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MCNP Sensitivity/Uncertainty Accomplishments for the Nuclear Criticality Safety Program

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INTRODUCTION

The DOE/NNSA Nuclear Criticality Safety Program (NCSP) supports research, development, maintenance, and verification and validation of the MCNP Monte Carlo radiation transport software package [1] for nuclear criticality safety (NCS) customers within DOE/NNSA. In recent years, the NCSP has been funding the development of sensitivity and uncertainty (S/U) capabilities in MCNP. Recent institutional needs at Los Alamos National Laboratory (LANL) related to the validation of MCNP for Pu operations have also spurred further development.

This paper gives an overview of the recent S/U-related developments and how, when applicable, have been applied at LANL for NCS needs. Specifically discussed are: enhancements to the MCNP6 continuous-energy nuclear data sensitivity capabilities that are available in MCNP6.1.1, a prototype for a fixed-source sensitivity capability that was applied to demonstrated by analyzing subcritical experiment at the National Critical Experiments Research Center (NCERC) in Nevada, research on methods for computing Doppler reactivity coefficients, the study of representations of nuclear covariance data, and the development S/U capabilities for determining baseline upper subcritical limits (USLs).

MCNP SENSITIVITY CAPABILITY UPDATE

In MCNP6.1, a new capability for generating nuclear data sensitivities with continuous-energy data [2]. Enhancements were made and are to be released in the next beta version, MCNP6.1.1. The first minor enhancement was the addition of writing a SCALE/TSUNAMI sensitivity data format (SDF) file, so MCNP results can be used with SCALE tools such as TSURFER. Secondly, the allowed reactions were limited, and a more extensive list of ENDF MT numbers is now allowed. The third enhancement, a completely new capability in Monte Carlo sensitivity methods, is the ability to compute sensitivities of Legendre scattering moments [3]; this is discussed in greater detail.

Legendre Moment Sensitivities

MCNP6.1 has the ability to compute sensitivities to the the scattering distributions as a function of incident and outgoing energy and scattering cosine. Such a format is often inconvenient because nuclear covariance data in ENDF is given as Legendre moments of the scattering distributions. Therefore, to be consistent with the nuclear covariance data, research was performed on how to take the energy-cosine resolved sensitivities and convert them to sensitivities of Legendre moments.

To do this, MCNP defines a uniform grid of scattering cosines. For each incident energy, the sensitivity is averaged over each cosine bin on the grid and constrained to satisfy normalization conditions on probability density functions. Also, MCNP tallies, for each incident energy zone specified, the bin-integrated scattering probability density function for each cosine bin and the scattering Legendre moments. Using simple midpoint integration, an expression to approximate the sensitivity of a Legendre scattering moment was developed and, for the ℓth moment, is

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

where i represents the index for the cosine bin with bounds μ_i and μ_{i+1}, $\hat{S}_{k,f,i+1/2}$ is the ith cosine bin-integrated constrained sensitivity, $F_{i+1/2}$ is the ith bin-integrated scattering probability density function tallied by MCNP, $P_\ell(\mu_{i+1/2})$ is the ℓth Legendre polynomial evaluated at the midpoint of cosine bin i, and f_ℓ is the ℓth Legendre moment of the scattering density function estimated by MCNP.

Verification was performed using simple multigroup test problems. Reference results were obtained with direct perturbations of the P_1 and P_2 Legendre scattering moments in the nuclear data files. The results of the sensitivity calculations with the new method agreed within statistical uncertainties of the reference, direct perturbation results. The Legendre moment sensitivities were then obtained for a variety of benchmark critical experiments. The findings are that for fast, bare and reflected benchmarks, P_1 elastic scattering moment is often a significant contributor toward determining k. Higher-order Legendre moments or inelastic moments do not appear to be significant in most bench-

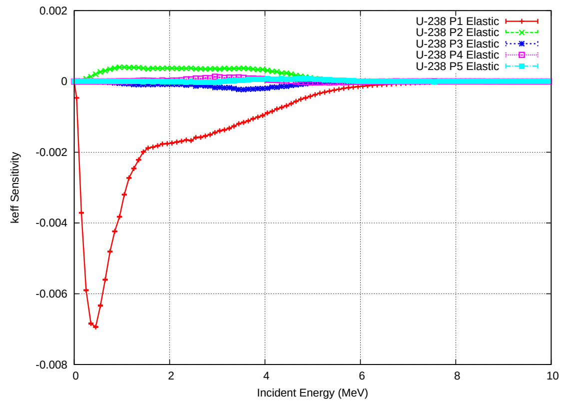

Fig. 1. Legendre moment elastic scattering sensitivities for ^{238}U in Flattop.

mark critical experiments. Also, the k of thermal systems are typically insensitive to the Legendre moments. An example of the Legendre moment sensitivities as a function of incident energy for ^{238}U in the Flattop critical experiment is given in Fig. 1.

FIXED-SOURCE SENSITIVITIES

Simulations of subcritical measurements are inherently fixed-source calculations, not eigenvalue calculations. For the purposes of analyzing nuclear data sensitivities of subcritical measurements at NCERC, research was performed on how this could be done, and a prototype version of MCNP6 was developed [4].

The sensitivity of response R with respect to nuclear data x can be obtained from perturbation theory:

$$S_{R,x} = \frac{x}{R}\left[\left\langle \frac{\partial f_R}{\partial x}, \psi \right\rangle + \left\langle \psi^\dagger, \frac{\partial Q}{\partial x} \right\rangle - \left\langle \psi^\dagger, \frac{\partial H}{\partial x}\psi \right\rangle\right]. \tag{2}$$

Here ψ is the neutron flux, $\psi^\dagger$ is its adjoint, the brackets denote integration over all phase space, and the three terms (from left to right) describe how the response function f_R, the fixed source Q, and the neutron transport (denoted with operator H) change with respect to nuclear data x.

Verification was performed using direct perturbations of the density (equivalent to the total cross section) for various test problems, and they agree within the statistical uncertainties.

Validation was performed by comparing with NCERC measurements of SNAP detector count rates of various mass substitutions (denoted perturbations A through F; see Ref. [4] for a detailed description) on the Thor core. The predicted change in the count rates R from the change in the source and transport ΔR_Q and ΔR_H for the experimental measurements are given in Table I along with the C/E for how well the perturbed measurement is predicted.

Table I. Sensitivities for Thor Core Glory Hole Mass

Pert.	$S_{R,x}$	ΔR_Q	ΔR_H	C/E
A	5.54E-02	-0.9	-1.3	0.948
B	7.12E-02	-1.5	-4.1	0.953
C	7.30E-02	-1.7	-5.7	1.009
D	1.63E-01	-2.8	-27.3	0.931
E	1.63E-01	-1.4	-12.8	0.961
F	1.63E-01	-2.1	-20.8	0.942

The sensitivity to the neutron source for spontaneous fission is assumed to be unity. It appears that the prototype capability underpredicts the change in the count rate by about 5% for this measurement. Nonetheless, these results do agree within 10%, which is better than the 20% bias observed for this experiment, suggesting this new capability has merit for small changes in mass in subcritical measurements.

DOPPLER REACTIVITY EFFECTS

Research was funded by the NCSP as part of a collaboration with the University of New Mexico to apply the continuous-energy sensitivity techniques to estimate temperature effects on k from Doppler broadening. Recently, efficient polynomial-fit representations of cross section variation with temperature were developed and implemented into MCNP6.1. By differentiating these analytic fits, temperature derivatives of cross sections may be obtained and inserted into the MCNP adjoint weighting routines. Figure 2 gives a representation of the temperature

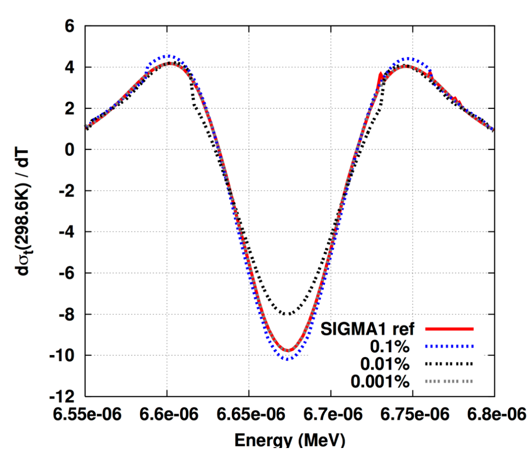

Fig. 2. Temperature derivative of the total cross section of ^{238}U for various fitting tolerances.

derivative of a cross section as a function of energy compared with a reference, central difference solution.

Preliminary results show that this approach can successfully compute Doppler reactivity coefficients, which can be used to quantify the effects of temperature variation in systems driven by thermal neutron fission [5]. Current work is proceeding on extending this approach to account for the variation in the scattering kinematics. Future plans involve possibly applying this approach to critical excursion transients.

DATA COVARIANCE STORAGE

The data format MCNP is able to read has no provision for covariances. The nuclear data libraries distributed with MCNP have grown to GB in size, and nuclear data covariances, preserving the fine-energy resolutions given in ENDF would increase them to make distribution of the nuclear data a practical challenge. As part of the S/U efforts, compact formats were investigated to compress the size of data [6].

Specifically, a principal eigenvector format was studied. This representation has shown great success for reducing the necessary size of nuclear data for prompt neutron fission spectra, which motivated the research. The idea is that a symmetric covariance matrix may be decomposed into real eigenvectors with corresponding eigenvalues. The relative magnitude of the eigenvalues represent the relative amount of information about the matrix that is stored in each eigenvector for reproducing the initial matrix. In many cases, such as for the prompt neutron fission spectrum, most of the information is captured with relatively few eigenvectors, and those few eigenvectors and eigenvalues alone can be used to reproduce the matrix to a very good approximation.

In these cases, significant compression of the nuclear data is possible. A study of this shows that for the cross sections of key actinides, the number of cross sections required ranges in the hundreds, as opposed to less than ten for the prompt neutron fission spectrum. The memory requirements (for all reactions with given covariance data in ENDF) compared with a compressed file generated by NJOY as a function of an error tolerance ϵ for estimating the uncertainty in k from the nuclear data are shown in Table II. The memory savings are significant (typically $> 50\%$), but perhaps not enough to justify the additional computational effort of reproducing the matrix.

Table II. Principal Eigenvector Memory Requirements (MB)

ϵ	Pu-239	U-235	U-238
10^{-2}	3.6	6.1	2.9
10^{-3}	4.8	15	5.5
10^{-4}	5.9	19	8.7
10^{-5}	6.0	20	11
NJOY	18	39	43

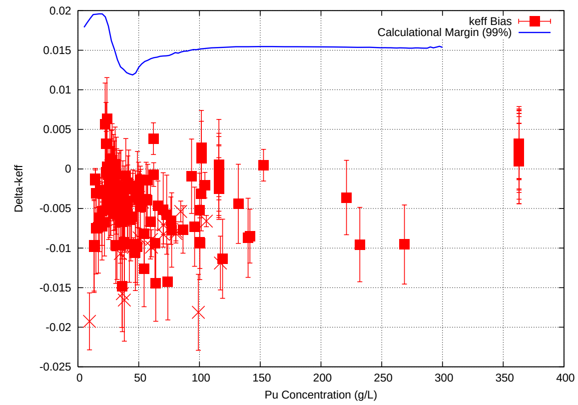

Fig. 3. Calculational margin for Pu metal-water mixes at varied concentrations.

BASELINE USL DETERMINATION

Recently, LANL performed a validation of MCNP calculations for Pu applications, and NCSP-funded S/U tools supported these efforts [7]. The goal of this effort was to develop a tool to estimate a baseline USL that NCS analysts may use to determine safe limits. Computing the baseline USL involves estimating calculational margins (biases plus their uncertainties) and scientifically-informed margins of subcriticality.

The computation of the calculational margin used a non-parametric, extreme value method. The calculational margin is defined as the value that to some confidence level (in this case 99%) that would bound the worst-case critical benchmark experiment bias, considering the benchmark uncertainties, of a weighted population of relevant benchmarks. The benchmarks were weighted using a nuclear data correlation coefficient c_k of the benchmark and the application model. The computation of the correlation coefficient uses the continuous-energy MCNP sensitivity profiles and the nuclear covariance data, which is the 44-group library distributed with SCALE6.1.

Figure 3 shows the calculational margin (the bias and calculational margin are defined consistent with the extreme-value method so that non-conservative, i.e., typically negative, values are treated as positive) that was produced for a parametric study of metal-water mixtures with varied Pu concentrations. The points in the figure represent the Pu thermal solution benchmark biases and their uncertainties; those points represented with an $\times$ were rejected in

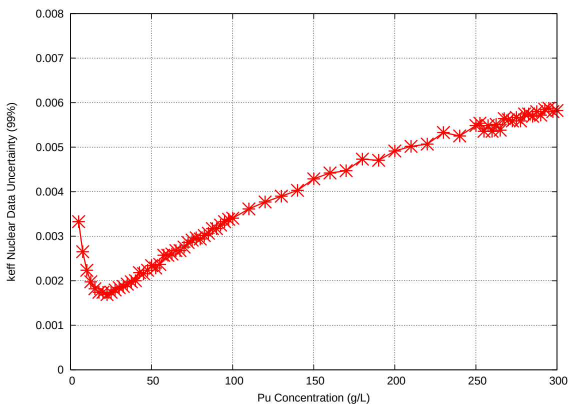

Fig. 4. Nuclear data uncertainties in k at the 99% confidence level for Pu metal-water mixes at varied concentrations.

a χ^2 minimization involving a nuclear data adjustment using generalized-linear least squares (GLLS), which is the same method in TSURFER, and therefore not used when computing the calculational margin.

The margin of subcriticality includes three factors: a margin for undetected errors in the transport software (a detection limit), uncertainties and variability in nuclear data, and an additional margin dependent upon the application. Discussions led to the establishment of a software margin of 0.005 for MCNP; this value was based upon the uncertainties of the highest quality critical benchmark experiments, the degree of support, development, and use of MCNP, as well as the degree to which MCNP has been benchmarked.

The nuclear data uncertainty was determined from the residual nuclear data uncertainty following the GLLS nuclear data adjustment at the 99% confidence level. This adjustment captures the uncertainty in k from nuclear data when considering the uncertainties of the differential measurements and their unknown dependencies upon the critical benchmark experiments, which are used in the data adjustment exercises. Figure 4 gives the uncertainty from nuclear data (2.6σ or 99% confidence level) as a function of Pu concentration of the metal-water mixtures. The steady increase represents that the nuclear data adjustment was unable to reduce the nuclear data uncertainties as the availability of benchmarks is increasingly sparse for higher Pu concentrations.

Additional margin may be applied by the analyst as appropriate to ensure subcriticality. This accounts for additional uncertainties about the process that cannot be accounted for in the computational analysis. From here these terms are combined to create a baseline USL as a function of a set of parameters. The NCS analysts may then use this baseline along with their expert judgment to help set the USL for the entire range of normal and credible abnormal conditions.

FUTURE WORK

Plans for FY2015 include the finalization of the nuclear data covariance format in ACE and the development of routines to process ENDF data into that format. Also, further development and integration is planned on the tools with MCNP to perform the setting of the baseline USLs and the nuclear data covariance data adjustments for uncertainty quantification.

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