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Title:	K-Eigenvalue Sensitivity Coefficients to Legendre Scattering Moments
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INTRODUCTION

The major source of uncertainty and bias in the effective multiplication k of fissioning systems is typically the nuclear data. For systems where leakage is particularly important, the angular scattering distributions may be a significant contributor. Until recently, most of the efforts related to sensitivity and uncertainty analysis have focused on the nuclear cross sections, fission neutron multiplicities ν, and fission emission spectra χ. The MCNP6 Monte Carlo code [1] has the ability to compute sensitivity profiles for scattering distributions as a function of incident and outgoing energies and scattering cosines [2].

Often times the scattering distributions and their covariance data are represented by their Legendre moments. To make the MCNP6 results consistent for data adjustment and uncertainty quantification, an approach has been developed to compute the sensitivities to the Legendre scattering moments. The method for doing so with the existing MCNP6 capability is shown, multigroup verification is performed, and Legendre moment sensitivity profiles are calculated for three fast critical assemblies. The results show that the P_1 elastic scattering moment may be significant for criticality.

THEORY

The scattering distribution $f^j(\mu, E|E')$ describes the probability density function (PDF) of a neutron emerging with outgoing energy E and scattering cosine μ given some incident energy E' for some isotope and scattering reaction j. For this summary and to keep the notation simple, $f(\mu)$ is used and the energy and isotope dependence is implied. The scattering PDF is often described by its Legendre moments:

$$f(\mu) = \sum_{\ell=0}^{\infty} \frac{2\ell+1}{2} P_\ell(\mu) f_\ell. \tag{1}$$

Here P_ℓ is the ℓth Legendre polynomial and f_ℓ is the corresponding Legendre moment of f. The ℓth Legendre moment may be found by

$$f_\ell = \int_{-1}^{1} d\mu \, P_\ell(\mu) f(\mu). \tag{2}$$

The relative change in k from the change in f may be estimated by

$$\frac{\Delta k}{k} = \int_{-1}^{1} d\mu \, \frac{\Delta f(\mu)}{f(\mu)} \hat{s}_{k,f}(\mu), \tag{3}$$

where $\hat{s}_{k,f}(\mu)$ is the sensitivity density (in units of per cosine). The hat implies that the sensitivity coefficient considers that the distribution f is constrained by a normalization to unity. Codes like MCNP do not compute the sensitivity density, but rather a bin-integrated sensitivity coefficient. If i is the cosine bin index, then

$$\hat{S}_{k,f,i+1/2} = \int_{\mu_i}^{\mu_{i+1}} \hat{s}_{k,f}(\mu). \tag{4}$$

Note that the integer values of i represent bin edges and the bin-integrated sensitivities are taken at bin centers or $i+1/2$. The constrained sensitivity is obtained by

$$\hat{S}_{k,f,i+1/2} = S_{k,f,i+1/2} - F_{i+1/2} S_{k,f} \tag{5}$$

Here $S_{k,f,i+1/2}$ represents the sensitivity coefficient for f if the distribution were left unnormalized, $F_{i+1/2}$ represents the bin-integrated cumulative density function (CDF) from

$$F_{i+1/2} = \int_{\mu_i}^{\mu_{i+1}} f(\mu), \tag{6}$$

and $S_{k,f}$ is given by

$$S_{k,f} = \sum_{i=0}^{N-1} S_{k,f,i+1/2}. \tag{7}$$

Note that N is the number of cosine bin edges for a total of $N-1$ bins.

The sensitivity coefficient $S_{k,f,i+1/2}$ is obtained from the result of linear-perturbation theory:

$$S_{k,f,i+1/2} = \frac{\langle \psi^\dagger, \iint_i dE' d\mathbf{\Omega}' \, \Sigma_s^j f^j \psi \rangle}{\langle \psi^\dagger, \iint dE' d\mathbf{\Omega}' \, \chi \nu \Sigma_f \psi \rangle}. \tag{8}$$

The brackets denote integration over the space, energy, and direction variables. The numerator is the adjoint-weighted scattering source for isotope and reaction j and the scattering integral is only over bin i, and the denominator is the adjoint-weighted fission source for the entire system.

MCNP6 calculates both $S_{k,f,i+1/2}$ and $F_{i+1/2}$ from internal tallies and uses those to compute an estimate of

$\hat{S}_{k,f,i+1/2}$. Unfortunately, these are as a function of cosine bin and not of the Legendre moments. To get the sensitivity to the ℓth Legendre moment of f, $\hat{S}_{k,f,\ell}$, more work is required.

Going back to Eq. (3), suppose the ℓth Legendre moment is perturbed by a multiplicative factor of $1 + p$ where p is small. The change in the scattering distribution Δf is then

$$\Delta f(\mu) = \frac{2\ell + 1}{2} P_\ell(\mu) f_\ell p. \tag{9}$$

Assuming that the binning is fine enough that midpoint integration is valid, Eq. (3) may be written in a discrete form:

$$\frac{1}{p}\frac{\Delta k}{k} = \frac{2\ell + 1}{2} f_\ell \sum_{i=0}^{N-1} (\mu_{i+1} - \mu_i) \frac{P_\ell(\mu_{i+1/2})}{f_{i+1/2}} \hat{s}_{k,f,i+1/2}. \tag{10}$$

The left-hand side is the relative change in k divided by the relative change in the Legendre moment f_ℓ, so that is the sensitivity coefficient for the ℓth Legendre moment by the definition of the sensitivity coefficient. Eq. (10) could be computed in principle, but MCNP only estimates the bin-integrated quantities. Again, assuming midpoint integration is valid, the PDF and sensitivity density for at the bin centers may be related to the bin-integrated values by

$$f_{i+1/2} = \frac{F_{i+1/2}}{\mu_{i+1} - \mu_i}, \tag{11}$$

$$\hat{s}_{k,f,i+1/2} = \frac{\hat{S}_{k,f,i+1/2}}{\mu_{i+1} - \mu_i}. \tag{12}$$

Substituting these into Eq. (10) the final result for the Legendre moment is obtained:

$$\hat{S}_{k,f,\ell} = \frac{2\ell + 1}{2} f_\ell \sum_{i=0}^{N-1} (\mu_{i+1} - \mu_i) \frac{P_\ell(\mu_{i+1/2})}{F_{i+1/2}} \hat{S}_{k,f,i+1/2}. \tag{13}$$

There still remains the task of computing the Legendre moment f_ℓ, which is done by midpoint integration:

$$f_\ell = \sum_{i'=0}^{N-1} F_{i'+1/2} P_\ell(\mu_{i'+1/2}). \tag{14}$$

Here the dummy index i' is used to delineate between the index i.

The implementation of solving for $\hat{S}_{k,f,\ell}$ is as follows: First, a cosine grid is created at problem setup. The user may provide one, and if not, a default of 200 equally spaced cosine intervals of width 0.01 is used. Note that in MCNP6, these scattering cosines and all calculations are in the reference frame of the table, which is usually the center-of-mass frame. During the calculation the Iterated Fission Probability method [3] is used to calculate the unconstrained sensitivity coefficients $S_{k,f,i+1/2}$, which involves creating an outer iteration around the standard power iteration

method used to solve the k-eigenvalue problem. At the end of each outer iteration, the unconstrained sensitivity coefficients and the bin-integrated CDFs $F_{i+1/2}$ are used to compute estimates of the constrained sensitivity coefficients $\hat{S}_{k,f,i+1/2}$ and the Legendre moments f_ℓ. These are then used to compute an estimate of $\hat{S}_{k,f,\ell}$, which is the score for this outer iteration. The final result is the mean of the Legendre moment sensitivity scores, and an estimate of its uncertainty is made using basic sample statistics.

The estimate of the Legendre moment sensitivity should be accurate if the cosine grid is a fine enough representation (the default has empirically been found to be good enough) and there are no negative scattering probabilities, which MCNP does not treat. Sometimes with Legendre expansion representations in ENDF, small amounts of unphysical negative scattering occurs. When the data is processed by NJOY, these negative regions are zeroed out or ignored. Should the data have significant amounts of negative scattering, estimates obtained by MCNP for the Legendre moment sensitivities will not be accurate. Then again, negative scattering is unphysical anyway, and the data representation should have used more Legendre moments for a more accurate representation of the scattering distribution.

VERIFICATION

This capability is verified in the multigroup mode of MCNP6. The verification is performed by seeing if the sensitivity coefficient generated by MCNP6 can be used to accurately predict the relative change in k from changing the Legendre scattering moment. The reference results are determined by taking the difference in k from two independent calculations: one with baseline nuclear data and another using the same data except that one of the Legendre scattering moments has been increased by ten percent.

Two test problems are presented.

Table I. Nuclear Data for Core of Verification Problem 1

g	σ_c	σ_f	ν	χ	$\sigma_{s0,g1}$	$\sigma_{s0,g2}$
1	1/2	2	5	1/2	1/2	0
2	1	2	3	1/2	0	2

Table II. Nuclear Data for Reflector of Verification Problem 1

g	σ_c	$\sigma_{s0,g1}$	$\sigma_{s0,g2}$	$\sigma_{s1,g1}$	$\sigma_{s1,g2}$
1	1	4	1	1	0
2	1	0	5	0	1

The first test problem has two regions and two energy

Table III. Nuclear Data for Verification Problem 2

σ_c	σ_f	ν	σ_{s0}	σ_{s1}	σ_{s2}
2	2	3	4	2	1

groups. The problem is a sphere of fissionable material (core) surrounded by a non-fissionable cylindrical reflector. The sphere has a radius of 3.4 cm and is centered at the origin having an atomic density of 0.05 atoms per barn cm. The cylinder is also centered about the origin, having a radius of 7 cm, a height of 20 cm, and an atomic density of 0.10 atoms per barn cm. The material cross sections for the core and reflector are given in Tables I and II respectively.

The baseline k is $1.00291(3)$. The P_1 within-group scattering cross section is increased from 1 b to 1.1 b ($p = 0.1$), and k becomes $0.99946(3)$, for a relative change in k of $-0.00344(4)$. The sensitivity to the P_1 Legendre moment of the group 1 predicted by MCNP6 is $-0.03410(9)$ or a predicted relative change in k for $p = 0.1$ of $-0.00341(1)$, which is within 1σ of the direct perturbation calculation.

The second test problem has one region and one energy group and the P_2 Legendre scattering moment is perturbed. The problem is a bare sphere with radius of 3.5 cm and a density of 0.1 atoms per barn cm. The cross sections are given in Table III.

The base k is $0.963207(5)$. The P_2 scattering cross section is perturbed by 10%, and the resultant k is $0.963389(5)$. The reference relative change in k is therefore $0.000189(7)$. The predicted relative change in k from the MCNP6 sensitivity theory is $0.000178(4)$, which agrees within 2σ.

CRITICAL EXPERIMENT RESULTS

Results are presented for three fast critical assemblies: Jezebel, Flattop with the Highly-Enriched Uranium (HEU) core, and the Copper-Reflected Zeus experiment. Sensitivities to the Legendre moments of relevant isotopes for elastic scattering are given for each from 0 to 10 MeV integrated over 0.1 MeV intervals. All calculations used ENDF/B-VII.0 nuclear data, and the MCNP models may be found in the ICSBEP Handbook [4].

Jezebel

Jezebel was a bare, nearly spherical assembly at Los Alamos during the 1950's. The model used for the calculations is the simplified bare sphere model. Curves for the sensitivities to the first five Legendre elastic scattering moments for Pu-239 are given in Fig. 1.

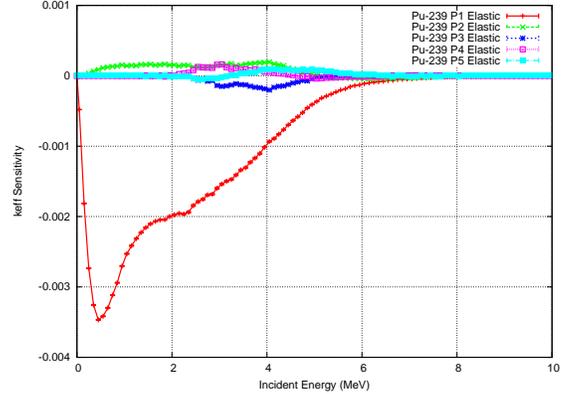The P_1 elastic moment is by far the most significant,

Fig. 1. Legendre moment elastic scattering sensitivities for Pu-239 in Jezebel.

being negative in sign indicating that, as expected, increasing the P_1 moment increases leakage and decreases k. The curve also peaks around 500 keV and not at the peak of the fission spectrum because for a few hundred keV, the scattering is mostly linearly anisotropic and therefore the P_1 component is dominant. As energy increases to several hundred keV and higher, higher Legendre moments are needed to describe the scattering and P_1 becomes less important. The higher moments are much less important overall because their increase leads to competing effects. For instance, increasing the P_2 scattering cross section both increases forward-peaked scattering and backscattering simultaneously, which tends to offset. It turns out that increasing P_2 scattering has a net positive effect in this case. The energy-integrated P_1, P_2, and P_3 sensitivities are -0.0905, 0.0056, and -0.0031 respectively.

Note that these results are somewhat contrary to those presented for Jezebel in Ref. [5], which had the P_1 peaking around a few MeV. This discrepancy makes sense, however, because the code used for their results is restricted to using P_1, i.e., all anisotropy has to be described only with one Legendre moment. Although, when integrating over all incident energies, the P_1 results show a similar magnitude. The Ref. [5] result is about -0.10 compared with -0.09.

Flattop, HEU Core

Flattop is a natural uranium reflected spherical assembly currently at the National Critical Experiments Research Center (NCERC) in Nevada. There are currently two central cores, one made of HEU and another of plutonium. The calculation model used is the simplified two concentric sphere model. Curves for the sensitivities to the first five Legendre elastic scattering moments for U-238 are given in Fig. 2.

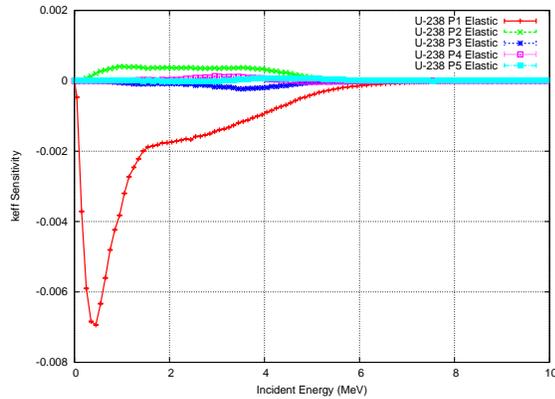The shapes of the curves in Fig. 2 are nearly iden-

Fig. 2. Legendre moment elastic scattering sensitivities for U-238 in Flattop.

Fig. 3. Legendre moment elastic scattering sensitivities for U-235 in Zeus.

tical to those in Fig. 1, however, their magnitudes are a bit higher. The energy-integrated P_1 through P_3 sensitivities for U-238 elastic scattering for this benchmark are about -0.1085, 0.0154, and -0.0054. The U-235 results were calculated, but the curves are not shown because they are of the same shape, but of smaller magnitude. The P_1 through P_3 U-235 elastic scattering sensitivities are -0.0381, 0.0006, and -0.0009.

Copper-Reflected Zeus

The Zeus experiment was conducted on the Comet machine, which is currently at NCERC. The experiment uses thin HEU cylindrical plates surrounded by a reflector; copper in this case. A detailed, 3-D model was used for the calculations, and sensitivities were obtained for Cu and U-235.

The Cu sensitivity curves show the same qualitative shapes as those of the other assemblies. The energy-integrated P_1 sensitivities for Cu-63 and Cu-65 are -0.0452 and -0.0223 respectively. The U-235 scattering distribution does not have as significant effect on criticality, but has a relatively significant P_2 moment compared to P_1. The energy-integrated sensitivity for P_1 is -0.0119 and for P_2 is 0.0067. The sensitivity profile for U-235 is shown in Fig. 3.

FUTURE WORK

In the near term, more calculations need to be performed with a broader selection of critical assemblies. Also, inelastic scattering should be considered as well, although this is more difficult because often the outgoing energy and angle are correlated and, unlike elastic scattering, one cannot necessarily be determined from the other. While covariance data for Legendre moments is currently limited
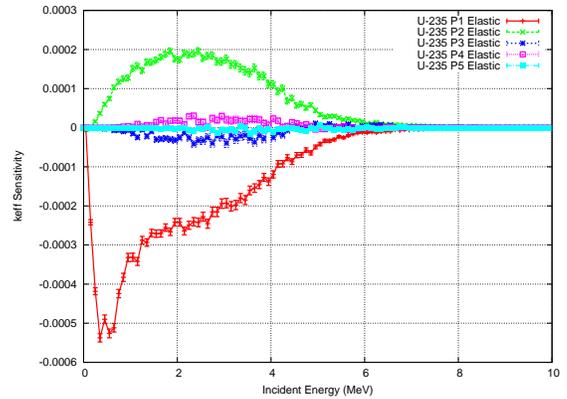
and almost always only for P_1, the results show that this may be enough to get reliable uncertainty estimates from scattering distributions for fast critical experiments. Therefore, these calculations will be attempted in the near future.

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