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Prototype Fixed-Source Sensitivity Capability in MCNP6 Applied to Subcritical Thor Core Measurements

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INTRODUCTION

A new capability was implemented into a research version of MCNP6 [1] that computes sensitivity profiles to responses (currents, fluxes, reaction rates) from nuclear data in fixed source calculations. This was done to support subcritical measurements done at the National Critical Experiment Research Center (NCERC) in Nevada. This summary discusses the theory and implementation of the new capability and its application to the recent subcritical Thor core measurements at NCERC. The results show that the new capability can predict the effect of small changes in mass to within 5-10%.

THEORY & METHOD

The sensitivity of response R is defined as the ratio of the predicted relative change in R as a result of a relative change in system paramter x. This is, in differential form,

$$S_{R,x} = \frac{x}{R}\frac{\partial R}{\partial x}. \tag{1}$$

Here R is taken to be a response such as a neutron flux, leakage current, or reaction rate, and x is taken here to be some nuclear data. For a reaction rate, the response R can be written as

$$R = \langle f_R, \psi \rangle . \tag{2}$$

Here f_R is the response function (often a cross section), ψ is the (forward) angular flux, and the brackets denote integration over all response positions, energies, and directions. The sensitivity of R can then be expressed as

$$S_{R,x} = \frac{x}{R}\left[\left\langle \frac{\partial f_R}{\partial x}, \psi \right\rangle + \left\langle f_R, \frac{\partial \psi}{\partial x} \right\rangle\right]. \tag{3}$$

The derivative on the left term is fairly simple to evaluate, and when multiplied by x, leads to just being the reaction rate if f_R is a function of x and zero otherwise. The second term may be found using perturbation theory. Consider the forward and adjoint transport equations:

$$H\psi = Q, \tag{4}$$

$$H^\dagger \psi^\dagger = f_R. \tag{5}$$

Here H is the (forward) transport operator containing the physics of leakage, total interactions, scattering, and fission, Q is the neutron source, and the daggers represent the adjoint operators or functions. Differentiating the forward transport equation, multiplying by the adjoint function $\psi^\dagger$, and integrating over all phase space yields

$$\left\langle \psi^\dagger, H\frac{\partial \psi}{\partial x} \right\rangle = \left\langle \psi^\dagger, \frac{\partial Q}{\partial x} \right\rangle - \left\langle \psi^\dagger, \frac{\partial H}{\partial x}\psi \right\rangle. \tag{6}$$

For the left hand side, applying the property of adjoints and substituting gives an expression for the unknown term in Eq. (3):

$$\left\langle \psi^\dagger, H\frac{\partial \psi}{\partial x} \right\rangle = \left\langle \frac{\partial \psi}{\partial x}, H^\dagger \psi^\dagger \right\rangle = \left\langle f_R, \frac{\partial \psi}{\partial x} \right\rangle. \tag{7}$$

By substitution, Eq. (3) can be rewritten as

$$S_{R,x} = \frac{x}{R}\left[\left\langle \frac{\partial f_R}{\partial x}, \psi \right\rangle + \left\langle \psi^\dagger, \frac{\partial Q}{\partial x} \right\rangle - \left\langle \psi^\dagger, \frac{\partial H}{\partial x}\psi \right\rangle\right]. \tag{8}$$

Multiplying through by x gives the final result to be evaluated by Monte Carlo:

$$S_{R,x} = \frac{\langle f_{R,x}, \psi\rangle + \langle \psi^\dagger, Q_x\rangle - \langle \psi^\dagger, H_x\psi\rangle}{R}. \tag{9}$$

Here $f_{R,x}$ is the portion of the response function that is an element of nuclear data x. For example, if $f_R = \nu\Sigma_f$, the total fission neutron production rate, and x is $\sigma_f^{U_{235}}$, the ^{235}U microscopic fission cross section, then $f_{R,x} = \nu^{U_{235}}\Sigma_f^{U_{235}}$, the fission neutron production exclusively from ^{235}U . The term Q_x represents the source term impacted by nuclear data x. For example, the ^{240}Pu density would impact a spontaneous fission source. The term H_x is the transport operators for nuclear data x, or the scattering and fission sources from x minus the interaction rate from x.

Implementation

MCNP6 was modified to incorporate the new capability in fixed-source mode. The current implementation only supports neutron problems, and the responses are limited to currents, fluxes, and reaction rates.

The physical meaning for the three terms in the numerator of Eq. (9) are: the response reaction rate from x, the importance-weighted source from x, and the importance-weighted interaction rate and scattering and fission sources from x. Each of these terms is handled separately.

The response term is handled upon a neutron scoring the tally response R. In addition to scoring R for the denominator of Eq. (9), the first term in the numerator is scored for each x. The middle term of Eq. (9), the effect of the source, is not yet implemented because it is not clear how to match user specified source distributions with the physical events (e.g., spontaneous fission, (α,n) of various nuclides). The third term for the adjoint-weighted transport is perhaps the most involved. The adjoint weighting routines for sensitivities of k in eigenvalue problems already handle this term and are fairly straightforward to adapt to fixed source mode – Ref. [2] gives details.

Verification

During the development of this capability, several test problems were performed. One such is presented here to demonstrate that the capability correctly finds the sensitivity to a response. The change in the response ΔR is predicted from two individual calculations, one with fixed, reference atomic densities, and another with the atomic density of nuclide x increased. Using the predicted $\Delta R/R$ and given $\Delta x/x$, the reference sensitivity is found.

The test case is as follows: A 10 cm radius sphere of a mix containing water and plutonium (20:1 ratio of water to plutonium being 80% ^{239}Pu and 20% ^{240}Pu by atom) is infinitely reflected by water. For simplicity, the atomic densities of both are 0.1 atoms per barn-cm. The source is uniformly sampled 1 MeV neutrons throughout the sphere. The response function f_R is $\nu\Sigma_f$ of ^{239}Pu exclusively, i.e., the fission neutron production in ^{239}Pu .

Reference sensitivities are generated for ^{1}H , ^{16}O , ^{239}Pu , and ^{240}Pu . The change in the response ΔR is predicted from two individual calculations, one with fixed, reference atomic densities, and another with the atomic density of response x increased. The $\Delta R/R$ is divided by the $\Delta x/x$ to get the reference sensitivity. A calculation of the sensitivities was made and the results compared to the reference cases are given in Table I with C/E values ($C/E = 1$ implies perfect agreement with the reference case). The statistical uncertainties of the reference results are about 2-3%. The sensitivities agree within these statistical uncertainties.

Table I. Sensitivities to Neutron Production for Water Reflected, Plutonium-Water Sphere.

x	$S_{R,x}$	C/E
^{1}H	2.3813	1.039
^{16}O	0.8847	1.021
^{239}Pu	2.2172	1.007
^{240}Pu	-0.4296	1.036

EXPERIMENTAL MEASUREMENT

Experiment Configurations

The purpose of this experiment is to provide benchmark data to validate recent improvements in computational tools and to provide a better understanding in the uncertainties associated with subcritical systems. This is the first in a series of subcritical experiments that investigated uncertainties and focused on subcritical plutonium systems. Use of the Thor core allows for samples to be placed inside the glory hole.

The Thor core [3, 4] is composed of three delta-phase plutonium components. The upper, center, and lower sections have masses of 3193 g, 4086 g, and 2174 g respectively. When put together, the three pieces form an approximate sphere with a total mass of 9453 g. All three components of the Thor core are clad with nominally 5 mils of nickel. The Thor core has a 0.5 inch glory hole in the center. 9.5 kg of delta-phase plutonium is a very significant quantity of nuclear material (15 and 7.3 kg are the approximate bare and water-reflected critical masses of delta-phase Pu), and this amount of material allows the added benefit of measuring a system with a high multiplication (the bare core has a multiplication of nearly 6).

Four radiation detectors were used to measure each configuration: two NPOD detectors, a SNAP detector, a LN_2-cooled HPGe detector. This sensitivity study focuses solely on the response of the SNAP detector.

Table II. Experimental Configurations Measured.

#	Lower	Center	Upper	G.H. Mass (g)
1	+			0
2		+		0
3		+		206.9
4			+	0
5	+	+		0
6	+	+		206.9
7	+		+	0
8		+	+	0
9		+	+	206.9
10	+	+	+	0
11	+	+	+	206.9
12	+	+	+	109.5
13	+	+	+	49.0

Table III. SNAP Measurements and Calculations.

#	mass (g)	Q	Expt.	MCNP	C/E
1	2174	4.36E+07	10	12	1.24
2	4086	8.17E+07	22	25	1.14
3	4293	8.49E+07	23	27	1.18
4	3193	6.36E+07	17	21	1.24
5	6260	1.07E+08	55	68	1.23
6	6467	1.10E+08	58	73	1.25
7	5367	1.07E+08	46	40	0.87
8	7279	1.45E+08	70	86	1.22
9	7486	1.49E+08	78	94	1.21
10	9453	1.89E+08	147	175	1.19
11	9660	1.92E+08	167	206	1.23
12	9563	1.91E+08	159	192	1.21
13	9502	1.90E+08	153	182	1.19

Table II shows 13 of the configurations that were measured for this experiment (G.H. = glory hole). A "+" symbol in the table represents that the component was present. Three different glory hole masses are used: 206.9 g is the mass when the glory hole is full, 109.5 g fills approximately half of the glory hole volume, and 49.0 g is approximately one-half the glory hole volume.

SNAP Measurements & Calculations

The SNAP count rates were taken for each of the experimental configurations for a time of 300 s. SOURCES-4C [5] was used to calculate the spontaneous fission sources, and those were used as the source multiplier in MCNP6 to estimate the count rates.

The measurements and calculations are given in Table III. Note that Q is the total number of neutrons emitted in 300 s, and the 1-σ statistical uncertainties of the calculated count rates are all about 3%. For most of the configurations, there is a consistent overprediction bias of about 20%, and better modeling of the detector should improve these results and is under investigation – Configuration 7 is also an outlier that is currently being investigated.

SENSITIVITY RESULTS

In this summary, two classes of sensitivities are investigated. The first are sensitivities to the various components of the experiment to see which have a significant effect on the count rate. The results of this show that the mass of the Thor core is most important (as expected), and then the effect of small changes in mass (i.e., insertion of material into the glory hole) is predicted by sensitivity theory and compared to the measured results.

Table IV. Sensitivities for Densities of Experiment Components

Component	$S_{R,x}$
Thor Core	5.75E+00
SNAP	8.76E-01
NPOD	-1.21E-02
HPGE	-3.54E-05
Tables	1.44E-02
Floor	2.05E-03

Experiment Component Sensitivities

The sensitivity to the SNAP count rate was found for the various objects that were part of the experiment: the Thor core, the SNAP (excluding the active ^{3}He gas), NPOD, and HPGE detectors, the tables, and the floor. The physical meaning of this sensitivity gives the effect of a uniform decrease in the density of these various objects, and their relative magnitudes denote the importance of each. Results are given only for configuration 11, the fully loaded Thor core.

Table IV gives the sensitivity for each component. The effect of the neutron source from spontaneous fission is assumed to be unity (the neutron emission rate scales linearly with the fissionable density). The results show that the most important element of the experiment is the fissionable material itself, confirming the expectation that the fissionable mass is the most important factor in determining the SNAP count rate. The SNAP detector has a lesser, but significant impact, the NPOD, tables, and floor have a minor, but non-negligible impact, and the HPGE does not impact the count rate much at all.

Thor Core Mass Sensitivities

The ability of the prototype MCNP capability to predict the effect small changes in mass in a subcritical multiplying system to the SNAP detector count rate is assessed. To do this, the region-wise density sensitivity is obtained for the plutonium in the glory hole for configurations 3, 6, 9, and 11. The perturbed cases (removal of mass) are 2, 5, and 8 for configurations 3, 6, and 9 respectively and configurations 10, 12, and 13 for configuration 11; these are

Table V. 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

referred to as perturbations A through F in that order.

The modified MCNP6 is used to estimate the sensitivity to the transport or multiplication within the Thor core. The sensitivity to the neutron source for spontaneous fission is assumed to be unity. Both of these effects were combined to predict the change in the experimental measurement of the case cases for the corresponding mass removals.

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 V along with the C/E for how well the perturbed measurement is predicted. 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.

SUMMARY & FUTURE EXTENSIONS

A prototype fixed-source sensitivity capability was implemented into a research version of MCNP6, and its theory and implementation were discussed in this summary. One of several verification problems was shown here, and the results show that the capability can predict response sensitivities. The recent subcritical measurements of the Thor core at NCERC were discussed, and calculations of the SNAP count rate with MCNP6.1 are compared with measurement, showing a relatively consistent bias of about $+20\%$. Sensitivities were computed for the most reactive configuration, and it appears the count rate is most driven by the mass in the Thor core. Sensitivities to the mass in the glory hole of the Thor core were calculated by MCNP and predicted changes in responses were compared to measurements; the results show about a -5% bias, which is smaller than the bias of the measurement itself. Better modeling of the experiment and the detector is currently being investigated, which should hopefully reduce the bias.

In the future, this capability needs to be extended to directly account for the effect of sources. Also, a methodology for multiplication measurements using coincident counting with the NPOD needs to be developed. Another application is an upcoming measurement involving a polyethylene reflector of a highly-enriched uranium sphere, the Flattop core.

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