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STATUS OF MCNP SENSITIVITY/UNCERTAINTY CAPABILITIES FOR CRITICALITY

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ABSTRACT

A new capability is being developed in MCNP6 to provide estimates of uncertainties in the effective multiplication k because of nuclear cross sections. This has been implemented in a prototype version of MCNP6. The version reads covariance data from the nuclear data libraries, runs a continuous-energy transport calculation to compute sensitivity profiles on the energy grids found in the covariance data, and convolves them to produce estimates of the k uncertainty. Results are shown for eight criticality benchmark experiments.

Key Words: Monte Carlo, covariance data, benchmarks

1. INTRODUCTION

For the previous decade, the U.S. DOE/NNSA Nuclear Criticality Safety Program has funded the development of sensitivity and uncertainty analysis tools for critical experiments and benchmark analysis. The first production release of MCNP6 [1] includes a capability to generate sensitivity profiles for the effective multiplication k from a continuous-energy calculation [2]. Subsequent development has focused upon extending this capability to process covariance libraries to estimate uncertainties in k.

Covariance libraries are prepared from the Evaluated Nuclear Data File (ENDF) processed by the NJOY nuclear data processing code [3]. These new libraries are then converted into a new A Compact ENDF (ACE) format [4] that can be read by MCNP. Each covariance matrix has its own energy grid, and upon MCNP reading them, the code automatically creates internal tallies to estimate sensitivity coefficients on those predefined energy grids. Once the calculation has been completed, MCNP uses the sensitivity results with the covariance data to produce estimates of the uncertainty of k. Results are given for the overall uncertainty and as a function of both isotope and reaction.

This paper discusses the methodology for the sensitivity profiles and the covariance libraries and how they are used in MCNP. Results are then provided for various criticality benchmark experiments.

2. BACKGROUND

A linear estimate of the uncertainty of a response can be made given derivatives of the response with respect to various parameters and covariance information about those parameters. The derivatives are contained in a vector of sensitivity coefficients $\mathbf{S}$. The sensitivity coefficient of k with respect to parameter

x is defined as

$$S_{k,x} = \frac{x}{k}\frac{dk}{dx}. \tag{1}$$

Here the parameter x is taken to be some nuclear data, e.g., cross section, prompt fission spectra, etc.

The ENDF libraries provide estimates of the experimental uncertainties in the nuclear data that can be represented as covariance matrices $\mathbf{C}$. Given the sensitivity vector and the covariance matrix, the uncertainty in k, δk, can be found via the sandwich rule, or

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

which is the sensitivity vector times the covariance matrix times the transpose of the sensitivity vector.

2.1. Computing the Sensitivity Vectors

The sensitivity vector $\mathbf{S}$ contains information about the sensitivities to various nuclear reactions as a function of neutron energy. This can be found from perturbation theory as a ratio of adjoint-weighted integrals:

$$S_{k,x} = -\frac{\left\langle \psi^\dagger, (\Sigma_x - \mathcal{S}_x - \lambda \mathcal{F}_x)\psi \right\rangle}{\langle \psi^\dagger, \lambda F \psi \rangle}. \tag{3}$$

Here ψ is the angular (forward) flux and $\psi^\dagger$ is its adjoint function. Σ_x is the cross section corresponding to x if x is a cross section, and zero otherwise (e.g., fission χ). $\mathcal{S}_x$ is the integral scattering operator for x if x is a scattering cross section or law [includes elastic, inelastic, (n,2n), etc.], and zero otherwise. $\mathcal{F}_x$ is the integral fission operator for x if x is a fission cross section, fission ν, or fission χ and zero otherwise. The quantity $\lambda = 1/k$ and the brackets denote integration over all phase space.

The adjoint-weighted integrals are computed by special tallies within MCNP using the iterated fission probability method [5].

The sensitivities computed by Eq. (1) are sufficient for cross section or fission neutron multiplicities ν, but do not account for the fact that neutron emission spectra from fission or scattering need to be renormalized such that the integral of the probability function comes to unity. In other words, the sensitivity represents some small increase of the data in some energy range, which needs to be offset by decreases elsewhere. There are many possible methods for doing this; MCNP uses a classic approach where the entire distribution is renormalized by a constant factor after the hypothetical increase. This renormalization can be taken into account by

$$\hat{S}_{k,f}(\mu, E, E') = S_{k,f}(\mu, E, E') - f(E' \to E, \mu) \int_0^\infty dE \int_{-1}^1 d\mu \, S_{k,f}(\mu, E, E'). \tag{4}$$

Here f represents the distribution, E' is in the incident neutron energy, E is the exiting neutron energy, and μ is the scattering cosine of the collision. The renormalized sensitivity $\hat{S}_{k,f}$ must be used when applying the sandwich rule in Eq. (2) for fission χ or scattering distributions.

2.2. Representing the Covariance Matrices

Covariance data may be found in the ENDF files in several formats. These are processed by NJOY to produce covariance matrices that correlate various isotopes and reactions on a unionized energy grid for each matrix. These NJOY-generated files are then further processed by external scripts and decomposed into their principal eigenvectors. The rationale for doing this is that often the covariance matrix may be represented to a good enough approximation with a much smaller amount of information than would be required for a triangular representation (the overall covariance matrix is guaranteed to by symmetric).

To summarize the process, the eigenvalues and eigenvectors of the full covariance matrix are found. The covariance matrix can be reproduced exactly by

$$\mathbf{C} = \mathbf{V}\mathbf{D}\mathbf{V}^T. \tag{5}$$

Here $\mathbf{V}$ is a matrix where the columns are the eigenvectors of $\mathbf{C}$, and $\mathbf{D}$ is a corresponding diagonal matrix of eigenvalues. Often a smaller subset of eigenvectors is only needed to reconstruct $\mathbf{C}$, which can be chosen based on the relative magnitudes of the eigenvalues – the eigenvectors corresponding to the largest eigenvalues contain the greatest amount of information for reproducing the covariance matrix.

This smaller subset of eigenvectors and eigenvalues are denoted by $\tilde{\mathbf{V}}$ and $\tilde{\mathbf{D}}$ respectively, and the covariance matrix can be approximated by

$$\mathbf{C} \approx \tilde{\mathbf{V}}\tilde{\mathbf{D}}\tilde{\mathbf{V}}^T. \tag{6}$$

This approximate matrix is used when MCNP computes δk via the sandwich rule. MCNP computes the elements of the covariance matrix as needed, and never actually reconstructs $\mathbf{C}$, only storing the principal eigenvalues and eigenvectors. How good an approximation this is depends upon the specific problem and the nuclear data; however, a previous study [6] shows that a the δk for various reactions can be estimated quite accurately with a memory compression often far exceeding 50% that of the triangular representation.

3. RESULTS

To test the new capability, ACE covariance libraries were prepared for ENDF/B-VII.1 [7] ^{1}H , ^{16}O , ^{235}U , ^{238}U , and ^{239}Pu . This process uncovered two issues with the NJOY routines for processing covariance data. The first is that NJOY has trouble with recursively creating covariances from partial reaction cross section, which was an issue when generating the ^{16}O library. Some manual fixes were made to remove unphysical values, but the ^{16}O results should be taken as preliminary until the fix in NJOY is completed. The second issue was with generating covariances for fission χ, and is also being investigated. A special library was prepared with a custom script for ^{239}Pu only to get some quantification of its impact. Also, ACE covariance data does not yet exist in ENDF/B-VII.1 for thermal scattering, so the effect on the uncertainty of hydrogen bonded to light water is not captured, and therefore the ^{1}H results may be significantly underpredicted.

Eight benchmark experiments were selected from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) Handbook [8]. Four of the benchmarks focused on ^{235}U as the dominant fissile isotope, whereas the others were for ^{239}Pu . The four ^{235}U benchmarks are Lady Godiva (HEU-MET-FAST-001), Flattop with the Highly-Enriched Uranium (HEU) core (HEU-MET-FAST-028), a uranium hydride experiment (HEU-COMP-INTER-003), and a light-water moderated Low-Enriched Uranium (LEU) lattice (LEU-COMP-THERM-008). The four ^{239}Pu benchmarks are Jezebel (PU-MET-FAST-001), Flattop with the Pu core (PU-MET-FAST-006), a light-water reflected lattice of Mixed-Oxide (MOX) fuel (MIX-COMP-THERM-001), and a Pu solution system (PU-SOL-THERM-009).

The results are presented such that the reaction uncertainties (on-diagonal terms) and the reaction correlations (off-diagonal terms) can be combined additively by taking their sign times their square and adding them up. The factor of two on the correlation terms is implicitly included in the reported results. In other words, if the uncertainties for each component are enumerated with an index i as $(\delta k)_i$, the overall uncertainty δk can be determined by

$$(\delta k)^2 = \sum_i \text{sgn}[(\delta k)_i]\,(\delta k)_i^2. \tag{7}$$

3.1. Lady Godiva (HEU-MET-FAST-001)

Lady Godiva was a bare, nearly spherical experiment consisting of mostly HEU at Los Alamos Scientific Laboratory (LASL) in the 1950's. The calculational uncertainty of the ICSBEP model for ^{235}U is 1188.2 pcm and for ^{238}U is 49.7 pcm for a combined uncertainty of 1189.2 pcm. Clearly, ^{235}U is the dominant source of uncertainty, which makes sense considering that it is predominantly composed of that isotope. Table I gives the covariances as a function of reaction where the contribution is greater than 100 pcm. The results show that the ^{235}U (n,γ) capture reaction drives most of the uncertainty in k for Lady Godiva, with fission ν, scattering (elastic and inelastic combined contribute 490.9 pcm), and fission being the other major contributors.

Table I. Major Contributors of k Uncertainty (pcm) in Lady Godiva

^{235}U	(n,γ)	(n,γ)	873.8
^{235}U	(n,n$'$)	(n,n$'$)	612.4
^{235}U	ν	ν	544.6
^{235}U	(n,n)	(n,n$'$)	-541.8
^{235}U	(n,n)	(n,γ)	341.5
^{235}U	(n,n)	(n,n)	294.1
^{235}U	(n,f)	(n,f)	268.9

3.2. Flattop with HEU Core (HEU-MET-FAST-026)

Flattop is a spherical reflected assembly with an interchangeable core (HEU or Pu) and a natural uranium reflector. The calculational uncertainty of the ICSBEP model is 1378.2 pcm, with ^{235}U contributing 1310.7 pcm and ^{238}U contributing only 425.9 pcm. Table II gives the individual reaction components greater than 100 pcm. Like with Lady Godiva, the dominant contributor to the uncertainty is the ^{235}U (n,γ) capture cross section. ^{238}U scattering would also be a very important contributor as well, except for the fact that the elastic and inelastic scattering reactions are strongly anticorrelated in the ENDF/B-VII.1 evaluation.

Table II. Major Contributors of k Uncertainty (pcm) in Flattop-HEU

^{235}U	(n,γ)	(n,γ)	1152.1
^{238}U	(n,n)	(n,n$'$)	-716.4
^{238}U	(n,n$'$)	(n,n$'$)	707.3
^{235}U	ν	ν	513.8
^{238}U	(n,n)	(n,n)	425.8
^{235}U	(n,n$'$)	(n,n$'$)	271.4
^{235}U	(n,f)	(n,f)	236.6
^{235}U	(n,n)	(n,n$'$)	-222.2
^{235}U	(n,n)	(n,γ)	192.2
^{235}U	(n,n)	(n,n)	104.7

3.3. Uranium-Hydride Benchmark (HEU-COMP-INTER-003)

This experiment consists of cylindrical cans of highly-enriched UH_3, and is interesting because it has an intermediate spectrum with about 60% of fissions being caused by neutrons between 0.625 eV and 100 keV. The calculational uncertainty in k from the nuclear data is 1587.2 pcm, with ^{1}H contributing 237.6 pcm, ^{235}U contributing 1512.6 pcm, and ^{238}U contributing 418.2 pcm. Table III gives the uncertainty contributors as a function of reaction ($>$ 100 pcm).

Table III. Major Contributors of k Uncertainty (pcm) in the UH_3 Experiment

^{235}U	(n,γ)	(n,γ)	1327.1
^{238}U	(n,n$'$)	(n,n$'$)	592.9
^{235}U	ν	ν	582.7
^{238}U	(n,n)	(n,n$'$)	-472.6
^{235}U	(n,n)	(n,γ)	320.4
^{235}U	(n,n$'$)	(n,n$'$)	265.8
^{1}H	(n,n)	(n,n)	237.6
^{238}U	(n,n)	(n,n)	213.5
^{235}U	(n,n)	(n,n$'$)	-179.1
^{235}U	(n,f)	(n,f)	160.8
^{235}U	(n,f)	(n,γ)	114.8

3.4. Light-Water Moderated LEU Lattice (LEU-COMP-THERM-008)

This benchmark is a reactor physics experiment consisting of LEU fuel pins moderated by light water. The overall calculational uncertainty in k from the nuclear data is 747.6 pcm. By isotope, ^{1}H contributes 189.7 pcm, ^{235}U contributes 666.8 pcm, and ^{238}U contributes 279.9 pcm. Table IV gives the contributions by reaction ($>$ 100 pcm). For this experiment, ^{235}U total ν is by far the largest contributor to the uncertainty.

Table IV. Major Contributors of k Uncertainty (pcm) in the LEU Lattice

^{235}U	ν	ν	625.8
^{238}U	(n,γ)	(n,γ)	264.2
^{1}H	(n,γ)	(n,γ)	181.3
^{235}U	(n,f)	(n,f)	144.6
^{235}U	(n,γ)	(n,γ)	131.5
^{235}U	(n,f)	(n,γ)	122.1

3.5. Jezebel (PU-MET-FAST-001)

Jezebel was a nearly spherical critical experiment consisting of mostly ^{239}Pu at LASL in the 1950's and 1960's. The uncertainty of k because of ^{239}Pu is 600.7 pcm. The uncertainty contributions by reaction (¿ 10 pcm) are given in Table V. The largest contributor is the scattering (inelastic and elastic) followed by fission, fission χ, and fission ν respectively.

Table V. Major Contributors of k Uncertainty (pcm) in Jezebel

^{239}Pu	(n,n$'$)	(n,n$'$)	868.8
^{239}Pu	(n,n)	(n,n$'$)	-865.0
^{239}Pu	(n,n)	(n,n)	455.9
^{239}Pu	(n,f)	(n,f)	331.0
^{239}Pu	χ	χ	173.9
^{239}Pu	ν	ν	81.6
^{239}Pu	(n,n)	(n,f)	-81.4
^{239}Pu	(n,γ)	(n,γ)	72.3
^{239}Pu	(n,n)	(n,γ)	36.1
^{239}Pu	(n,2n)	(n,2n)	10.4

3.6. Flattop with Pu Core (PU-MET-FAST-006)

This experiment is like the previous Flattop case, except that it has a Pu spherical core as opposed to a HEU one. The overall calculational uncertainty of k is 572.4, with ^{238}U contributing 415.7 pcm, and ^{239}Pu contributing 393.4 pcm. Table VI gives the uncertainty contributor by reaction ($>$ 100 pcm). ^{238}U scattering is the largest source of uncertainty, followed by ^{239}Pu fission and fission χ.

3.7. MOX Lattice in Light Water (MIX-COMP-THERM-001)

This benchmark is a lattice of MOX fuel pins immersed in light water. The predicted uncertainty in k from the nuclear data is 700.5 pcm. By isotope, ^{1}H contributes 375.2 pcm, ^{16}O 176.8 pcm, ^{238}U 199.1 pcm, and ^{239}Pu 528.2 pcm. Table VII gives the listing of uncertainty contributors by reaction.

Table VI. Major Contributors of k Uncertainty (pcm) in Flattop-Pu

^{238}U	(n,n)	(n,n′)	-825.5
^{238}U	(n,n′)	(n,n′)	777.3
^{238}U	(n,n)	(n,n)	487.9
^{239}Pu	(n,n)	(n,n′)	-317.1
^{239}Pu	(n,n′)	(n,n′)	300.3
^{239}Pu	(n,f)	(n,f)	286.1
^{239}Pu	χ	χ	192.4
^{239}Pu	(n,n)	(n,n)	175.0
^{239}Pu	(n,γ)	(n,γ)	110.4

Table VII. Major Contributors of k Uncertainty (pcm) in MOX Lattice

^{1}H	(n,n)	(n,n)	317.7
^{239}Pu	(n,γ)	(n,γ)	275.0
^{239}Pu	(n,f)	(n,f)	260.6
^{239}Pu	χ	χ	250.6
^{239}Pu	(n,f)	(n,γ)	222.3
^{238}U	(n,n′)	(n,n′)	213.9
^{1}H	(n,γ)	(n,γ)	199.6
^{16}O	(n,n)	(n,n)	176.7
^{239}Pu	ν	ν	150.0
^{238}U	(n,n)	(n,n′)	-112.9

3.8. Pu-Light Water Solution (PU-SOL-THERM-009)

The benchmark experiment is a spherical tank of plutonium nitrate solution. The uncertainty in k from the nuclear data is 1295.0 pcm, with ^{1}H contributing 1040.6 pcm and ^{239}Pu contributing 771.0 pcm. Table VIII gives the most important reactions for the uncertainty in k.

Table VIII. Major Contributors of k Uncertainty (pcm) in the Pu Solution

^{1}H	(n,γ)	(n,γ)	1034.0
^{239}Pu	(n,f)	(n,f)	628.4
^{239}Pu	(n,f)	(n,γ)	339.1
^{239}Pu	(n,γ)	(n,γ)	216.0
^{239}Pu	ν	ν	168.9
^{1}H	(n,n)	(n,n)	116.8
^{239}Pu	χ	χ	96.8

4. SUMMARY, CONCLUSIONS, & FUTURE WORK

A capability for estimating the uncertainty in k with MCNP has been developed. A new ACE covariance format has been developed, and coding has been implemented into a prototype MCNP to process the new format. Covariance data libraries have been prepared using NJOY and ENDF/B-VII.1 nuclear data, and these files have been processed to make the new ACE format.

Calculations were run on eight ICSBEP benchmarks, and estimates on the uncertainty in k were obtained. The results show that for fast HEU systems, the ^{235}U (n,γ) capture cross section is the largest source of uncertainty. For thermal HEU systems, it appears that the ^{235}U fission ν is a dominant source of calculational uncertainty in k. For fast Pu systems, ^{239}Pu neutron elastic and inelastic scattering together appear to be driving much of the uncertainty, with smaller contributions from fission, fission ν, and fission χ. For thermal Pu systems tested, the ^{239}Pu fission and (n,γ) capture cross sections are a major source of uncertainty in k.

One isotope that appears to drive a significant amount of the uncertainty is ^{1}H . Unfortunately, because there is no thermal scattering law covariance data in ENDF/B-VII.1, the uncertainties for scattering may be significantly underpredicted because hydrogen bonded to light water is neglected. In the future, MCNP may approximate this by treating scattering off isotopes in molecules and crystalline lattices as free should no data be provided.

Also, fission χ covariance data was only generated for ^{239}Pu . This was done specially as NJOY currently has difficulties generating a correct covariance library. This issue is currently under investigation and hopefully a fix will be soon forthcoming so that fission χ covariance data for other actinides may be obtained. Furthermore, covariances were generated for none of the angular scattering distributions (i.e., no $\bar{\mu}$ uncertainties yet). Recently, a method was developed to handle this for Legendre moments [9], which is how the angular covariance data is represented, and hopefully soon uncertainties estimates can be made for these as well.

Otherwise, development will continue on this new capability. The new ACE covariance format will be refined, and NJOY will be modified to generate these libraries directly. Development will continue in MCNP with the ultimate goal of providing criticality safety practitioners with a simple and efficient means of finding calculational uncertainty estimates of k from nuclear data.

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