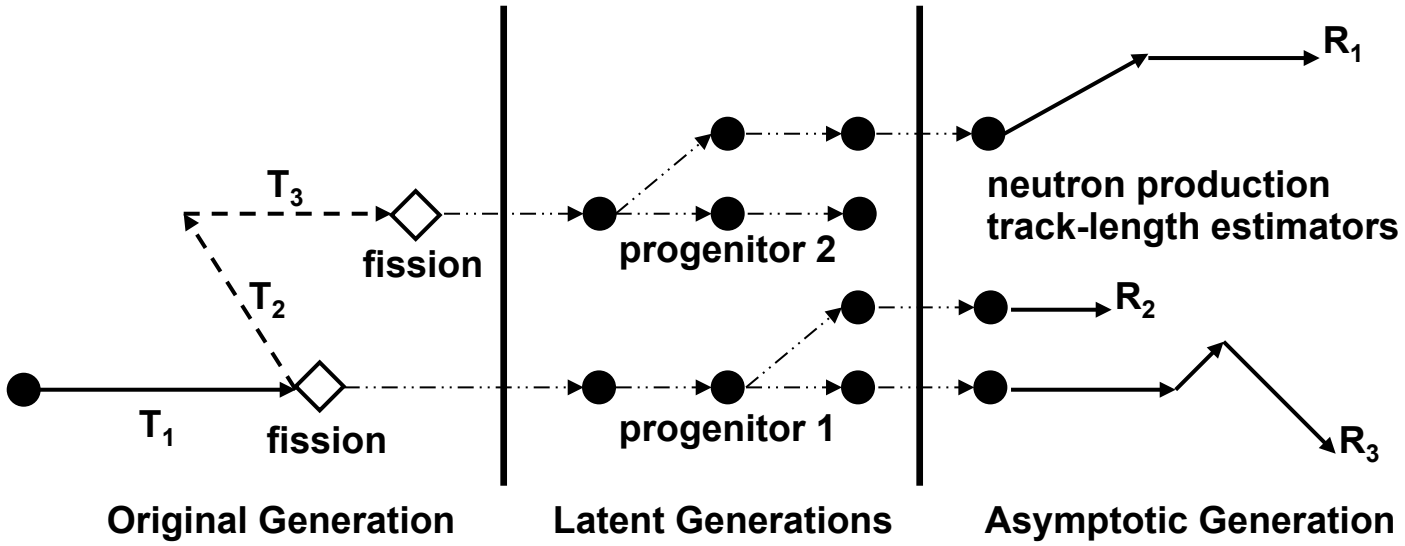
Neutrons spending significant time deep in the reflector are unlikely to cause fission and are therefore unimportant



Important neutrons are often short-lived

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

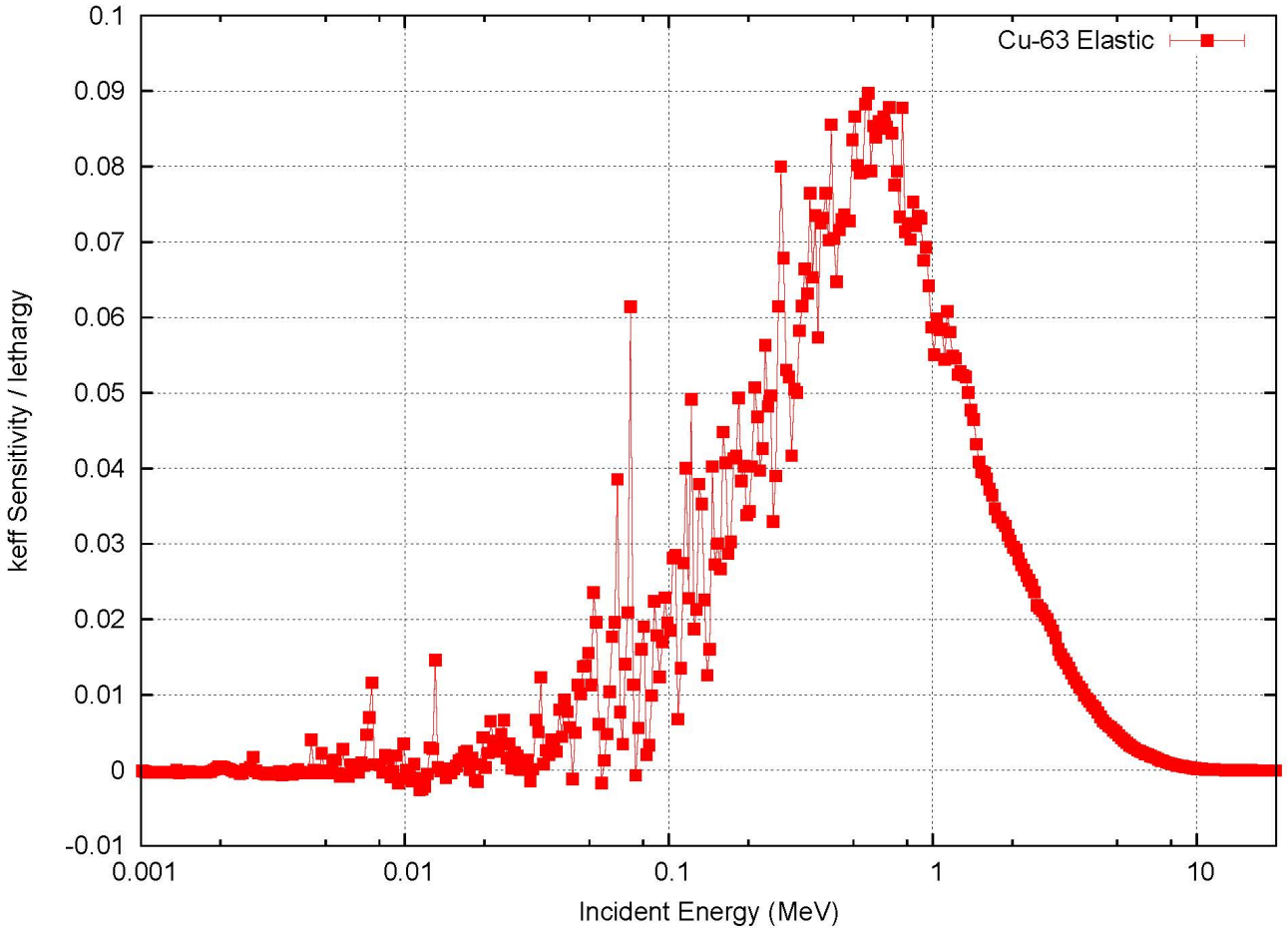
- MCNP performs adjoint-weighting of tallies using a technique called the iterated fission probability
- MCNP breaks active cycles into consecutive ***blocks***:
  - Tally contributions collected in first generation, progenitor neutrons tagged and linked with tally contributions.
  - All subsequent progeny within the block remember their progenitor.
  - After *N* cycles, the population of progeny from each progenitor is measured. This is multiplied by the previously recorded tally contributions to form a tally score.



Example Sensitivity Coefficient Profile

Cu-63: Elastic Scattering Sensitivity

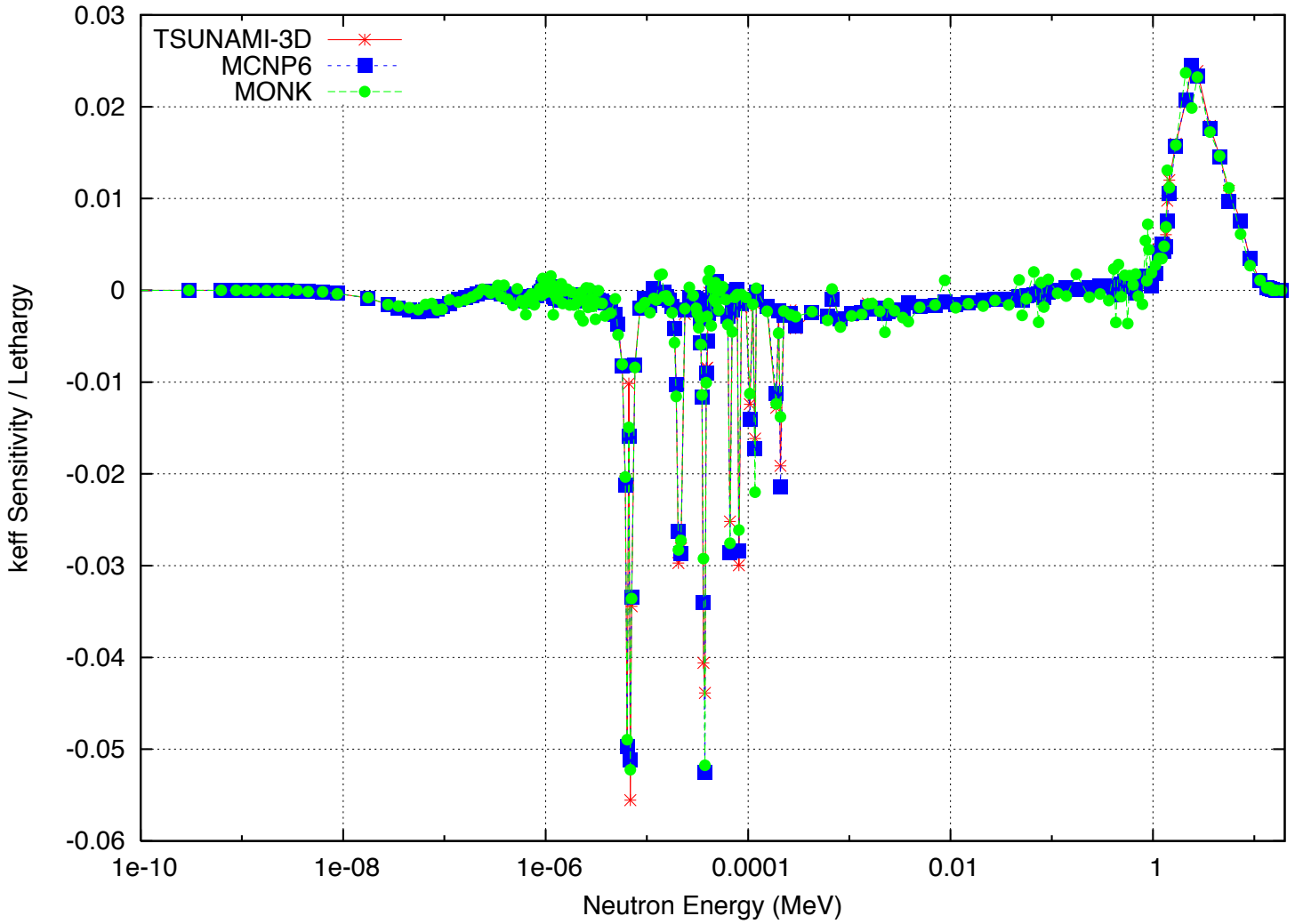
Copper-Reflected Zeus experiment:



Example Sensitivity Coefficient Profile

U-238: total cross-section sensitivity

OECD/NEA UACSA Benchmark Phase III.1

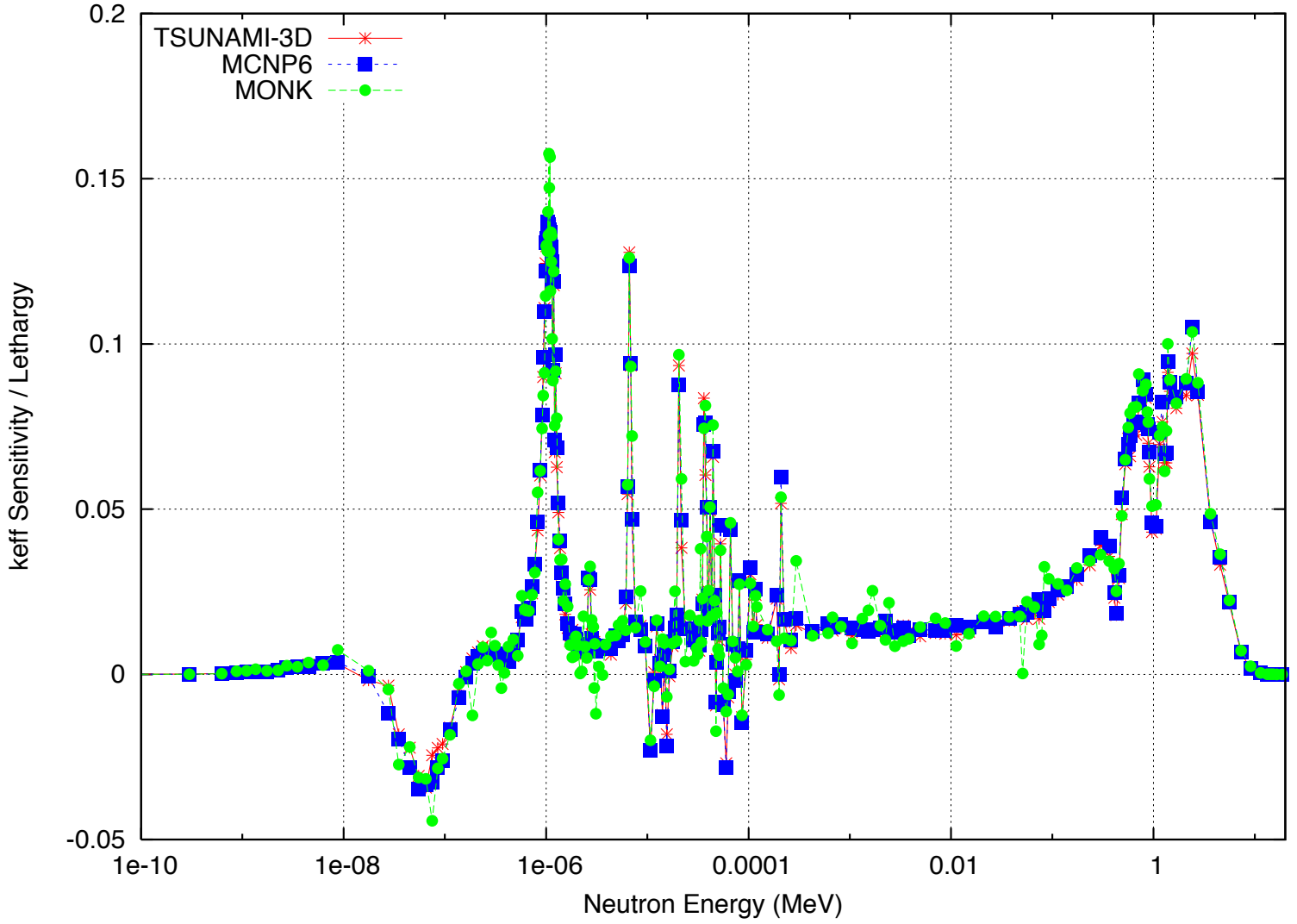


Example Sensitivity Coefficient Profile

Monte Carlo Codes
XCP-3, LANL

H-1: elastic scattering cross-section sensitivity

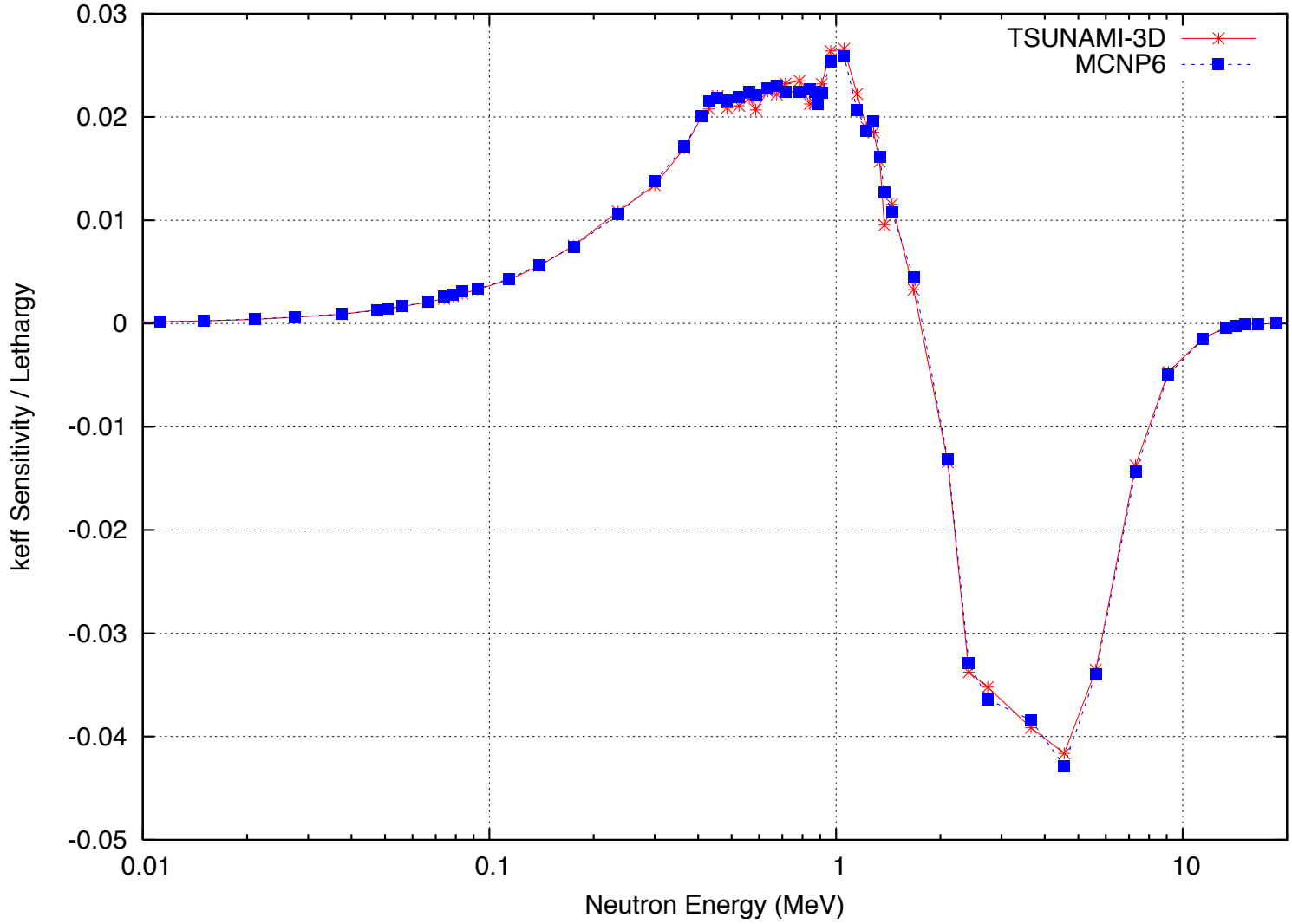
OECD/NEA UACSA Benchmark Phase III.1



Example Sensitivity Coefficient Profile

- **Pu-239: fission chi(E) sensitivity**

OECD/NEA UACSA Benchmark Phase III.1



MCNP6 - KOPTS Card

- KOPTS controls many special features for KCODE calculations
- For keff sensitivity calculations, KOPTS is used to control the following:
  - Size of the blocks (default is 10 cycles)
  - Sensitivity output printing (default is just to the output file).
- Format:

  KOPTS BLOCKSIZE= N KSENTAL= FILEOPT

- For now, the only "FILEOPT" allowed is MCTAL, which has MCNP produce a special MCTAL results file

MCNP6 - KSEN Card

- **Format for nuclear data:**

  KSEN*j* XS ISO= ZAID1 ZAID2 … RXN= MT1 MT2 …

  ERG= E1 E2 …

- **Notes:**
  - ***j* is an arbitrary user index (> 0).**
  - **XS defines the type of sensitivity (XS only allowed for now).**
  - **ISO is followed by a list of ZAIDS or S(a,b) identifiers (e.g., 92235.70c, default is all isotopes).**
  - **RXN is a list of MT numbers (default is total, see next slide for a shortened list).**
  - **ERG is a user-defined energy grid in MeV (default 0 to infinity).**
  - **More options available for secondary distributions (e.g., chi).**
  - **Multiple instances of KSEN are allowed, so long as they have a different user index *j*.**

MCNP6 - KSEN Reaction MT numbers

Monte Carlo Codes
XCP-3, LANL

- **Partial list of valid reaction MTs for KSEN**

– Total	1
– Capture	-2
– N,Gamma	102
– Elastic Scattering	2
– Inelastic Scattering	4
– Fission	-6
– Fission Nu	-7
– N,2N	16
– Fission Chi	-1018
– Elastic Law	-1002

MCNP6 - KSEN Examples

- **Capture cross section sensitivity for all isotopes**

```
ksen1    xs    rxn= -2
```

- **U-238 elastic and inelastic scattering sensitivities**

```
ksen2    xs    iso= 92238.70c    rxn=  2   4
```

- **H-1 and light-water S(a,b) total sensitivity with uniform lethargy grid from 1e-5 eV to 100 MeV**

```
ksen3    xs    iso= 1001.70c  lwtr.10t    rxn=    1
                     erg= 1.e-11 12ilog 1e+2
```

MCNP6 Example 1: KSEN Card

- Copy puc6.txt from SOLUTIONS directory to ksen1.txt.
- Find sensitivities to 3 x 2 array of cans containing plutonium nitrate solution.
  - Set KCODE card to use 5000 neutrons per cycle, skip 50, and run 250 cycles total.
  - Set KOPTS card to have a BLOCKSIZE of 5.
  - Add a cross section sensitivity card with no arguments, i.e., use all defaults

```
kcode    5000    1.0    50   250
...
c
c ### keff sensitivity cards
c
kopts    blocksize = 5
c
c default ksen, get total xs sensitivity to all isotopes
ksen1    xs
```

- Run the problem and analyze output.

MCNP6 Exercise 1: Results

Monte Carlo Codes
XCP-3, LANL

```
 nuclear data keff sensitivity coefficients

  sensitivity profile      1

        energy range:    0.0000E+00   1.0000E+36 MeV

  isotope        reaction        sensitivity    rel. unc.

 1001.70c          total          4.7564E-01      0.0589
 7014.70c          total         -1.0670E-02      0.5088
 8016.70c          total          1.2197E-01      0.1225
24050.70c          total         -9.1837E-05      4.4999
24052.70c          total          2.5948E-03      0.3650
24053.70c          total          7.2096E-04      0.8493
24054.70c          total          1.5180E-05      7.5290
26054.70c          total         -4.5558E-04      0.8763
26056.70c          total          1.3197E-02      0.1791
26057.70c          total          7.9241E-04      0.5101
...
94239.70c          total          8.1218E-02      0.0919
94240.70c          total         -4.5498E-02      0.0288
94241.70c          total          7.6258E-04      0.1957
94242.70c          total         -6.0798E-05      0.0480
 lwtr.10t          total          1.6518E-01      0.1716
```

- Total cross section sensitivities can also be thought of as the sensitivity to the atomic density
- Observations:
  - Water (hydrogen and oxygen) have the most impact on k in this system.
  - Pu-239 has a significant, but smaller impact.
  - Other significant, but less important, isotopes are Pu-240 and Fe-56.
- Pu-239 total sensitivity is small for a dominant fissile isotope
  - Investigate this by decomposing this into specific reactions

MCNP6 Exercise 2: Sensitivities by Reaction

- Copy ksen1.txt to ksen2.txt.

- Find sensitivities of total, capture, elastic, inelastic, and fission for H-1, light-water S(a,b), O-16, and Pu-239
  - Delete the old KSEN card and insert a new one

```
c
c ### keff sensitivity cards
c
kopts   blocksize= 5
c
c reaction sensitivities for h-1, o-16, pu-239
c capture, elastic, inelastic, fission
ksen2   xs   iso= 1001.70c lwtr.10t 8016.70c 94239.70c
             rxn=   1 -2  2  4 -6
```

- Run the problem and analyze output.

MCNP6 Exercise 2: Results

Monte Carlo Codes
XCP-3, LANL

1001.70c	total	4.7564E-01	0.0589
1001.70c	capture	-4.1980E-02	0.0110
1001.70c	elastic	5.1762E-01	0.0541
1001.70c	inelastic	0.0000E+00	0.0000
1001.70c	fission	0.0000E+00	0.0000
lwtr.10t	total	1.6518E-01	0.1716
lwtr.10t	capture	0.0000E+00	0.0000
lwtr.10t	elastic	0.0000E+00	0.0000
lwtr.10t	inelastic	1.6518E-01	0.1716
lwtr.10t	fission	0.0000E+00	0.0000
8016.70c	total	1.2197E-01	0.1225
8016.70c	capture	-1.3346E-03	0.0491
8016.70c	elastic	1.2219E-01	0.1219
8016.70c	inelastic	1.1203E-03	0.2583
8016.70c	fission	0.0000E+00	0.0000
94239.70c	total	8.1218E-02	0.0919
94239.70c	capture	-3.0413E-01	0.0076
94239.70c	elastic	-1.3872E-03	1.2795
94239.70c	inelastic	6.1685E-04	0.8563
94239.70c	fission	3.8605E-01	0.0140

- **Elastic scattering with H-1 and O-16 are important, as is inelastic thermal scattering with H-1 in H2O molecule.**
- **Pu-239 fission and capture are of similar opposing magnitude, which is the cause of a lower than normal sensitivity to keff.**
- **Analyze Pu-239 capture and fission as function of energy.**

MCNP6 Exercise 3: Sensitivities by Energy

- Copy ksen2.txt to ksen3.txt.

- Find sensitivities of Pu-239 capture and fission as function of energy.
  - Delete the old KSEN card and insert a new one.
  - For the energy bins, use 0 to 0.625 eV, 0.625 eV to 100 keV, and 100 keV to 100 MeV as thermal, intermediate, and fast.

```
c
c ### keff sensitivity cards
c
kopts   blocksize = 5
c
c pu-239 capture and fission sensitivity for thermal,
intermediate, and fast
ksen3   xs    iso = 94239.70c
              rxn = -2 -6
              erg = 0  0.625e-6   0.1   100
```

- Run the problem and analyze output.

MCNP6 Exercise 3: Results

Monte Carlo Codes
XCP-3, LANL

94239.70c capture

energy range (MeV)		sensitivity	rel. unc.
0.0000E+00	6.2500E-07	-2.7413E-01	0.0084
6.2500E-07	1.0000E-01	-2.9833E-02	0.0124
1.0000E-01	1.0000E+02	-1.7170E-04	0.0066

94239.70c fission

energy range (MeV)		sensitivity	rel. unc.
0.0000E+00	6.2500E-07	3.3226E-01	0.0184
6.2500E-07	1.0000E-01	4.2493E-02	0.0556
1.0000E-01	1.0000E+02	1.1298E-02	0.1122

- Most of the effect for fission and capture are in the thermal range (as expected).
- Both thermal and intermediate Pu-239 capture and fission are of similar magnitude.
- Fast Pu-239 capture is negligible relative to Pu-239 fission.

MCNP6 - KSEN with Secondary Distributions

- **More complete KSEN:**

KSEN*j* XS ISO = ZAID1 ZAID2 … RXN = MT1 MT2 …
ERG = E1 E2 … COS = C1 C2 …
EIN = I1 I2 …
CONSTRAIN = YES/NO

- **Comments:**
  - **For secondary distributions ERG is with respect to outgoing energies (default 0 to infinity).**
  - **COS defines direction cosine changes from the collision (default -1 to 1)**
  - **EIN defines the incident energy range (default 0 to infinity)**
  - **CONSTRAIN tells MCNP whether the distribution must be renormalized to preserve probability (default is YES)**
  - **If cross sections or fission nu listed in RXN, MCNP will calculate those as normal.**

MCNP6 - Constrained Chi Sensitivity Example

- **KSEN card of Pu-239 chi sensitivity:**

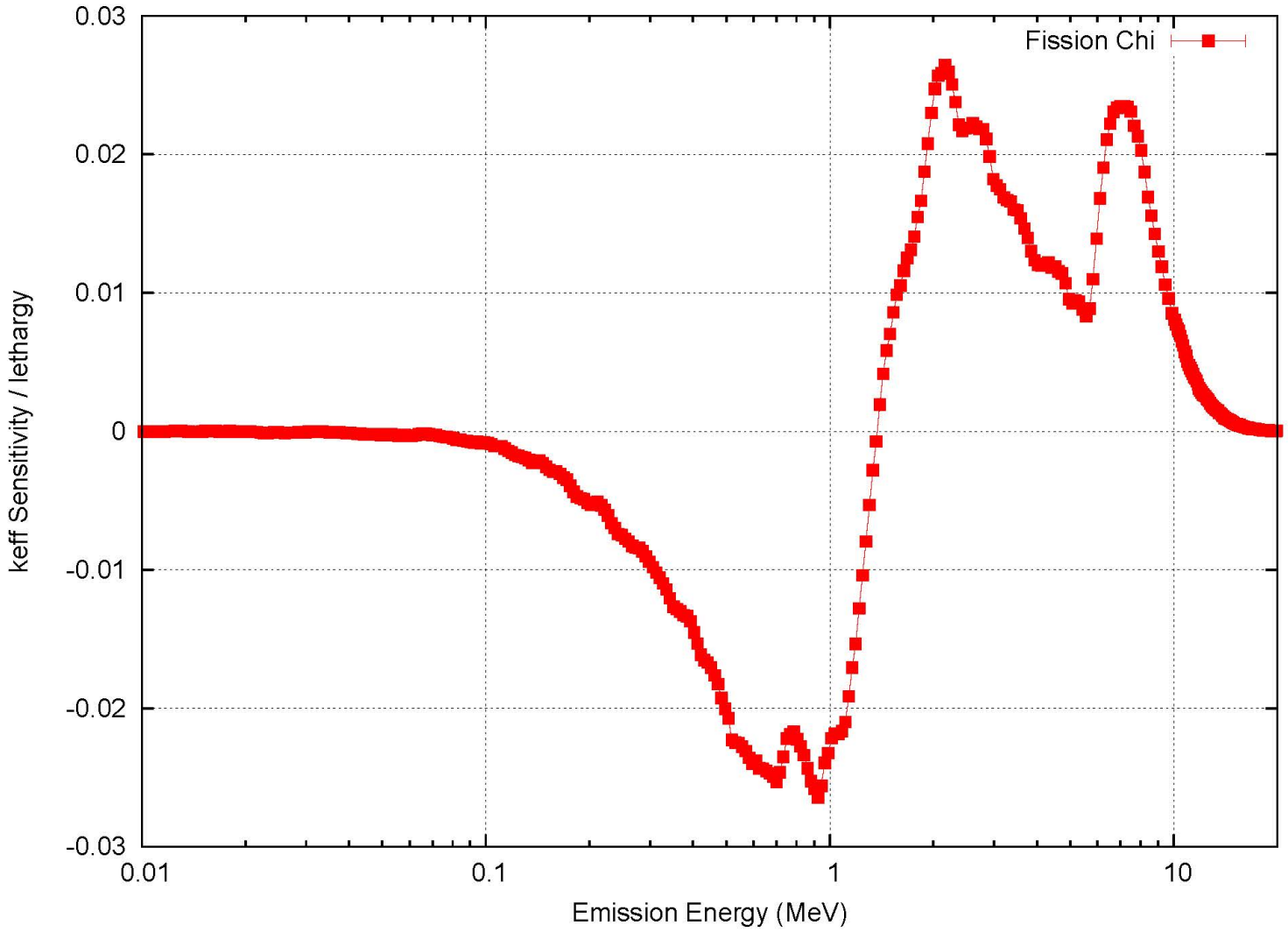
```
ksen94  xs   iso= 94239.70c
             rxn= -1018
             erg= 1e-11 999ilog 20
             ein= 0 19i 20
             constrain= yes
```

- **Comments:**
  - **Fine outgoing energy binning in lethargy**
  - **Incident energy bins are in 1 MeV intervals from 0 to 20 MeV**
  - **MCNP should give a sensitivity to a distribution that is renormalized**

Constrained Chi Sensitivity Example

Monte Carlo Codes
XCP-3, LANL

- **Pu-239 chi sensitivity in Jezebel (Pu Sphere):**



Covariance Data

Cross-section Covariance Data (1)

- For a given isotope, these 12 cross-sections & sensitivities are used within Whisper:

MT	reaction
2	elastic scatter
4	inelastic
16	n,2n
18	fission
102	n,γ
103	n,p
104	n,d
105	n,t
106	n,^{3}He
107	n,α
452	ν
1018	χ

Cross-section Covariance Data (2)

- MCNP uses continuous-energy cross-section data & collision physics, but sensitivity profiles are tallied in 44 energy bins

- The 44 energy bins reflect the cross-section covariance data files obtained for each isotope & reaction from the SCALE system

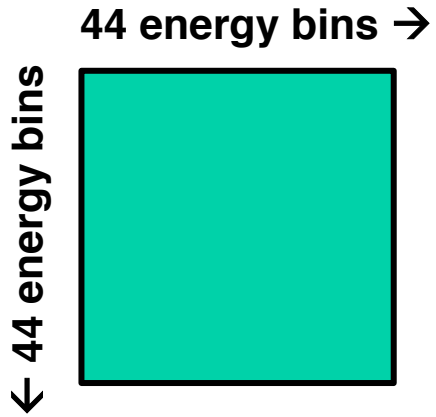
Energy bin bounds (MeV)

```
1.0000e-11 3.0000e-09 7.5000e-09 1.0000e-08 2.5300e-08 3.0000e-08
4.0000e-08 5.0000e-08 7.0000e-08 1.0000e-07 1.5000e-07 2.0000e-07
2.2500e-07 2.5000e-07 2.7500e-07 3.2500e-07 3.5000e-07 3.7500e-07
4.0000e-07 6.2500e-07 1.0000e-06 1.7700e-06 3.0000e-06 4.7500e-06
6.0000e-06 8.1000e-06 1.0000e-05 3.0000e-05 1.0000e-04 5.5000e-04
3.0000e-03 1.7000e-02 2.5000e-02 1.0000e-01 4.0000e-01 9.0000e-01
1.4000e+00 1.8500e+00 2.3540e+00 2.4790e+00 3.0000e+00 4.8000e+00
6.4340e+00 8.1873e+00 2.0000e+01
```

- When better cross-section covariance data become available, more energy bins will be used

Cross-section Covariance Data (3)

- For a particular isotope & particular reaction (MT), the nuclear data uncertainties are a G x 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 (4)

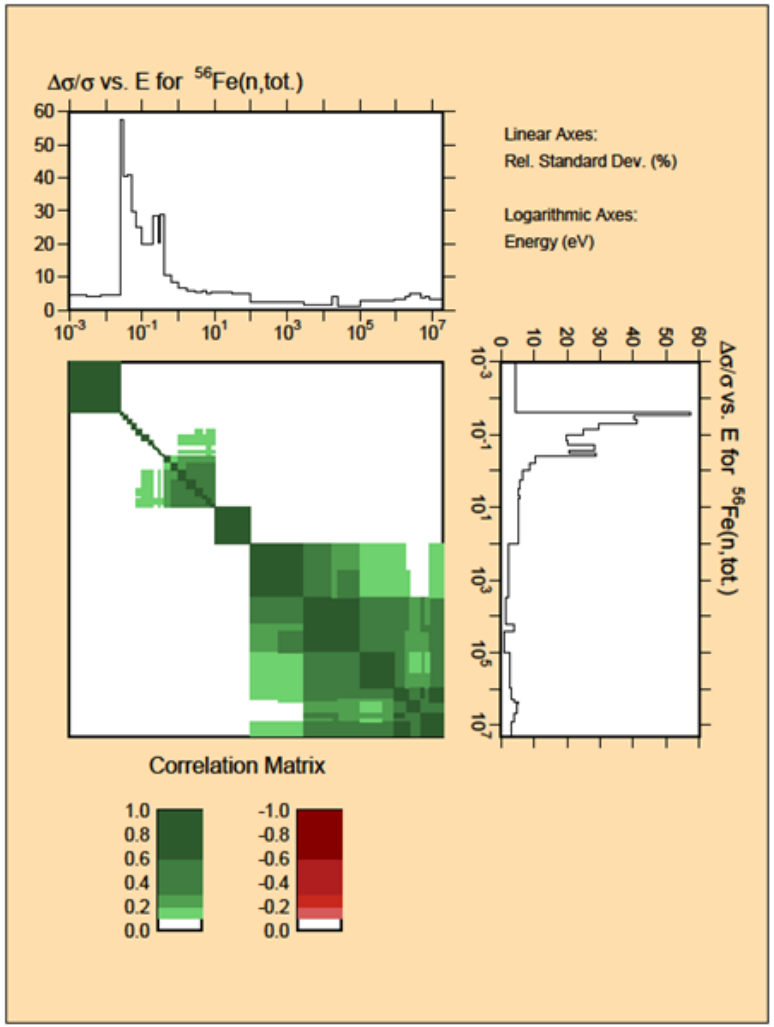


FIG. 9: A typical NJOY-generated plot of ENDF/B-VII.0 data downloaded from the National Nuclear Data Center, BNL, USA.

Cross-section Covariance Data (5)

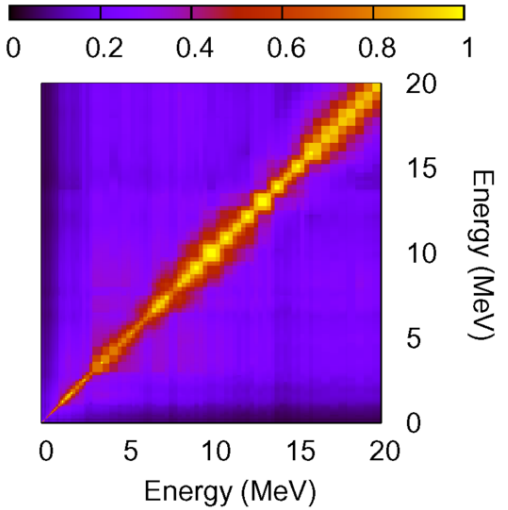


FIG. 3: Correlation matrix for the neutron-induced fission cross section on ^{235}U. It was evaluated by Pronyaev *et al.* as part of the cross section standards evaluation [19].

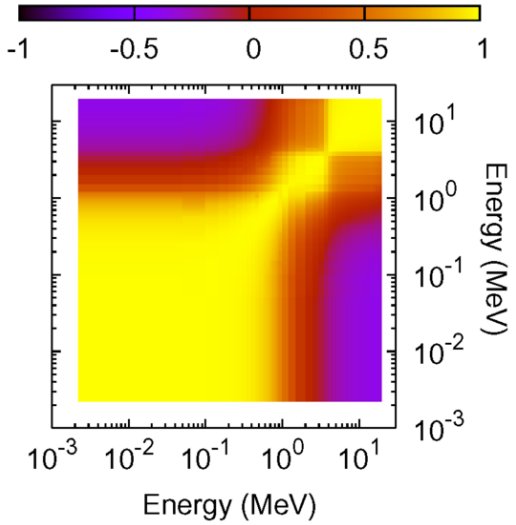


FIG. 6: Correlation matrix for the capture cross section of n+^{235}U.

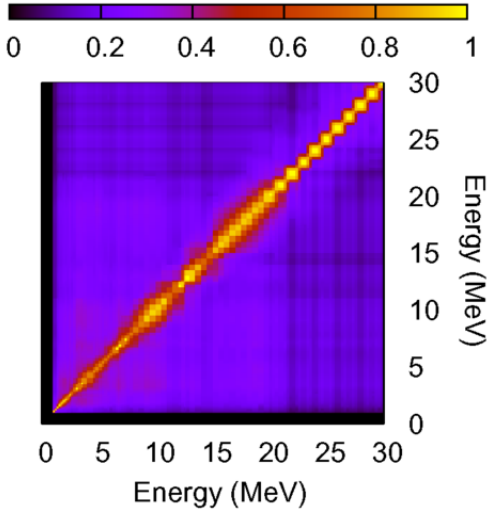


FIG. 13: ^{238}U fission cross-section correlation matrix.

Covariance plots on this & next page taken from:

P. Talou, P.G. Young, T. Kawano, M. Rising, M.B. Chadwick, "Quantification of Uncertainties for Evaluated Neutron-Induced Reactions on Actinides in the Fast Energy Range", Nuclear Data Sheets 112, 3054–3074 (2011)

Cross-section Covariance Data (6)

Monte Carlo Codes
XCP-3, LANL

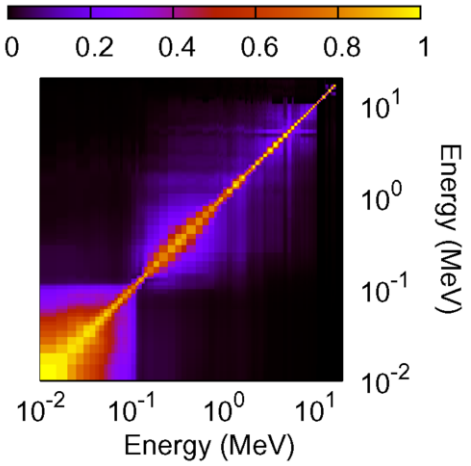


FIG. 25: Correlation matrix evaluated for the ^{238}Pu (n,fission) cross section.

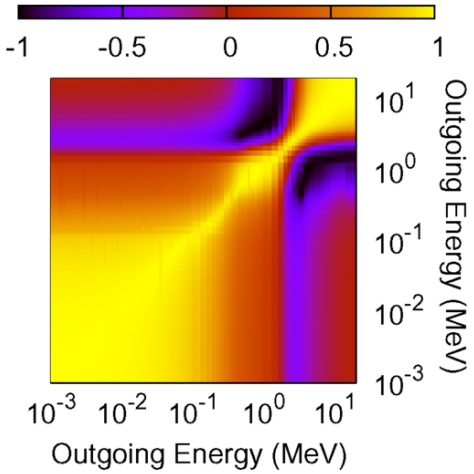


FIG. 40: Correlation matrix evaluated for the n(0.5 MeV)+^{239}Pu prompt fission neutron spectrum.

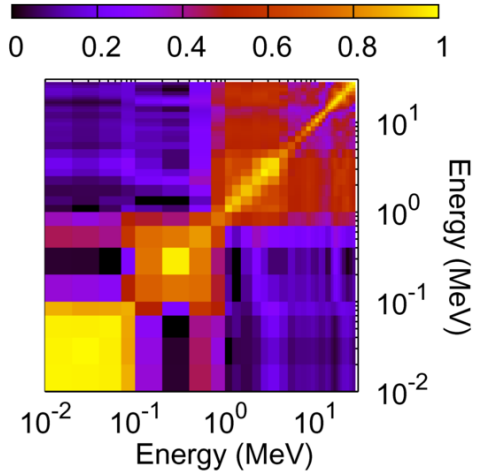


FIG. 43: Evaluated correlation matrix for the neutron-induced fission cross section of ^{240}Pu in the fast energy range.

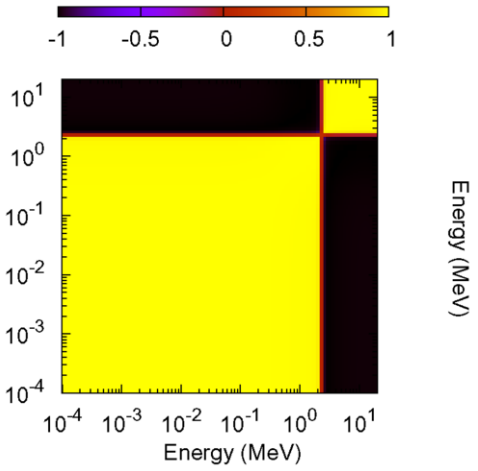


FIG. 30: Correlation matrix for the n(0.5 MeV)+^{238}Pu prompt fission neutron spectrum.

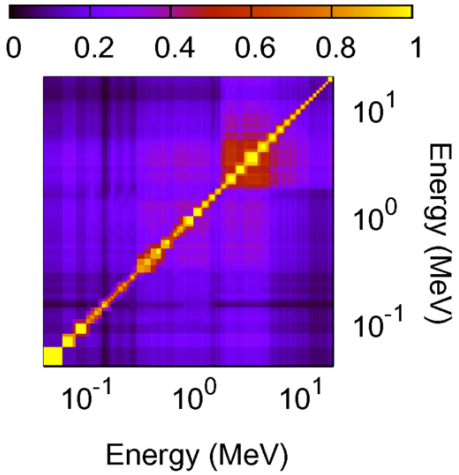


FIG. 45: ^{240}Pu (n,total) cross section correlation matrix.

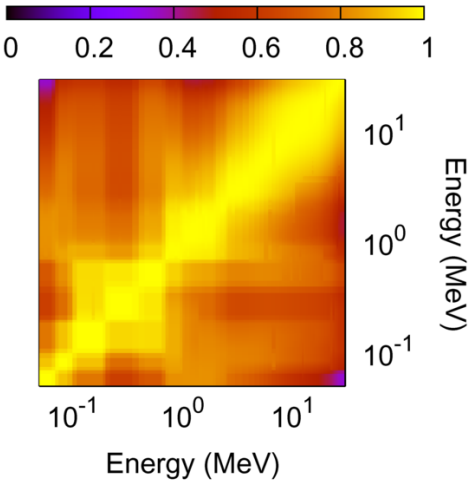


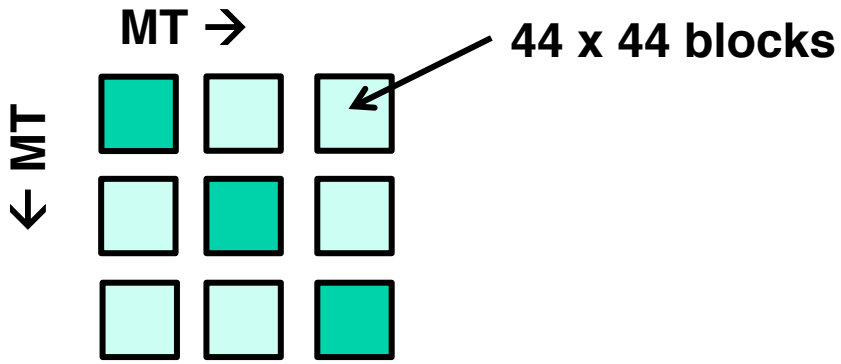
FIG. 47: Correlation matrix for the n+^{240}Pu capture cross section. Large off-diagonal elements are due mostly to model uncertainties, since no experimental data exist above 300 keV.

Cross-section Covariance Data (7)

- **For each isotope, with 44 energies & 12 reactions:**

  C_{xx}^{Iso} : c(44, 44, 12, 12)

  - Each diagonal element of C_{xx} is the variance of the cross-section for a particular MT & energy bin
  - Off-diagonal elements of C_{xx} are the shared variance between pairs of MT-E & MT'-E' (Off-diagonal MT-MT' blocks would generally be 0)

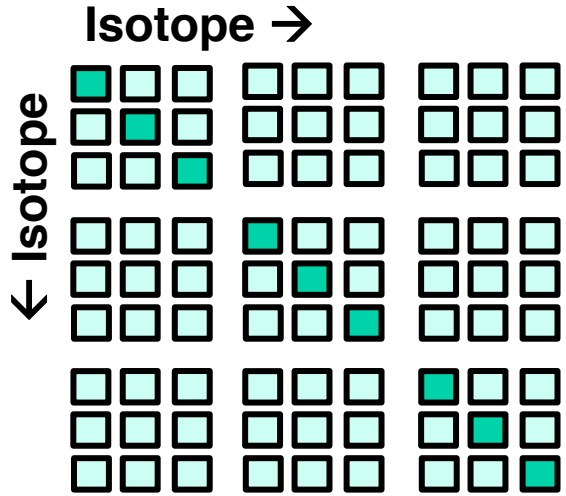


  - Each C_{xx}^{Iso} entry is produced by SCALE or NJOY based on covariance data from the ENDF/B libraries (with some adjustments if needed)
  - The C_{xx} data is universal, independent of benchmark or application problem

Cross-section Covariance Data (8)

- **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**

C_{xx} =



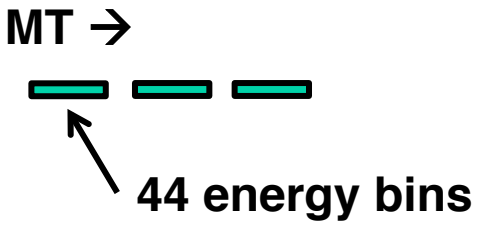
  - Each diagonal element of C_{xx} is the variance of the cross-section for a particular isotope, MT, & energy bin
  - Off-diagonal elements of C_{xx} are the shared variance between pairs of Iso-MT-E & Iso'-MT'-E'
  - Very sparse (lots of zeros), block-structured matrix
    (Off-diagonal I-I' blocks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

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 Keff 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, & energy bin

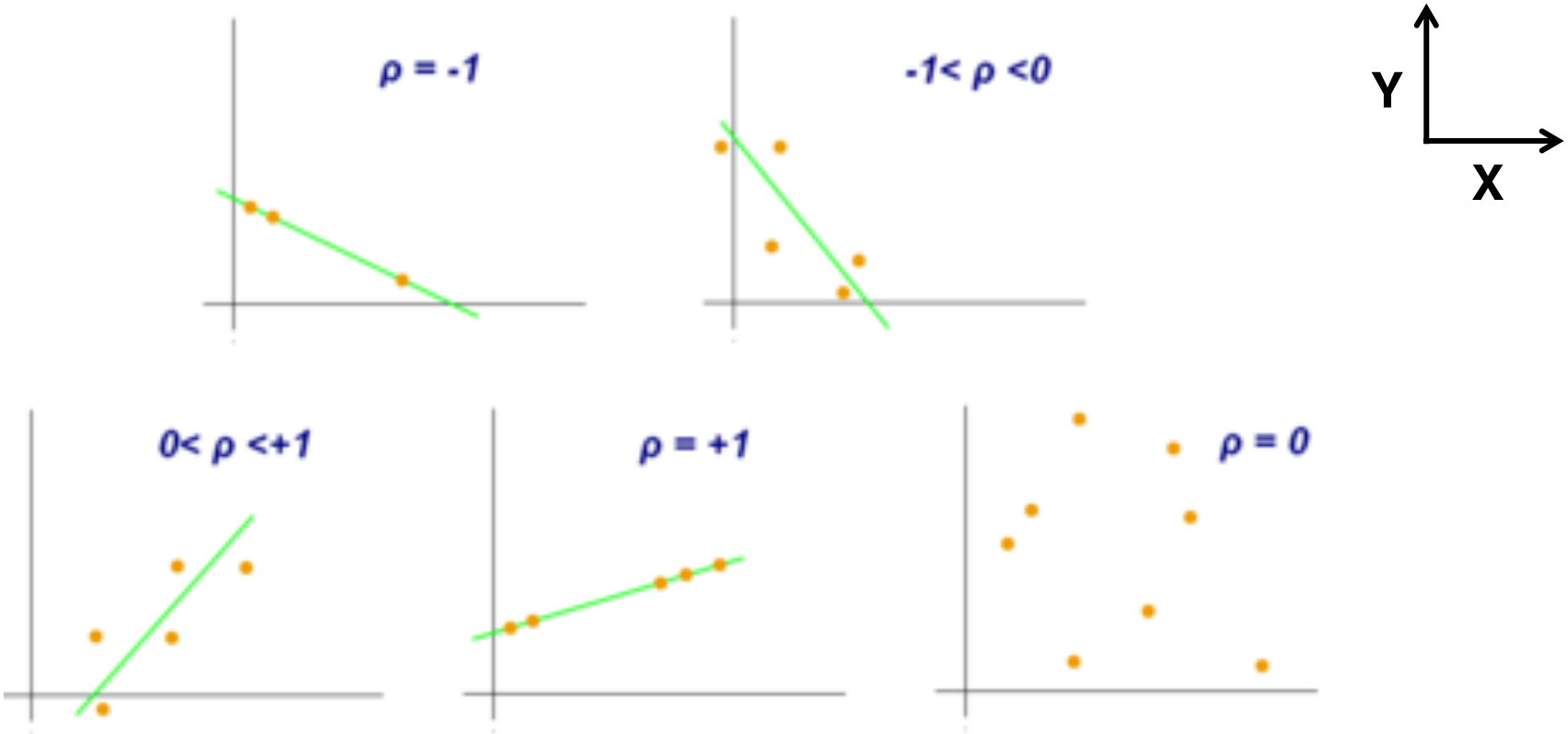


- For a particular application problem, A, the sensitivity profiles for all isotopes are combined into one sensitivity vector S_A

Correlation Coefficients

Correlation Coefficient (1)

- **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
    - $\rho = 0$ no correlation



Correlation Coefficient (2)

- **Population correlation coefficient, ρ**
  - **Distribution of X, with mean μ_x, standard deviation σ_x**
  - **Distribution of Y, with mean μ_y, standard deviation σ_y**

$$\rho_{X,Y} = \frac{\mathrm{cov}(X,Y)}{\sigma_X \cdot \sigma_Y} = \frac{E[(X-\mu_X)(Y-\mu_Y)]}{\sigma_X \cdot \sigma_Y} = \frac{E(XY)-E(X)\cdot E(Y)}{\sigma_X \cdot \sigma_Y}$$

$$\mu_X = E(X) \qquad \sigma_X^2 = E[(X-E(X))^2] = E(X^2)-E(X)^2$$

$$\mu_Y = E(Y) \qquad \sigma_Y^2 = E[(Y-E(Y))^2] = E(Y^2)-E(Y)^2$$

- **Sample correlation coefficient, r**
  - **Dataset for X: { x_1, x_2, ..., x_n }, mean x-bar, std dev s_x**
  - **Dataset for Y: { y_1, y_2, ..., y_n } mean y-bar, std dev s_y**

$$r = r_{xy} = \frac{\frac{1}{n}\sum x_i y_i - \overline{x}\cdot\overline{y}}{s_x \cdot s_y}$$

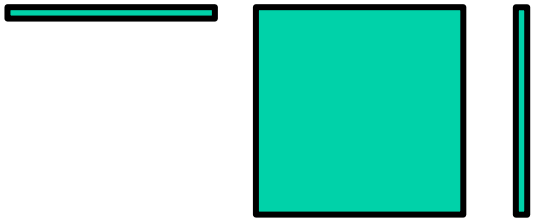
Variance in Keff & Correlation Between Problems

- **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:**

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

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



= scalar

- **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

Monte Carlo Codes
XCP-3, LANL

- **Matrix-vector operations**

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

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

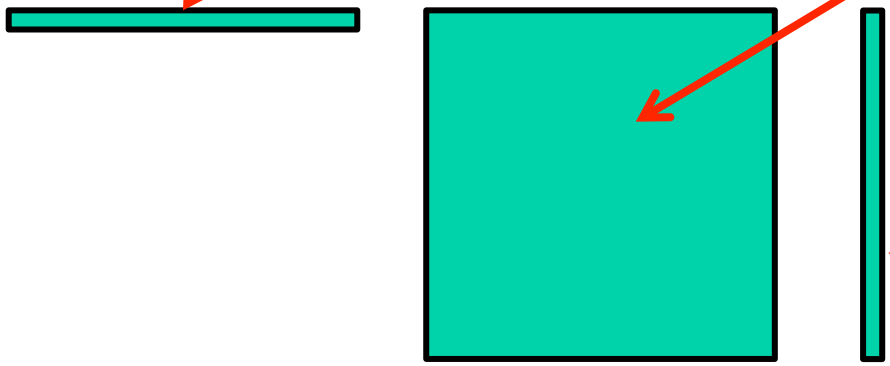
Problem-dependent sensitivity vector, S.

Based on flux spectrum, adjoint spectum, nuclear data, problem isotopes, geometry, temperature

Size = G x MT x NI

Nuclear Data Covariances

Size= (G x MT x NI)^2



= scalar

S^T

Error Propagation (1)

- **Define a linear relationship**

$$\mathbf{y} = \mathbf{A}\mathbf{x} + \mathbf{b}$$

- **Determine expected (mean) value of y**

$$\mu_{\mathbf{y}} = E[\mathbf{y}] = E[\mathbf{A}\mathbf{x} + \mathbf{b}] = \mathbf{A}E[\mathbf{x}] + \mathbf{b} = \mathbf{A}\mu_{\mathbf{x}} + \mathbf{b}$$

- **Determine covariance matrix of y**

$$\begin{aligned}
\mathbf{C}_{\mathbf{y}} &= \mathrm{cov}(\mathbf{y},\mathbf{y}) = E[(\mathbf{y} - \mu_{\mathbf{y}})(\mathbf{y} - \mu_{\mathbf{y}})^T] \\
&= E[(\mathbf{A}\mathbf{x} + \mathbf{b} - \mathbf{A}\mu_{\mathbf{x}} - \mathbf{b})(\mathbf{A}\mathbf{x} + \mathbf{b} - \mathbf{A}\mu_{\mathbf{x}} - \mathbf{b})^T] \\
&= E[(\mathbf{A}(\mathbf{x} - \mu_{\mathbf{x}}))(\mathbf{A}(\mathbf{x} - \mu_{\mathbf{x}}))^T] \\
&= E[\mathbf{A}(\mathbf{x} - \mu_{\mathbf{x}})(\mathbf{x} - \mu_{\mathbf{x}})^T \mathbf{A}^T] \\
&= \mathbf{A}\, E[(\mathbf{x} - \mu_{\mathbf{x}})(\mathbf{x} - \mu_{\mathbf{x}})^T]\mathbf{A}^T \\
&= \mathbf{A}\,\mathrm{cov}(\mathbf{x},\mathbf{x})\,\mathbf{A}^T \\
\mathbf{C}_{\mathbf{y}} &= \mathbf{A}\,\mathbf{C}_{\mathbf{x}}\,\mathbf{A}^T
\end{aligned}$$

"Sandwich" Rule!

Error Propagation (2)

- **First-order Taylor series expansion of k about cross section, Σ**

$$k(\Sigma_1^{'},\Sigma_2^{'},\ldots,\Sigma_N^{'}) \cong k(\Sigma_1^0,\Sigma_2^0,\ldots,\Sigma_N^0) + \sum_{i=1}^{N} \left.\frac{\partial k}{\partial \Sigma_i}\right|_{\Sigma_i^0} (\Sigma_i^{'} - \Sigma_i^0)$$

- **Define vectors for cross sections and sensitivity profiles**

$$\vec{\Sigma}^{'} = \begin{bmatrix} \Sigma_1^{'} & \Sigma_2^{'} & \cdots & \Sigma_N^{'} \end{bmatrix}$$

$$\vec{\Sigma}^{0} = \begin{bmatrix} \Sigma_1^{0} & \Sigma_2^{0} & \cdots & \Sigma_N^{0} \end{bmatrix}$$

$$\vec{S} = \begin{bmatrix} \left.\frac{\partial k}{\partial \Sigma_1}\right|_{\Sigma_1^0} & \left.\frac{\partial k}{\partial \Sigma_2}\right|_{\Sigma_2^0} & \cdots & \left.\frac{\partial k}{\partial \Sigma_N}\right|_{\Sigma_N^0} \end{bmatrix}$$

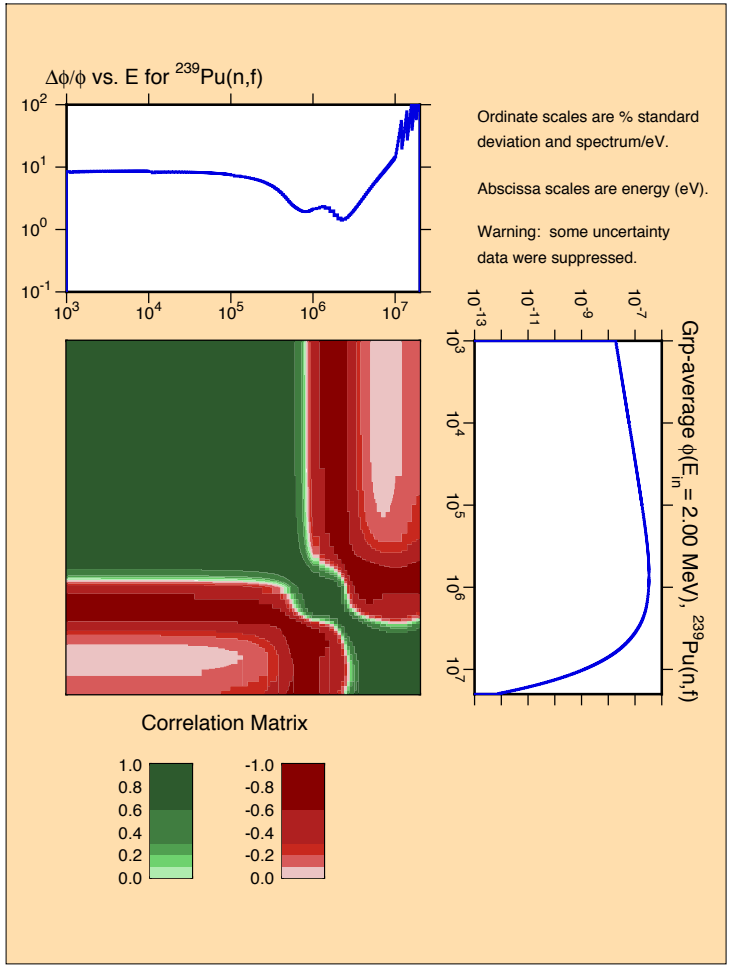
- **Determine covariance matrix (variance) of k**

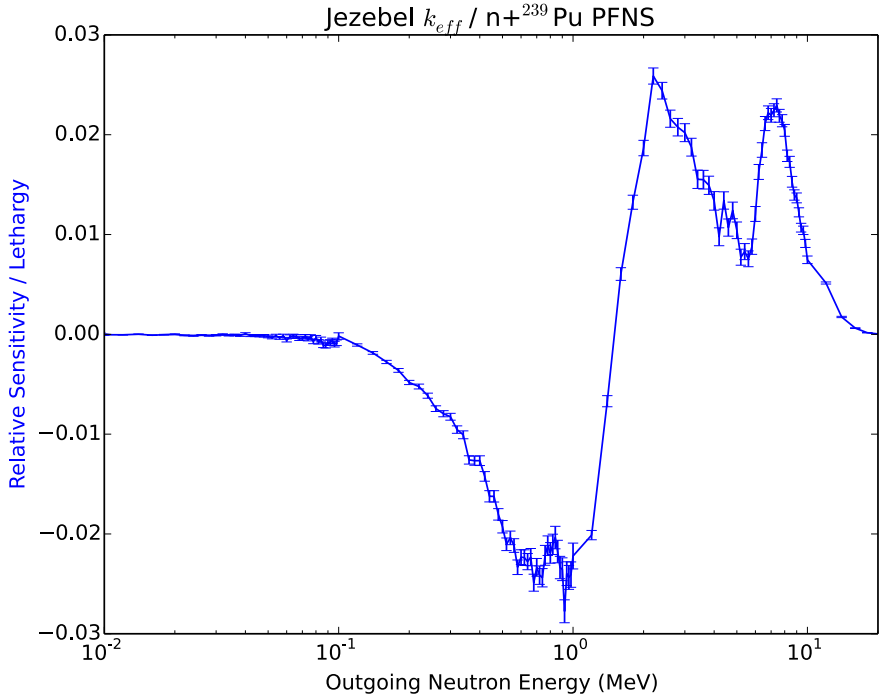
$$\begin{aligned} k(\vec{\Sigma}^{'}) &\cong k(\vec{\Sigma}^0) + \vec{S}(\vec{\Sigma}^{'} - \vec{\Sigma}^0)^T \\ &= \vec{S}\,\vec{\Sigma}^{'T} + \left[k(\vec{\Sigma}^0) - \vec{S}\,\vec{\Sigma}^{0T}\right] \\ &= \mathbf{Ax} \quad + \quad \mathbf{b} \end{aligned}$$

$$\boxed{\mathbf{C}_k = \vec{S}\,\mathbf{C}_\Sigma\,\vec{S}^T}$$

Error Propagation (3)

- **Example using sandwich rule, ^{239}Pu PFNS impact on *k***





Uncertainty in *k* due to ^{239}Pu PFNS only!

$$\sigma_k^2 = \vec{S}\,\mathbf{C}_X\,\vec{S}^T$$

$$\frac{\sigma_k}{k} \cong 0.160\%$$

Whisper

Software for Sensitivity-Uncertainty-based Nuclear Criticality Safety Validation

Whisper – Summary

Whisper - Software for Sensitivity-Uncertainty-Based Nuclear Criticality Safety Validation

Whisper is computational software designed to assist the nuclear criticality safety (NCS) analyst with validation studies with the Monte Carlo radiation transport package MCNP. Standard approaches to validation rely on the selection of benchmarks based upon expert judgment. Whisper uses sensitivity/uncertainty (S/U) methods to select relevant benchmarks to a particular application or area of applicability (AOA), or set of applications being analyzed. Using these benchmarks, Whisper computes a calculational margin from an extreme value distribution. In NCS, a margin of subcriticality (MOS) that accounts for unknowns about the analysis. Typically, this MOS is some prescribed number by institutional requirements and/or derived from expert judgment, encompassing many aspects of criticality safety. Whisper will attempt to quantify the margin from two sources of potential unknowns, errors in the software and uncertainties in nuclear data. The Whisper-derived calculational margin and MOS may be used to set a baseline upper subcritical limit (USL) for a particular AOA, and additional margin may be applied by the NCS analyst as appropriate to ensure subcriticality for a specific application in the AOA.

Whisper provides a benchmark library containing over 1,100 MCNP input files spanning a large set of fissionable isotopes, forms (metal, oxide, solution), geometries, spectral characteristics, etc. Along with the benchmark library are scripts that may be used to add new benchmarks to the set; this documentation provides instructions for doing so. If the user desires, Whisper may analyze benchmarks using a generalized linear least squares (GLLS) fitting based on nuclear data covariances and identify those of lower quality. These may, at the discretion of the NCS analyst and their institution, be excluded from the validation to prevent contamination of potentially low quality data. Whisper provides a set of recommended benchmarks to be optionally excluded.

Whisper also provides two sets of 44-group covariance data. The first set is the same data that is distributed with SCALE 6.1 in a format that Whisper can parse. The second set is an adjusted nuclear data library based upon a GLLS fitting of the benchmarks following rejection. Whisper uses the latter to quantify the effect of nuclear data uncertainties within the MOS. Whisper also has the option to perform a nuclear covariance data adjustment to produce a custom adjusted covariance library for a different set of benchmarks.

Whisper

- **Whisper History, Background, SQA Status, Documentation**

- **Whisper Methodology**
  - Capabilities
  - Correlation Coefficients
  - Cross-section Covariance Data
  - Sensitivity Profiles
  - Variance in Keff & Correlation Between Problems
  - Determining benchmark C_k's
  - Determining bias & bias uncertainty
  - Determining portions of the MOS

- **Using Whisper for Validation**
  - Overview
  - Using whisper_mcnp
  - Using whisper_usl
  - Examples

Whisper Methodology for Validation & USLs (2)

- **Whisper ICSBEP Benchmark Suite**
  - **1101 ICSBEP benchmark problems from Mosteller, Kahler, others**
  - **Sensitivity profiles from adjoint-weighting for all isotopes/reactions/benchmarks**
- **Whisper methodology –** LA-UR-14-26558, LA-UR-14-26436, LA-UR-14-23352
  - **Validation benchmarks**
    - Estimate missing uncertainties
    - Reject inconsistent benchmarks via iterated diagonal chi-squared method (~12%)
    - Correlation data from DICE; covariance data from ORNL (10% diag for missing)
    - Automated benchmark selection for AOA problem using sensitivity data to determine C_k values; C_k values used for weighting
  - **Calculational Margin**
    - Determine bias from non-parametric method based on Extreme Value Theory, using weighting determined from C_k values
    - Determine bias uncertainty numerically from distribution of worst-case k_{eff} bias
  - **Margin of Subcriticality**
    - Margin of 0.0050 for unknown code errors (expert judgment)
    - Margin for nuclear data uncertainty from GLLS method
    - Additional margin – analyst judgment for AOA & problem, conservatism, etc.
  - **USL = 1.0 – Calculational Margin – Margin of Subcriticality**

Whisper SQA

- **Whisper is part of the MCNP software package**
  - Will be distributed to the criticality-safety community via future RSICC releases of MCNP
  - Feedback from criticality-safety analysts at DOE sites will be factored into future development
  - Potential for world-wide feedback/review/improvements
- **Maintained under MCNP version control system (GIT, TeamForge)**
  - LANL standard
  - WHISPER GIT Module for checkout into MCNP source tree
  - All revisions, additions, improvements tracked under Artifact 36407
- **MCNP SQA methodology**
  - Encompasses Whisper
  - Previous audits & reviews of MCNP SQA determined that methodology was compliant with DOE/ASC & LANL P1040 requirements
  - Review is in progress to assess current MCNP SQA P1040 compliance, and make any revisions required to continue compliance

Whisper Documentation

- **THEORY**

  B.C. Kiedrowski, F.B. Brown, et al., "Whisper: Sensitivity/Uncertainty-Based Computational Methods and Software for Determining Baseline Upper Subcritical Limits", Nuc. Sci. Eng. Sept. 2015, LA-UR-14-26558 (2014),

  B.C. Kiedrowski, "Methodology for Sensitivity and Uncertainty-Based Criticality Safety Validation", LA-UR-14-23202 (2014)

- **USER MANUAL**

  B.C. Kiedrowski, "User Manual for Whisper (v1.0.0), Software for Sensitivity- and Uncertainty-Based Nuclear Criticality Safety Validation", LA-UR-14-26436 (2014)

- **APPLICATION**

  B.C. Kiedrowski, et al., "Validation of MCNP6.1 for Criticality Safety of Pu-Metal, -Solution, and -Oxide Systems", LA-UR-14-23352 (2014)

- **SOFTWARE QUALITY ASSURANCE**

  R.F. Sartor, F.B. Brown, "Whisper Program Suite Validation and Verification Report", LA-UR-15-23972 (2015-05-28)

  R.F. Sartor, F.B. Brown, "Whisper Source Code Inspection Report", LA-UR-15-23986 (2015-05-28)

  R.F. Sartor, B.A. Greenfield, F.B. Brown, "MCNP6 Criticality Calculations Verification and Validation Report", LA-UR-15-23266 (2015-04-30)

  Monte Carlo Codes Group (XCP-3), "Whisper - Software for Sensitivity-Uncertainty-based Nuclear Criticality Safety Validation", LANL TeamForge Tracker system, Artifact artf36407 (2015)

  Monte Carlo Codes Group (XCP-3), WHISPER module in LANL TeamForge GIT repository (2015)

  Monte Carlo Codes Group (XCP-3), MCNP6 module in LANL TeamForge GIT repository

  Monte Carlo Codes Group (XCP-3), "MCNP Process Documents", LANL Teamforge wiki for MCNP

  Monte Carlo Codes Group (XCP-3), "Software Quality Assurance", LANL Teamforge wiki for MCNP, P1040-rev9 requirements

Whisper Methodology

Whisper Methodology

- **MCNP6**
  - Determine Sensitivity Profiles for Benchmarks B_1 ... B_N
  - Determine Sensitivity Profiles for Application A

- **Whisper – Determine Benchmark c_k's**
  - For each benchmark B_J, determine $c_k^{(J)}$ correlation coefficient between A & B_J

- **Whisper – Determine Benchmark Weights & Select Benchmarks**
  - Iterative procedure using $c_k^{(J)}$ values, $c_{k,max}$, $c_{k,acc}$

- **Whisper – Determine Calculational Margin (CM)**
  - Extreme Value Theory, with weighted data, nonparametric
  - Compute bias & bias uncertainty
  - Adjustment for non-conservative bias
  - Handling small sample sizes

- **Whisper – Determine portions of MOS**

Whisper Capabilities

Monte Carlo Codes
XCP-3, LANL

Admin

- Install code, scripts, benchmarks, covariance files, correlations
- Test the installation
- Identify inconsistent benchmarks to be rejected
- Estimate missing benchmark uncertainties
- Can add additional benchmarks
- Can reject additional benchmarks

User

- Use whisper_mcnp script to run MCNP6 for process models, to obtain k_{eff} & sensitivity profiles for all isotopes & reactions
- Use whisper_usl script to run Whisper for process models
  - Whisper matches process model sensitivity profiles with benchmark library profiles, selects most similar benchmarks
  - Compute calculational margin for each process model, based on selected benchmarks (bias + bias uncertainty)
  - Estimate cross-section portion of MOS based on GLLS
  - Use 0.005 for code unknowns portion of MOS
  - Estimate baseline USL for each process model (not including additional AOA or other margin)

Using Whisper for Validation

- **As part of Whisper installation (not day-to-day use),**
  - **For each of the 1100+ benchmarks**
    - MCNP6 is run to generate the sensitivity vector S_B for that benchmark
    - The sensitivity vector S_B for each benchmark is saved in a folder
  - **The nuclear data covariance files are saved in a folder**
  - **Benchmarks are checked for consistency, some may be rejected**
  - **Missing uncertainties for some benchmarks are estimated**
  - **Details will be covered later. All of this is the responsibility of the Admin person & needs to be done only once at installation (or repeated if the code, data, or computer change)**

- **To use Whisper for validation:**

  - **Use the whisper_mcnp script to make 1 run with MCNP6 for a particular application, to generate the sensitivity vector for the application, S_A**

  - **Run Whisper, using the whisper_usl script**

Whisper – Overview of Application Use

- **Given S_A for an application, the nuclear data covariance files, and the collection of 1100+ S_B vectors for the benchmarks**
  - **For each of the benchmarks, compute the correlation between the benchmark & application problem, $c_k(A,B)$**
  - **Use the $c_k(A,B)$ values for the benchmarks to compute relative weights for each benchmark**
  - **Select the a set of benchmarks with the highest weights (i.e., the highest neutronics correlations between benchmarks & application)**
  - **Using the selected benchmarks, compute bias, bias uncertainty, & extra margin based on nuclear data uncertainty**
  - **There are of course details, such as acceptable c_k values, determining weights using c_k values, extra penalty if not enough similar benchmarks, benchmark correlation, …..**

Whisper Details – Compute c_k Values

- **Given:**
  - Problem A, Application Sensitivity S_A computed by MCNP
  - Problem B_J, Benchmark Sensitivity S_{Bj} computed by MCNP, J = 1, ..., N (N = number of benchmarks)
- **Find correlation between Application A & Benchmark B_J, J = 1 ... N:**

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

- **Eliminate any negative correlation coefficients**
  - If $c_k^{(J)} < 0$, set $c_k^{(J)} = 0$, J = 1 ... N
- **Determine maximum $c_k^{(J)}$, $c_{k,max}$**

Whisper Details – Benchmark Weights (1)

- **Benchmarks are assigned weights w_J based on their $c_k^{(J)}$ values, $c_{k,max}$, and a (to-be-determined) acceptance threshold, $c_{k,acc}$**
  - **Benchmarks similar to the application, $c_k^{(J)} > c_{k,acc}$: $0 < w_J \leq 1$**
  - **Benchmarks not similar to the application, $c_k^{(J)} < c_{k,acc}$: $w_J = 0$**
  - **Scheme for determining w_J is on next slide**
- **The minimum required total weight, w_{req}, for the set of selected benchmarks is:**

$$w_{req} = w_{min} + (1 - c_{k,max})^* w_{penalty}$$

where $w_{min} = 25$ (default, user opt)
$w_{penalty} = 100$ (default, user opt)

  - **That is, must select enough benchmarks so that $\text{sum}\{ w_J \} \geq w_{req}$**
  - **Rationale**
    - 25 or more are needed for reliable statistical treatment
    - If benchmarks are not close to application ($c_{k,max}$ not close to 1.0), want to require more of them. Simple linear penalty.

- **The determination of benchmark weights is iterative, based on an acceptance criteria $c_{k,acc}$**
  - **$c_{k,acc}$ is the minimum threshold for $c_k^{(J)}$ values**
  - **Benchmarks with $c_k^{(J)} < c_{k,acc}$ are assigned $w_J = 0$**
  - **Benchmarks with $c_k^{(J)} \geq c_{k,acc}$ are assigned weight**

$$w_J = \frac{c_k^{(J)} - c_{k,acc}}{c_{k,max} - c_{k,acc}}$$

- **Iterative procedure determines largest $c_{k,acc}$ that satisfies requirement that $sum\{ w_J \} \geq w_{req}$**
  - **Select a value for $c_{k,acc}$ close to $c_{k,max}$**
  - **Determine benchmark weights (by above scheme)**
  - **If $sum\{ w_J \} < w_{req}$, decrease $c_{k,acc}$ by 10^{-5} & repeat above step**
  - **The iteration ends when enough benchmarks with highest w_J's are selected so that $sum\{ w_J \} \geq w_{req}$**

If not enough benchmarks to satisfy total weight requirement, adjustment scheme is used. Discussed later, at end.....

Whisper Details – Calculational Margin (1)

- **Whisper uses a nonparametric statistical approach to determining the calculational margin (bias + bias uncertainty)**
  - **Does not rely on assumption that ($k_{calc} – k_{bench}$) is normally distributed for the set of benchmarks**
  - **Can handle weighted benchmarks (Tsunami rank-order scheme can't)**
  - **Based on Extreme Value Theory**
    - The addition of less-relevant benchmarks cannot reduce the calculational margin
    - Irrelevant benchmarks (i.e., low c_k) will not non-conservatively affect results
    - Accounting for weighting avoids overly conservative calculational margin
- **Whisper uses EVT to to find the value of a calculational margin that bounds the worst-case bias to some probability of a weighted population**

Note in following discussion:

- **There is the fundamental assumption that for a single benchmark, the bias for that benchmark is normally distributed, according to the experimental uncertainty & Monte Carlo statistics**
- **There is no assumption of normality across the collection of benchmarks, however. The method is nonparametric.**

Whisper Details – Calculational Margin (2)

- Let $\beta_J = k_{calc\ J} - k_{bench\ J}$ and $\sigma^2_J = \sigma^2_{bench\ J} + \sigma^2_{calc\ J}$
  - For convenience, the X_J below are opposite in sign to β_J
- For a set of N benchmarks, let X_J be a random variable normally distributed about β_J with uncertainty σ_J. The cumulative distribution function (CDF) for X_J is

$$F_J(x) = \text{Prob}(X_J < x) = \frac{1}{\sqrt{2\pi}\cdot\sigma_J}\int_{-\infty}^{x} \exp\left[-\frac{1}{2}\left(\frac{y+\beta_J}{\sigma_J}\right)^2\right]dy = \frac{1}{2}\left[1 + \text{erf}\left(\frac{x+\beta_J}{\sqrt{2\sigma_J^2}}\right)\right]$$

Note: $+\beta_J$, due to opposite sign

- Let the random variable X be the maximum (opposite-signed) bias for the benchmark collection:

$$X = \max\{ X_1, \ldots, X_N \}$$

- The cumulative distribution function (CDF) for X is

$$F(x) = \text{Prob}(X \le x) = \prod_{J=1}^{N} F_J(x)$$

Whisper Details – Calculational Margin (3)

- When benchmarks are weighted, the following form is used for $F_J(x)$

$$F_J(x) = (1 - w_J) + \frac{w_J}{2}\left[1 + \text{erf}\left(\frac{x + \beta_J}{\sqrt{2\sigma_J^2}}\right)\right]$$

- For all benchmarks J = 1, ..., N, Whisper computes
  - Benchmark weight, w_J
  - Bias, β_J
  - Bias uncertainty, σ_J

- Those quantities & the weighted $F_J(x)$ determine F(x):

$$F(x) = \prod_{J=1}^{N} F_J(x)$$

- Whisper determines the calculational margin (bias + bias uncertainty) by numerically solving:

F(CM) = .99 (.99 is default, user opt)

CM is the calculational margin that bounds the worst-case benchmark bias & bias uncertainty with probability .99 (default)

Whisper Details – Calculational Margin (4)

- **Bias & bias uncertainty**

  USL = 1 - CM - MOS

  = 1 + bias - bias-uncert - $\Delta_{\text{non-conserv}}$ - MOS

  – **ANSI/ANS-8.24:**

  "Individual elements (e.g., bias and bias uncertainty) of the calculational margin need not be computed separately. Methods may be used that combine the elements into the calculational margin."

- **Whisper computes CM by numerically solving** **F(CM) = .99**

- **Whisper computes bias & bias uncertainty numerically as:**

$$\text{bias} = -\int_{-\infty}^{\infty} x \cdot f(x)\,dx = -\int_{-\infty}^{\infty} xF(x)\sum_{J=1}^{N} w_J \frac{f_J(x)}{F_J(x)}\,dx$$

$$\sigma_{\text{bias}} = CM + \text{bias}$$

- **If the bias is non-conservative (positive), then the CM is adjusted so that no credit is taken for non-conservative bias**

  if bias>0, CM = CM + bias

What if there are not enough benchmarks to meet the requirement that sum{ w_J } = w_{req} ?

- **Define these quantities:**

  W_{sum} = sum{ w_J } - **sum of all benchmark weights, $w_{sum} < w_{req}$**

  CM_0 = calculational margin computed with all benchmark weights set to 1.0

  - CM_0 is an upper bound, wide application space but not specific enough for the application being analyzed
  - Typically large & very over-conservative

  CM' = calculation margin with weighted benchmarks, but $w_{sum} < w_{req}$

  - Note that $CM_0 \geq$ CM'

- **Compute CM from:** $$CM = CM' \cdot \frac{W_{sum}}{W_{req}} + CM_0 \cdot \left(1 - \frac{W_{sum}}{W_{req}}\right)$$

- **Should probably question the benchmark suite, & include extra conservative margin of subcriticality**

Margin of Subcriticality

$$MOS = MOS_{software} + MOS_{data} + MOS_{application}$$

- **MOS = additional margin "that is sufficiently large to ensure that the calculated conditions will actually be subcritical" (ANSI/ANS-8.24)**

- **$MOS_{software}$ (for MCNP)**
  - **No approximations from mesh or multigroup**
  - **Exact answers to analytical benchmarks with given xsecs**
  - **Many years testing with collision physics & random sampling**
  - **Only realistic concern is unknown bugs**
    - MCNP is used a lot, for many different criticality applications
    - Bugs that produce $\Delta k < 0.0010$ are difficult to distinguish from data uncertainties
    - Past bugs that produced $\Delta k > 0.0020$ are very few, but reported & fixed
    - Historical detection limit for bugs is $\Delta k \sim 0.0020$
    - Expert judgment, conservative: $MOS_{software} = 0.0050$
      → Any unknown bug larger than this would have certainly been found & fixed
    - Other MC codes should almost certainly use a larger margin
    - **Analysts may use a larger number, but have no basis for a smaller number**

Margin of Subcriticality

$$MOS = MOS_{software} + MOS_{data} + MOS_{application}$$

- $MOS_{application}$
  - Analyst: analyses, scoping, judgment
  - Consider uncertainties in dimensions, densities, isotopics, etc.
  - Consider the number of similar benchmark cases
  - Consider area-of-applicability

  - Expert judgment, backed up by analysis

Margin of Subcriticality

$$MOS = MOS_{software} + MOS_{data} + MOS_{application}$$

- **MOS_{data}**
  - **The largest portion of MOS comes from uncertainties in the nuclear cross-section data**
  - **Data uncertainties could be as large as 0.5% - 1% in extra MOS, possibly more, possibly less**
  - **MOS_{data} depends on the application**
    - For common applications, where there are lots of benchmark experiments, the relevant ENDF/B-VII data was adjusted based on those benchmarks
    - For less common applications, where there are few benchmark experiments, ENDF/B-VII adjustments for benchmarks plays little or no role in the data
  - **In the past, very difficult to assess MOS_{data}, which led to large conservative margins**
  - **Whisper (LANL) & Tsunami (ORNL) both use essentially the same methodology to address MOS_{data} – GLLS**
  - **Generalized Linear Least Squares (GLLS) takes into account the experiments, calculations, sensitivities, & data covariance data to predict MOS_{data}**

- **The goal of GLLS:** **(start at the end.....)**
  - **Determine adjustments to the nuclear data, Δx, which produce changes in computed k_{eff} for benchmarks, Δk, such that this quantity is minimized for the set of benchmarks:**

$$\chi^2 = \Delta\vec{k} \cdot \bar{C}_{kk} \cdot \Delta\vec{k}^T + \Delta\vec{x} \cdot \bar{C}_{xx} \cdot \Delta\vec{x}^T$$

  - **Δk is a vector of the relative changes in the ratio of calculated k to benchmark k, due to the change in cross-section data Δx. The length of Δk is the number of benchmarks**
  - **Δx is a vector of the relative differences of cross-section data from their mean values. The length of Δx is (isotopes)*(reacions)*(energies)**
  - **C_{kk} is the relative covariance matrix for the benchmark experiment k's**
    - Diagonal elements are variance of each benchmark experiment
    - Off-diagonals are correlation between benchmark measurements. (From DICE, often zero or not well-known)
  - **C_{xx} is the relative covariance matrix for the nuclear data**
  - **GLLS finds Δx (and the resulting Δk) such that χ^2 is minimized**

- **The goal of GLLS:**
  - Determine adjustments to the nuclear data, Δx, which produce changes in computed k_{eff} for benchmarks, Δk, such that this quantity is minimized for the set of benchmarks:

$$\chi^2 = \Delta\vec{k} \cdot \bar{C}_{kk} \cdot \Delta\vec{k}^T + \Delta\vec{x} \cdot \bar{C}_{xx} \cdot \Delta\vec{x}^T$$

  - With no data adjustment, Δx = 0, so χ^2 determined only by differences in calculated & benchmark k's
  - If data is adjusted to decrease 1st term, then 2nd term increases
  - GLLS determines optimum tradeoff (minimum χ^2) between Δx & Δk

Measured k_{eff} values for benchmarks:

$$\vec{m} = (m_i), \qquad i = 1,...I \qquad (I = \#\ \text{benchmarks})$$

Covariance matrix for $\vec{m}$, relative to calculated k_{eff}'s:

$$\bar{C}_{mm} = \left(\frac{m_i}{k_i} \bullet \frac{\text{cov}(m_i, m_j)}{m_i m_j} \bullet \frac{m_j}{k_j} \right), \qquad i, j = 1,...,I$$

Covariance between measured benchmark k's (m's) & cross-section data:

$$\bar{C}_{xm} = \left(\frac{\text{cov}(x_n, m_i)}{x_n m_i} \bullet \frac{m_i}{k_i} \right), \qquad n = 1,...,M \quad i = 1,...,I$$

This represents correlations between cross-section data & the measured benchmark k's. At present, these data do not exist. Neither Tsunami nor Whisper use C_{xm}.

Linear changes in calculated k_{eff} due to perturbation in data, $\vec{x}$:

$$k_i(\vec{x}') = k_i(\vec{x} + \delta\vec{x}) = k_i(\vec{x}) + \delta k_i = k_i(\vec{x}) \bullet \left[1 + \sum_{n=1}^{M} S_n^{(i)} \bullet \frac{\delta x_n}{x_n} \right]$$

Recall that:

Sensitivity matrix for a set of benchmarks:

$$\bar{S}_k = \left(\frac{x_n}{k_i} \bullet \frac{\partial k_i}{\partial x_n} \right) \qquad i = 1,...,I \text{ (rows)} \qquad n = 1,...,M \text{ (cols)}$$

Covariance matrix for nuclear data, $\vec{x}$:

$$\bar{C}_{xx} = \left(\frac{\text{cov}(x_n, x_p)}{x_n x_p} \right) \qquad n = 1,...,M \qquad p = 1,...,M$$

Uncertainty matrix for the set of benchmarks, due to data:

$$\bar{C}_{kk} = \bar{S}_k \cdot \bar{C}_{xx} \cdot \bar{S}_k^T$$

Express the relative changes in k for a set of benchmarks due to data perturbations:

$$\frac{k_i(\vec{x}') - m_i}{k_i(\vec{x})} = \frac{k_i(\vec{x}) - m_i}{k_i(\vec{x})} + \left[\sum_{n=1}^{M} S_n^{(i)} \bullet \frac{\delta x_n}{x_n} \right]$$

or

$$\vec{y} \quad = \quad \vec{d} \quad + \quad \bar{S}_k \bullet \vec{z}$$

For the vector $\vec{d}$, $(d_i) = \dfrac{k_i(\vec{x}) - m_i}{k_i(\vec{x})} \qquad i = 1,...,I$

the uncertainty matrix for the set of benchmarks is

$$\begin{aligned}\bar{C}_{dd} &= \bar{C}_{kk} + \bar{C}_{mm} - \bar{S}_k\bar{C}_{xm} - \bar{C}_{mx}\bar{S}_k^T \\ &= \bar{S}_k\bar{C}_{xx}\bar{S}_k^T + \bar{C}_{mm} - \bar{S}_k\bar{C}_{xm} - \bar{C}_{mx}\bar{S}_k^T\end{aligned}$$

GLLS involves minimizing this quantity:

$$Q(\vec{z},\vec{y}) = (\vec{y},\vec{z}) \bullet \begin{pmatrix} \bar{C}_{mm} & \bar{C}_{mx} \\ \bar{C}_{xm} & \bar{C}_{xx} \end{pmatrix}^{-1} \bullet (\vec{y},\vec{z})^T,$$

subject to the constraint $\vec{y} = \vec{d} + \bar{S}_k\vec{z}$

This is accomplished using Lagrange multipliers & minimizing this quantity:

$$R(\vec{z},\vec{y}) = Q(\vec{z},\vec{y}) + 2\lambda(\bar{S}_k\vec{z} - \vec{y})$$

$\vec{z}$ and $\vec{y}$ satisfy these relations:

$$\frac{\partial R(\vec{z},\vec{y})}{\partial \vec{z}} = \frac{\partial R(\vec{z},\vec{y})}{\partial \vec{y}} = 0$$

The results, giving the adjusted data & k's that minimize R are:

Δdata: $\qquad \vec{z} = \left(\bar{C}_{xm} - \bar{C}_{xx}\bar{S}_k^T\right) \cdot \bar{C}_{dd}^{-1} \cdot \vec{d}$

Δk : $\qquad \vec{y} = \left(\bar{C}_{mm} - \bar{C}_{mx}\bar{S}_k^T\right) \cdot \bar{C}_{dd}^{-1} \cdot \vec{d}$

GLLS

GLLS gives the data adjustments (& resulting Δk's) that minimize the Q or R functions (also called χ^2)

The adjustments also give reduced uncertainties:

$$\bar{C}_{m'm'} = \bar{C}_{mm} - \left(\bar{C}_{mm} - \bar{C}_{mx}\bar{S}_k^T\right)\cdot\bar{C}_{dd}^{-1}\cdot\left(\bar{C}_{mm} - \bar{S}_k\bar{C}_{xm}\right)$$

$$\bar{C}_{x'x'} = \bar{C}_{xx} - \left(\bar{C}_{xm} - \bar{C}_{xx}\bar{S}_k^T\right)\cdot\bar{C}_{dd}^{-1}\cdot\left(\bar{C}_{mx} - \bar{S}_k\bar{C}_{xx}\right)$$

The adjusted uncertainty matrix in k for a set of applications is:

$$\bar{C}_{k'k'} = \bar{S}_{k,A}\cdot\bar{C}_{x'x'}\cdot\bar{S}_{k,A}^T$$

where each row of $\bar{S}_{k,A}$ is the sensitivity vector for an application.

The square roots of diagonal elements in $\bar{C}_{k'k'}$ are the relative 1σ uncertainties in k for the adjusted data.

For a particular application i, the portion of MOS for nuclear data uncertainty is:

$$MOS_{data} = n_\sigma\cdot\sqrt{\left(\bar{C}_{kk}\right)_{i,i}}$$

where n_σ = 2 for 95% confidence, 2.6 for 99%

Upper Subcritical Limit

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

$$K_{calc} < USL$$

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

$$MOS = MOS_{data} + MOS_{code} + MOS_{application}$$

- 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.

Whisper
Usage

Using Whisper for Validation

- **As part of Whisper installation (not day-to-day use),**
  - **For each of the ~1100 benchmarks**
    - MCNP6 is run to generate the sensitivity vector S_B for that benchmark
    - The sensitivity vector S_B for each benchmark is saved in a folder
  - **The nuclear data covariance files are saved in a folder**
  - **Benchmarks are checked for consistency, some may be rejected**
  - **Missing uncertainties for some benchmarks are estimated**
  - **All of this is the responsibility of the Admin person & needs to be done only once at installation (or repeated if the code, data, or computer change)**

- **To use Whisper for validation:**
  - **Use the whisper_mcnp script to make 1 run with MCNP6 for a particular application, to generate the sensitivity vector for the application, S_A**
  - **Run Whisper, using the whisper_usl script**

To try it, on Moonlight HPC:

- **Set & export WHISPER_PATH environment variable**
  - bash:

```
export WHISPER_PATH
WHISPER_PATH="/usr/projects/mcnp/ncs/WHISPER"
export PATH
PATH="$WHISPER_PATH/bin:$PATH"
```

  - csh, tcsh:

```
setenv  WHISPER_PATH  "/usr/projects/mcnp/ncs/WHISPER"
setenv  PATH          "$WHISPER_PATH/bin:$PATH"
```

- **Make a directory with input files**
  - No blanks in pathname, directory name, input file names
  - Put mcnp6 input files in the directory
- **Run**

```
whisper_mcnp.pl    -walltime 02:00:00      myjob*.i
..... wait till jobs complete
whisper_usl.pl
```

Using whisper_mcnp (1)

- **From the front-end on an HPC system:**

```
whisper_mcnp   Inp1.txt
```

  - **Inp1.txt is an MCNP6 input file**
    - Must NOT include any of these cards: `kopts, ksen, prdmp`
    - May list more than 1 input file on whimcnp command line
    - For now, input file names must be 40 chars or less
    - May include time limit for MCNP jobs before the list of input files,

```
walltime hh:mm:ss
```

  - **Creates files & dirs:**
    - **MCNPInputList.toc**
    - **Calcs/**
    - **Calcs/Inp1.txt** ← **modified to include kopts, ksen, prdmp, & new kcode**
    - **KeffSenLib/**
  - **Submits jobs to HPC compute nodes**
    - **Single-node jobs, 16 threads each**
    - **Default time limit of 1 hr**

Using whisper_mcnp (2)

- **For each MCNP6 input file listed on the whisper_mcnp command line:**
  - **KCODE line is deleted & these lines are inserted:**

```
kcode    100000   1.0    100    600
kopts blocksize= 5
ksen1 xs
      rxn= +2 +4 -6 +16 102 103 104 105 106 107 -7 -1018
      erg= 1.0000e-11 3.0000e-09 7.5000e-09 1.0000e-08 2.5300e-08 3.0000e-08
           4.0000e-08 5.0000e-08 7.0000e-08 1.0000e-07 1.5000e-07 2.0000e-07
           2.2500e-07 2.5000e-07 2.7500e-07 3.2500e-07 3.5000e-07 3.7500e-07
           4.0000e-07 6.2500e-07 1.0000e-06 1.7700e-06 3.0000e-06 4.7500e-06
           6.0000e-06 8.1000e-06 1.0000e-05 3.0000e-05 1.0000e-04 5.5000e-04
           3.0000e-03 1.7000e-02 2.5000e-02 1.0000e-01 4.0000e-01 9.0000e-01
           1.4000e+00 1.8500e+00 2.3540e+00 2.4790e+00 3.0000e+00 4.8000e+00
           6.4340e+00 8.1873e+00 2.0000e+01
prdmp j 9999999
```

- **After using whisper_mcnp, after the MCNP6 jobs complete:**
  - **The Calcs/ directory will contain these files**
    - Inp1.txt — modified MCNP6 input file, with kcode, ksen, kopts, prdmp
    - Inp1.txto — output file from MCNP6 jobs
    - Inp1.txtr — runtpe file
    - Inp1.txts — srctp file

whisper_mcnp.pl - Usage

Monte Carlo Codes
XCP-3, LANL

```
whisper_mcnp.pl [Options]  Filelist

Options:
         -help               print this information
         -local              run MCNP jobs locally, on this computer
         -submit             submit batch MCNP jobs, using msub    [default]
         -walltime x         walltime limit for submitted batch jobs (eg, 01:00:00)
         -mcnp x             pathname for MCNP6 executable
         -xsdir x            pathname for MCNP6 xsdir file
         -data x             pathname for MCNP6 data, DATAPATH
         -threads x          number of threads for MCNP6
         -neutrons x         number of neutrons/cycle for MCNP6
         -discard x          number of inactive cycles for MCNP6
         -cycles x           total number of cycles for MCNP6
Filelist:
         Names of MCNP6 input files. The names should not contain blanks.
         The files must include a KCODE card (that will be replaced), &
         must not contain KSENn, KOPTS, or PRDMP cards (they will be supplied)

Defaults:                    **for local**                **for submit**
         -submit
         -mcnp               hardwired in script      /usr/projects/mcnp/mcnpexe  -6
         -xsdir              hardwired in script   /usr/projects/mcnp/MCNP_DATA/xsdir_mcnp6.1
         -data               hardwired in script      /usr/projects/mcnp/MCNP_DATA
         -walltime                                         01:00:00
         -threads            12                            16
         -neutrons           10000                         100000
         -discard            100                           100
         -cycles             600                           600
```

Using whisper_usl (1)

- From the front-end on an HPC system, in the same directory where whisper_mcnp was executed, run Whisper using the whisper_usl script:

  whisper_usl

  - Can optionally include ExcludeFile.dat, list of benchmark files to exclude from Whisper calculations
  - Runs Whisper for application(s) Inp1.txt (etc)

- For each input file listed in `MCNPInputList.toc`:
  - Extract sensitivity profiles from `Calcs/Inp1.txto`, place into directory `KeffSenLib/`
  - Create (or add to) file `KeffSenList.toc`
  - Run Whisper using the sensitivity profiles for the application (Inp1.txt) and the collection of Whisper benchmark sensitivity profiles
  - Output to screen & file `Whisper.out`

Using whisper_usl (2)

- After running whisper_mcnp & whisper_usl:

```
whisper_mcnp    Inp1.txt    Inp2.txt
whisper_usl
```

Files created by whisper_mcnp, mcnp6, & whisper_usl:

```
Inp1.txt                ← original
Inp2.txt                ← original
MCNPInputlist.toc
Calcs/
      Inp1.txt Inp1.txto Inp1.txtr Inp1.txts
      Inp2.txt Inp2.txto Inp2.txtr Inp2.txts
KeffSenList.toc
KeffSenLib/
      Inp1.txtk
      Inp2.txtk
Whisper.out
```

Whisper-1.1.0 Demo

- **Whisper-1.1.0, whisper_mcnp.pl, whisper_usl.pl**
  - **whisper_mcnp.pl**
    - set up & run mcnp6 for application to generate application sensitivity profiles
  - **whisper_usl.pl**
    - use whisper to select benchmarks based on comparing application sensitivity profiles to benchmark sensitivity profiles
    - compute USL using selected benchmarks (weighted)

- **Benchmarks for this demo**
  - **Don't use 1101 Whisper benchmark set – takes too long on laptop to compare application with 1101 benchmark profiles**
  - **Instead: use 246 problems from NCS Validation Suite (from 2015)**
    (not including 15 pu-met-fast-042-* problems)

- **Application for this demo**
  - **in-28-2-1 (from Salazar, 11/06/2014)**

whisper_mcnp.pl

Monte Carlo Codes
XCP-3, LANL

```
bash:   whisper_mcnp.pl -local -neutrons 10000 -discard 25 \
                        -cycles 225 -threads 4   in-28-2-1.txt

******************
*                *
*  whisper_mcnp  *      a utility script to set up input & run MCNP for Whisper
*                *
******************

        Input File TOC           = MCNPInputList.toc
        Calculation directory    = Calcs
        Sensitivity directory    = KeffSenLib

        Neutrons/cycle           = 10000
        Cycles to discard        = 25
        Total Cycles to run      = 225

        MCNP6 executable         = /Users/fbrown/LANL/MCNP_CODE/bin/mcnp6
        XSDIR file               = /Users/fbrown/LANL/MCNP_DATA/xsdir_mcnp6.1
        DATAPATH                 = /Users/fbrown/LANL/MCNP_DATA
        Threads                  = 4

        All jobs will be run locally on this computer

        ...process  mcnp input file:  in-28-2-1.txt
        ...modified mcnp input file:  Calcs/in-28-2-1.txt

        ...run mcnp on this computer:  in-28-2-1.txt
 mcnp     ver=6     , ld=06/23/14  02/07/16 14:44:03
          Code Name & Version = MCNP, 6.1.1b
```

whisper_usl.pl (1)

Monte Carlo Codes
XCP-3, LANL

```
bash: whisper_usl.pl

******************
*                *
*  whisper_usl   *      set up & run Whisper validation calculations
*                *
******************

   =====> setup files for whisper

        ---> setup for problem in-28-2-1.txt
               ...extract sensitivity profile data from:  Calcs/in-28-2-1.txto
               ...copy    sensitivity profile data to:    KeffSenLib/in-28-2-1.txtk
               ...extract calc Keff & Kstd    data from:  Calcs/in-28-2-1.txto
               ...  KeffCalc= 0.96740 +- 0.00057,  ANECF= 1.4904E+00 MeV,  EALF= 1.2150E-01 MeV

   =====> run whisper

/Users/fbrown/CODES/WHISPER/WHISPER.git/bin/whisper -a KeffSenList.toc -ap KeffSenLib
 whisper-1.1.0                    2016-02-02   (Copyright 2016 LANL)
 WHISPER_PATH                   = /Users/fbrown/CODES/WHISPER/WHISPER.git
 Benchmark TOC File             = /Users/fbrown/CODES/WHISPER/WHISPER.git/Benchmarks/TOC/BenchmarkTOC.dat
 Benchmark Sensitivity Path     = /Users/fbrown/CODES/WHISPER/WHISPER.git/Benchmarks/Sensitivities
 Benchmark Correlation File     =
 Benchmark Exclusion File       =
 Benchmark Rejection File       =
 Covariance Data Path           = /Users/fbrown/CODES/WHISPER/WHISPER.git/CovarianceData/SCALE6.1
 Covariance Adjusted Data Path  =
 Application TOC File           = KeffSenList.toc
 Application Sensitivity Path   = KeffSenLib/
 User Options File              =
 Output File                    = Whisper.out
```

whisper_usl.pl (2)

Monte Carlo Codes
XCP-3, LANL

```
........

 Reading benchmark data ...
 Reading application data ...
 Reading covariance data ...
 Reading adjusted covariance data ...
 Calculating application nuclear data uncertainties ...
 Calculating upper subcritical limits ...
......case     1  Ck=  0.41263
......case     4  Ck=  0.36554
......case     3  Ck=  0.63497

         ........

......case   246  Ck=  0.18901
                                        calc        data unc    baseline    k(calc)
    application                         margin      (1-sigma)   USL         > USL

    in-28-2-1.txt                       0.01329     0.00120     0.97860    -0.00972
```

Whisper.out (1)

Monte Carlo Codes
XCP-3, LANL

```
whisper-1.1.0                    2016-02-02   (Copyright 2016 LANL)
WHISPER_PATH                   = /Users/fbrown/CODES/WHISPER/WHISPER.git
Benchmark TOC File             = /Users/fbrown/CODES/WHISPER/WHISPER.git/Benchmarks/TOC/BenchmarkTOC.dat
Benchmark Sensitivity Path     = /Users/fbrown/CODES/WHISPER/WHISPER.git/Benchmarks/Sensitivities
Benchmark Correlation File     =
Benchmark Exclusion File       =
Benchmark Rejection File       =
Covariance Data Path           = /Users/fbrown/CODES/WHISPER/WHISPER.git/CovarianceData/SCALE6.1
Covariance Adjusted Data Path  =
Application TOC File           = KeffSenList.toc
Application Sensitivity Path   = KeffSenLib/
User Options File              =
Output File                    = Whisper.out

Reading benchmark data ...
                         benchmark     k(bench)     unc          k(calc)     unc          bias         unc
             pu-comp-inter-001-001.i     1.00000     0.01100     1.01174     0.00007    -0.01174     0.01100
             pu-comp-mixed-001-001.i     0.99860     0.00410     1.02477     0.00009    -0.02617     0.0041

                     ..........

  246 benchmarks read,       0 benchmarks excluded.

Reading application data ...
                               application      k(calc)      unc
                              in-28-2-1.txt     0.96802     0.00052

Reading covariance data ...
 Reading covariance data for 1001 ...

                     ..........

Reading adjusted covariance data ...
 Reading covariance data for 1001 ...
```

Whisper.out (2)

Monte Carlo Codes
XCP-3, LANL

```
Calculating application nuclear data uncertainties ...
    application                                adjusted    prior
    in-28-2-1.txt                              0.00209     0.01221

 Calculating upper subcritical limits ...
                                               calc        data unc    baseline    k(calc)
    application                                margin      (1-sigma)   USL         > USL
    in-28-2-1.txt                              0.01334     0.00209     0.97623    -0.00686

    Benchmark population    =   48
    Population weight       =  28.56732
    Maximum similarity      =   0.96434

    Bias                    =   0.00850
    Bias uncertainty        =   0.00484
    Nuc Data uncert margin  =   0.00209
    Software/method margin  =   0.00500
    Non-coverage penalty    =   0.00000

    benchmark                                  ck          weight
    pu-met-fast-011-001.i                      0.9643      1.0000
    pu-met-fast-044-002.i                      0.9641      0.9958
    pu-met-fast-021-002.i                      0.9618      0.9545
    pu-met-fast-003-103.i                      0.9602      0.9252
    pu-met-fast-026-001.i                      0.9594      0.9099
    pu-met-fast-025-001.i                      0.9584      0.8912
    pu-met-fast-032-001.i                      0.9572      0.8699
    pu-met-fast-016-001.i                      0.9546      0.8221
    pu-met-fast-027-001.i                      0.9546      0.8217
                        .........
    pu-met-fast-012-001.i                      0.9167      0.1283
    pu-met-fast-040-001.i                      0.9166      0.1269
    pu-met-fast-045-003.i                      0.9163      0.1209
    pu-met-fast-045-004.i                      0.9147      0.0909
    pu-met-fast-002-001.i                      0.9145      0.0874
```

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

Benchmark rankings shown below

Comments & Discussion

- Traditional validation methods are 40+ years old; S/U methods are new
- Should not argue for exclusive use of either traditional or S/U methods
- The foundation of criticality safety includes conservatism, continuous improvement, state-of-the-art tools & data, thorough checking, …..
- The next 5 years or so should be a transition period, where both traditional & S/U methods should be used
  - 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 selection
  - Traditional methods use $MOS_{data+code}$ of 2-5%.
    Quantitative, physics-based, repeatable $MOS_{data+code}$ from S/U usually smaller
- Traditional & S/U methods complement each other, & provide greater assurance for setting USLs
- In today's environment of audits, reviews, & "justify everything", it is prudent to use both traditional & S/U methods for validation

References for Whisper & MCNP6 (1)

Abstract

- Whisper - abstract from LANL TeamForge Tracker system, Artifact artf36407 (2015)

Theory

- B.C. Kiedrowski, F.B. Brown, et al., "Whisper: Sensitivity/Uncertainty-Based Computational Methods and Software for Determining Baseline Upper Subcritical Limits", Nuc. Sci. Eng. Sept. 2015, LA-UR-14-26558 (2014)
- B.C. Kiedrowski, "Methodology for Sensitivity and Uncertainty-Based Criticality Safety Validation", LA-UR-14-23202 (2014)

User Manual

- B.C. Kiedrowski, "User Manual for Whisper (v1.0.0), Software for Sensitivity- and Uncertainty-Based Nuclear Criticality Safety Validation", LA-UR-14-26436 (2014)
- B.C. Kiedrowski, "MCNP6.1 k-Eigenvalue Sensitivity Capability: A Users Guide", LA- UR-13-22251 (2013)

Application

- B.C. Kiedrowski, et al., "Validation of MCNP6.1 for Criticality Safety of Pu-Metal, - Solution, and -Oxide Systems", LA-UR-14-23352 (2014)

References for Whisper & MCNP6 (2)

Monte Carlo Codes XCP-3, LANL

Software Quality Assurance

- R.F. Sartor, F.B. Brown, "Whisper Program Suite Validation and Verification Report", LA-UR-15-23972 (2015-05-28)
- R.F. Sartor, F.B. Brown, "Whisper Source Code Inspection Report", LA-UR-15-23986 (2015-05-28)
- R.F. Sartor, B.A. Greenfield, F.B. Brown, "MCNP6 Criticality Calculations Verification and Validation Report", LA-UR-15-23266 (2015-04-30)
- Monte Carlo Codes Group (XCP-3), "Whisper - Software for Sensitivity-Uncertainty-based Nuclear Criticality Safety Validation", LANL TeamForge Tracker system, Artifact artf36407 (2015)
- Monte Carlo Codes Group (XCP-3), WHISPER module in LANL TeamForge GIT repository (2015)
- Monte Carlo Codes Group (XCP-3), MCNP6 module in LANL TeamForge GIT repository
- Monte Carlo Codes Group (XCP-3), "MCNP Process Documents", LANL Teamforge wiki for MCNP
- Monte Carlo Codes Group (XCP-3), "Software Quality Assurance", LANL Teamforge wiki for MCNP, P1040-rev9 requirements

Recent MCNP6 & ENDF/B-VII.1 Verification/Validation

- F.B. Brown, "MCNP6 Optimization and Testing for Criticality Safety Calculations", Trans. ANS 111, LA-UR-15-20422 (2015)
- Monte Carlo Codes XCP-3, LANL F.B. Brown, B.C. Kiedrowski, J.S. Bull, "Verification of MCNP6.1 and MCNP6.1.1 for Criticality Safety Applications", LA-UR-14-22480 (2014).
- F.B. Brown, B.C. Kiedrowski, J.S. Bull, "Verification of MCNP5-1.60 and MCNP6.1 for Criticality Safety Applications", LA-UR-13-22196 (2013).
- L.J. Cox, S.D. Matthews, "MCNP6 Release 1.0: Creating and Testing the Code Distribution", LA-UR-13-24008 (2013)

References for Whisper & MCNP6 (3)

Recent MCNP6 & ENDF/B-VII.1 Verification/Validation (cont'd)

- R.D. Mosteller, F.B. Brown, B.C. Kiedrowski, "An Expanded Criticality Validation Suite for MCNP", LA-UR-11-00240 (2011).
- R.D. Mosteller, "An Expanded Criticality Validation Suite for MCNP", LA-UR-10-06230 (2010).
- R.C. Little, "V&V of MCNP and Data Libraries at Los Alamos", LA-UR-12-26307 (2012) A. Sood, R.A. Forster, D.K. Parsons, "Analytic Benchmark Test Set for Criticality Code
- Verification", LA-13511 and LA-UR-01-3082 (2001)
  XCP Data Team, "LANL Data Testing Support for ENDF/B-VII.1", LA-UR-12-20002 LA-UR-12-20002 (2012)

General References on Adjoints, Perturbation, and Sensitivity Analysis

- B.C. Kiedrowski, F.B. Brown, et al., "MCNP Sensitivity/Uncertainty Accomplishments for the Nuclear Criticality Safety Program", Trans. Am. Nuc. Soc 111, Nov 2014, LA-UR-14- 24458 (2014)
- B.C. Kiedrowski, "Adjoint Weighting Methods Applied to Monte Carlo Simulations of Applications and Experiments in Nuclear Criticality" seminar at University of Michigan, March 2014, LA-UR-14-21608 (2014)
- B.C. Kiedrowski, "MCNP Continuous-Energy Sensitivity and Uncertainty Progress and Application", Presentation at DOE-NNSA Nuclear Criticality Safety Program Technical Review, 26-27 March 2014, LA-UR-14-21919 (2014)
- B.C. Kiedrowski, "Application of Covariance Data in Nuclear Criticality", Nuclear Data Covariance Workshop, April 28 - May 1, Santa Fe, NM, LA-UR-14-22972 (2014)

References for Whisper & MCNP6 (4)

General References on Adjoints, Perturbation, and Sensitivity Analysis (cont'd)

- B.C. Kiedrowski & F.B. Brown, "Applications of Adjoint-Based Techniques in Continuous-Energy Monte Carlo Criticality Calculations", Supercomputing in Nuclear Applications and Monte Carlo 2013, Paris, Oct 27-31, LA-UR-13-27002 (2013)
- B.C. Kiedrowski, "Importance of Scattering Distributions on Criticality", ANS NCSD- 2013, Wilmington, NC, Sept 29 - Oct 1, LA-UR-13-24254 (2013).
- B.C. Kiedrowski, A.C. Kahler, M.E. Rising, "Status of MCNP Sensitivity/Uncertainty Capabilities for Criticality", ANS NCSD-2013, Wilmington, NC, Sept 29 - Oct 1, LA-UR- 13-24090 (2013)
- B.C. Kiedrowski, "K-Eigenvalue Sensitivity Coefficients to Legendre Scattering Moments", ANS 2013 Winter Meeting, LANL report LA-UR-13-22431 (2013)
- B.C. Kiedrowski, F.B. Brown, "Applications of Adjoint-Based Techniques in Continuous- Energy Monte Carlo Criticality Calculations", submitted to SNA+MC-2013, Paris, France [also LA-UR-12-26436] (2012)
- B.C. Kiedrowski, F.B. Brown, "K-Eigenvalue Sensitivities of Secondary Distributions of Continuous-Energy Data," M&C 2013, Sun Valley, ID, May 2013, report LA-UR-12- 25966, talk LA-UR-13-23208 (2013)
- B.C. Kiedrowski, F.B. Brown, "Methodology, Verification, and Performance of the Continuous-Energy Nuclear Data Sensitivity Capability in MCNP6," M&C 2013, Sun Valley, ID, May 2013, report LA-UR-12-25947, talk LA-UR-13-23199 (2012)
- B.C. Kiedrowski, F.B. Brown, "MCNP6 Nuclear Data Sensitivity Capability: Current Status and Future Prospects", presentation at MCNP/ENDF/NJOY Workshop, 2012-10- 30, LANL, LA-UR-12-25560 (2012)
- B.C. Kiedrowski, F.B. Brown, "Nuclear Data Sensitivities in Fast Critical Assemblies", presentation at NECDC-2012, LA-UR-12-25144 (2012)

References for Whisper & MCNP6 (5)

General References on Adjoints, Perturbation, and Sensitivity Analysis (cont'd)

- B.C. Kiedrowski, F.B. Brown, "Adjoint-Based k-Eigenvalue Sensitivity Coefficients to Nuclear Data Using Continuous-Energy Monte Carlo", submitted to Nuclear Science & Engineering [also LA-UR-12-22089] (2012)
- B.C. Kiedrowski, "MCNP6 Results for the Phase III Sensitivity Benchmark of the OCED/NEA Expert Group on Uncertainty Analysis for Criticality Safety Assessment", LA-UR-12-21048 (2012)
- B.C. Kiedrowski & F.B. Brown, “Continuous-Energy Sensitivity Coefficient Capability in MCNP6”, Trans. Am. Nuc. Soc. 107, LA-UR-12-21010,
  presentation at 2012 ANS Winter Meeting, San Diego, CA, LA-UR-12-25949 (2012)
- B.C. Kiedrowski & F.B. Brown, “Comparison Of The Monte Carlo Adjoint-Weighted And Differential Operator Perturbation Methods”, SNA+MC-2010, Tokyo, Oct 17-20, LA-UR- 10-05215 (2010)
- B.C. Kiedrowski, J.A. Favorite, & F.B. Brown, “Verification of K-eigenvalue Sensitivity Coefficient Calculations Using Adjoint-Weighted Perturbation Theory in MCNP”, Trans. Am. Nuc. Soc, 103, Nov 2010, LA-UR-10-04285 (2010)
- B.C. Kiedrowski, F.B. Brown, & P. Wilson, “Adjoint-Weighted Tallies for k-Eigenvalue Calculations with Continuous-Energy Monte Carlo”, Nucl. Sci. Eng. 168, 38-50, 2011, LA-UR-10-01824, (2010).
- B.C. Kiedrowski & F.B. Brown, “Adjoint-Weighting for Critical Systems with Continuous Energy Monte Carlo”, ANS NCSD-2009, Richland, WA, Sept 13-17, paper LA-UR-09- 2594, presentation LA-UR-09-5624 (2009)