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Title: Eigenvalue Sensitivity Analysis Using the MCNP5 Perturbation Capability

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EIGENVALUE SENSITIVITY ANALYSIS USING THE MCNP5 PERTURBATION CAPABILITY

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The MCNP5 perturbation capability can be used to estimate k_{eff} *sensitivities to isotopic reaction cross sections. Only the first-order Taylor term is needed, and the computed sensitivities are independent of the size of the perturbation. Accuracy of the perturbation estimate can always be tested for the total cross section. Two test problems are presented, a one-group fast reflected sphere and a continuous-energy homogeneous thermal sphere. Comparisons are made with direct estimates obtained by directly perturbing the one-group data and with TSUNAMI-3D results, respectively. The PERT card RXN keyword reaction numbers corresponding to TSUNAMI-3D reactions are given. The MCNP5 method becomes inaccurate when the fission source distribution is perturbed and is inaccurate for* k_{eff} *sensitivities to some scattering cross sections.*

I. INTRODUCTION

The differential operator method for estimating the sensitivity of a response to a cross section in a general three-dimensional Monte Carlo calculation was developed by Hall.[1] McKinney[2] implemented the method in an earlier version (4B) of the MCNP5 Monte Carlo code.[3] Rief[4] realized that the linear term of Refs. 1 and 2 was the first-order term in a Taylor series expansion of a perturbation and derived the second-order Taylor term, which was subsequently implemented[3] in MCNP. There has been recent renewed interest in using MCNP for three-dimensional sensitivity and uncertainty analysis.[5]

In this paper, the perturbation capability is used to compute k_{eff} sensitivities in a one-group and a continuous-energy problem. The one-group problem is a spherical reflected fast system; exact sensitivities are obtained for comparison by directly perturbing the cross sections. Continuous-energy problems present difficulties because there is no direct method of obtaining the exact sensitivities, except for energy-integrated sensitivities to total cross sections. Thus, a comparison is made with results from the TSUNAMI-3D sequence[6,7] of the SCALE code.[8] The continuous-energy test problem is a homogeneous sphere of UF_4 (enriched to 2%) and paraffin.[9]

II. TAYLOR SERIES, SENSITIVITIES, AND MCNP PERTURBATIONS

A Taylor series expansion of a response k with respect to some reaction cross section σ_x is

$$k(\sigma_x) = k_0 + \left.\frac{dk}{d\sigma_x}\right|_{\sigma_{x,0}} \Delta\sigma_x + \frac{1}{2}\left.\frac{d^2k}{d\sigma_x^2}\right|_{\sigma_{x,0}} (\Delta\sigma_x)^2 + \cdots, \tag{1}$$

where $\sigma_{x,0}$ is the reference value of the cross section, $k_0 \equiv k(\sigma_{x,0})$ is the reference value of the response, and

$$\Delta\sigma_x \equiv \sigma_x - \sigma_{x,0}. \tag{2}$$

For later convenience, define the first- and second-order Taylor terms as

$$\left[\Delta k(\Delta\sigma_x)\right]_{\text{1st}} = \frac{dk}{d\sigma_x}\Delta\sigma_x \tag{3}$$

and

$$\left[\Delta k(\Delta\sigma_x)\right]_{\text{2nd}} = \frac{1}{2}\frac{d^2k}{d\sigma_x^2}(\Delta\sigma_x)^2, \tag{4}$$

respectively; all derivatives are assumed to be evaluated at the reference value $\sigma_{x,0}$. The two-term Taylor series representation of the k perturbation Δk associated with the cross section perturbation $\Delta\sigma_x$ is

$$\left[\Delta k(\Delta\sigma_x)\right]_{\text{PERT}} = \left[\Delta k(\Delta\sigma_x)\right]_{\text{1st}} + \left[\Delta k(\Delta\sigma_x)\right]_{\text{2nd}}. \tag{5}$$

The subscript PERT is used because, at present, the MCNP5 perturbation capability, invoked with the PERT card, uses a two-term Taylor expansion.

Define the relative cross-section perturbation p_x as

$$p_x \equiv \Delta\sigma_x / \sigma_{x,0} \tag{6}$$

so that the cross section varies as

$$\sigma_x = \sigma_{x,0}(1 + p_x). \tag{7}$$

Using Eq. (6) in Eq. (3), the first-order Taylor term is

$$\left[\Delta k(\Delta\sigma_x)\right]_{\text{1st}} = p_x\sigma_{x,0}\frac{dk}{d\sigma_x}. \tag{8}$$

The *sensitivity* of k to cross section σ_x is defined as

$$S_{k,\sigma_x} \equiv \frac{\sigma_{x,0}}{k_0}\frac{dk}{d\sigma_x}. \tag{9}$$

The sensitivity is related to the first-order Taylor term of Eq. (8):

$$S_{k,\sigma_x} = \frac{1}{k_0 p_x}\left[\Delta k(\Delta\sigma_x)\right]_{\text{1st}}. \tag{10}$$

Equation (10) provides a prescription for computing k_{eff} sensitivities to cross sections using the MCNP5 perturbation capability. In particular, note that only the first-order term should be used[1,4] (METHOD=2 on the PERT card). Because $\left[\Delta k(\Delta\sigma_x)\right]_{\text{1st}}$ is linear with respect to the size of the perturbation p_x [Eq. (8)] the computed sensitivity is independent of p_x; any non-zero value can be used. This insight is useful for users of MCNP5 who may be unable to modify the source code to print more digits in the "predicted changes in keff…for perturbations" output; they can increase p_x to populate as many digits of the FORTRAN `0pf17.5` format as desired.

Generally speaking, the MCNP perturbation capability is sensitive to three sources of error. The first is the lack of third- and higher-order terms in the Taylor expansion and the second is the lack of second-order cross terms.[10] For sensitivity analysis, only the first-order term is needed, so these errors are generally irrelevant. Occasionally the second-order term might be used for comparison with the first-order term to help diagnose problems. Normally, however, the advice[3] about comparing the second- and first-order terms to estimate the accuracy of the second-order Taylor expansion does not apply to sensitivity analysis.

The third source of error in MCNP k_{eff} perturbation calculations is that the fission source is approximated as unperturbed. This approximation can lead to serious errors in sensitivity results.

Using Eq. (7) in Eq. (9) yields

$$S_{k,\sigma_x} = \frac{\sigma_{x,0}}{k_0}\frac{dk}{dp_x}\frac{dp_x}{d\sigma_x} = \frac{1}{k_0}\frac{dk}{dp_x}. \tag{11}$$

Equation (11) suggests that sensitivities are additive. If $\sigma_x = \sum_{i=1}^{I}\sigma_i$, where I is the number of reactions included in reaction x, then $S_{k,\sigma_x} = \sum_{i=1}^{I} S_{k,\sigma_i}$. However, the second-order terms in the Taylor series are not additive in this way.

The statistical relative uncertainty in the sensitivity is given by the usual propagation of errors formula to be

$$\frac{s_{S_{k,\sigma_x}}}{S_{k,\sigma_x}} = \sqrt{\left(\frac{s_{\Delta k_1}}{\Delta k_1}\right)^2 + \left(\frac{s_{k_0}}{k_0}\right)^2}, \tag{12}$$

where s_x^2 is the variance of quantity x and $\Delta k_1 \equiv \left[\Delta k(\Delta\sigma_x)\right]_{1\text{st}}$. Equation (12) assumes that Δk_1 and k_0 are uncorrelated, which is not true if they are computed using the same set of histories but which is nevertheless a common approximation.

An example showing how to set up a perturbed material and modify its density on the PERT card in order to perturb a specific reaction in a specific isotope of a material is given in Chapter 3 of the MCNP5 manual.[3] However, the example incorrectly implies that the default METHOD (1) should be used. In fact, METHOD=2 should be used, because only the first derivative is needed [Eqs. (9) and (10)].

III. ONE-GROUP TEST PROBLEM

The one-group k_{eff} test problem is a homogeneous spherical fuel region (radius 6.12745 cm) surrounded by a spherical reflector shell (thickness 3.063725 cm). It is problem 16 from Ref. 11. The macroscopic cross sections are listed in Table I. Scattering is isotropic. These one-group data were put into a continuous-energy format for use by MCNP.

Table I. Isotopes Used in the One-Group k_{eff} Problem

Material	ν	Σ_f (cm^{-1})	Σ_c (cm^{-1})	Σ_s (cm^{-1})	Σ_t (cm^{-1})
Fuel[a]	2.797101	0.065280	0.013056	0.248064	0.32640
Reflector[b]	0.0	0.0	0.032640	0.293760	0.32640

[a] U-235 (b), Table 9, Ref. 11.
[b] H_2O (refl), Table 9, Ref. 11.

The analytic value of k_{eff} for this problem is k_{eff} = 1. Using 3×10^5 neutrons per cycle, 20 settle cycles, 300 active cycles, and an initial guess of 1, the MCNP5 track-length estimate of k_{eff} was 0.999916 ± 0.000067, having an error of –0.008% or 1.25 standard deviations (the track-length estimate was used for consistency with the Δk_{eff} estimates of the perturbation feature). Note that the MCNP5 output was modified to print more digits for both the track-length k_{eff} and its standard deviation (from FORTRAN `f12.5,f16.5` to `1p2e14.5`) and the perturbation result and its standard deviation (from `0pf17.5,f12.5` to `1pe17.5,e12.5`).

Table II.One-Group k_{eff} Eigenvalue Sensitivities

		Direct	PERT Estimate	Difference Rel. to Direct
Fuel	S_{k_{eff},σ_t}	0.75801 ± 0.04%	0.73178 ± 0.09%	–3.460%
	S_{k_{eff},σ_f}	0.68296 ± 0.04%	0.67463 ± 0.02%	–1.219%
	S_{k_{eff},σ_c}	–0.06416 ± 0.46%	–0.06507 ± 0.06%	1.417%
	S_{k_{eff},σ_s}	0.13917 ± 0.21%	0.12222 ± 0.52%	–12.178%
	S_{k_{eff},σ_t}, sum	0.75797 ± 0.07%	0.73178 ± 0.09%	–3.455%
Refl.	S_{k_{eff},σ_t}	0.10891 ± 0.28%	0.12381 ± 0.16%	13.676%
	S_{k_{eff},σ_c}	–0.01825 ± 1.64%	–0.02137 ± 0.15%	17.076%
	S_{k_{eff},σ_s}	0.12742 ± 0.23%	0.14517 ± 0.15%	13.931%
	S_{k_{eff},σ_t}, sum	0.10917 ± 0.38%	0.12381 ± 0.18%	13.405%

Derivatives were calculated using a direct approach. Libraries were created containing the perturbed cross sections (with individual reaction cross-section perturbations of ±10% and ±20%; the total cross section was also adjusted consistently) and these were used to construct a k_{eff} vs. p_x curve for each reaction x. The slope of this curve at $p_x = 0$ is the required derivative in Eq. (11). A χ^2 minimization (the Marquardt method[12]) of a linear fit was used to obtain the slope. This method allows an estimate of the uncertainty in the fitted parameters. These calculations all used 3×10^5 neutrons per cycle, 20 settle cycles, 300 active cycles, an initial guess of 1, and a different random number seed. The k_{eff} vs. p_x curves were all examined to ensure that a linear fit was appropriate.

MCNP perturbation estimates of the sensitivities for the k_{eff} problem are shown and compared with the direct results in Table II. Except for the scattering cross section, the sensitivities for the fuel cross sections are within 4% of the direct values. However, the differences are well outside the reported standard deviations. Sensitivities for the reflector cross sections are within only 13-17% of the direct values, which may be accurate enough for some applications. The differences are very far outside the reported standard deviations. Inaccurate MCNP k_{eff} perturbation results for spatially localized perturbations have been seen before, both in sensitivity analysis[13] and in reactivity worth calculations.[14] References 13 and 14 both dealt with material mass density perturbations, not reaction cross-section perturbations.

To investigate these results further, the equivalent fixed-source problem was used. The fission source distribution from a k_{eff} problem using 3×10^4 neutrons per cycle, 20 settle cycles, and 300 active cycles was used as the source; there were a bit over 9×10^6 source neutrons. Fission was treated as capture. The appropriate

Table III. One-Group k Response Sensitivities

		Direct	PERT Estimate	Difference Rel. to Direct
Fuel	S_{k,σ_t}	0.73442 ± 0.12%	0.73162 ± 0.21%	–0.381%
	S_{k,σ_f}	0.67776 ± 0.13%	0.67561 ± 0.10%	–0.318%
	S_{k,σ_c}	–0.06498 ± 1.39%	–0.06518 ± 0.16%	0.312%
	S_{k,σ_s}	0.12120 ± 0.74%	0.12119 ± 1.13%	–0.002%
	S_{k,σ_t}, sum	0.73398 ± 0.21%	0.73162 ± 0.21%	–0.321%
Refl.	S_{k,σ_t}	0.12438 ± 0.72%	0.12330 ± 0.41%	–0.866%
	S_{k,σ_c}	–0.02026 ± 4.44%	–0.02128 ± 0.35%	5.029%
	S_{k,σ_s}	0.14526 ± 0.62%	0.14458 ± 0.38%	–0.467%
	S_{k,σ_t}, sum	0.12500 ± 1.02%	0.12330 ± 0.45%	–1.358%

quantity of interest k is

$$k = \int dV \, \nu\Sigma_f(r)\phi(r), \tag{13}$$

where $\phi(r)$ is the scalar neutron flux. This k should be equal to the k_{eff} of the eigenvalue problem, which is 1 analytically. The MCNP5 value of k was 1.00016 ± 0.020%, which is in error by 0.168% or 0.80 standard deviations. The difference between this problem and the eigenvalue problem is that here the source really is fixed and unaffected by perturbations.

Direct sensitivities were computed using the perturbed cross-section libraries and χ^2 minimization of a linear fit as in the k_{eff} problem. These values are compared with MCNP5 perturbation estimates in Table III. The perturbation estimates are now much closer to the direct results, all within 1½% and ~2 standard deviations of the direct results, except for the sensitivity to capture in the reflector, for which the difference is 5% but still within one standard deviation.

In the MCNP perturbation k_{eff}-eigenvalue sensitivity results of Table II, there is only one source of error: the approximation that the perturbation does not affect the fission source distribution (errors associated with second- and higher-order Taylor terms do not affect sensitivity calculations). This source of error is removed in the MCNP perturbation k-response sensitivity results of Table III.

Thus, assuming that the fission source distribution is unaffected by the perturbation is the cause of the MCNP perturbation errors in Table II. Some work has been done in MCNP to implement a method of estimating the change in k_{eff} due to a perturbed fission source distribution,[15] but that was only done for the density (or total cross section), and it is not presently a usable feature of any public (i.e., outside the MCNP development team) version of MCNP.

The implicit effects of perturbed isotope self-shielding[9] were not accounted for in this analysis.

IV. CONTINUOUS-ENERGY TEST PROBLEM

IV.A. Problem Description

The problem of this section has been used before for TSUNAMI-3D tests[9]; it "is based on an unreflected rectangular parallelepiped consisting of a homogeneous mixture [of] UF_4 and paraffin with an enrichment of 2% in ^{235}U. The H/^{235}U atomic ratio is 293.9:1." The material composition is given in Table IV. As in Ref. 9, the experiment was modeled as a homogeneous sphere with a radius of 38.50 cm. The calculations used ENDF-VI cross sections (".60c") and the lwtr.60t $S(\alpha,\beta)$ table for consistency with recent TSUNAMI-3D results. The reference MCNP5 (track-length) value of k_{eff} was 1.00149 ± 0.00025, obtained using 60,000 neutrons per cycle, 20 settle cycles, and 340 active cycles. The KENO-V.a value of k_{eff} was 1.00782 ± 0.00099 (more details on this calculation will be given in Sec. IV.C.2).

Table IV. U(2)F_4 Material

Isotope	Atom Density (at/bn·cm)
^{235}U	0.00013303
^{238}U	0.006437
^{1}H	0.039097
C	0.018797
^{19}F	0.02628
Total	0.09074403

IV.B. Reaction Numbers for Comparison with TSUNAMI-3D

In the TSUNAMI-3D output, reactions are identified with words rather than specific MT numbers. The corresponding reaction numbers to use on the MCNP5 PERT card RXN keyword are given in Table V. In some cases, particularly for scattering, these were determined by trial and error. Only the five isotopes in the UF_4/paraffin test problem (Table IV) have been tested in this way so far. There may be surprises when other isotopes are used, especially with $S(\alpha,\beta)$ tables.

Table V. Reaction Sensitivity Types for Comparing TSUNAMI-3D and MCNP5 Results

Reaction	SCALE Identifier	MCNP5 PERT RXN
Sum of scattering	scatter	2 16 51 39i 91 [and 4 for $S(\alpha,\beta)$[a]]
Total	total	1
Elastic scattering	elastic	2 [and 4 for $S(\alpha,\beta)$[a]]
Inelastic scattering	n,n'	51 39i 91
n,2n	n,2n	16
Fission	fission	–6
Neutron disappearance	capture	–2
n,γ	n,gamma	102
n,p	n,p	103
n,d	n,d	104
n,t	n,t	105
n,^{3}He	n,he-3	106
n,α	n,alpha	107

[a] Only ^{1}H has been tested.

IV.C. Energy-Integrated Sensitivities

IV.C.1. Total Sensitivities

There is one direct sensitivity calculation that users can do to test the applicability of the differential operator method used in the MCNP5 perturbation capability. Since an isotopic total cross section perturbation is the same as an isotopic density perturbation, the k_{eff} sensitivity to a total isotopic cross section can be estimated directly using a central difference approximation in Eq. (11),

$$S_{k,\sigma_x} \approx \frac{1}{k_0}\frac{k(p_{x+})-k(p_{x-})}{p_{x+}-p_{x-}} = \frac{k(p_{x+})-k(-p_{x+})}{2k_0 p_{x+}}, \tag{14}$$

where $p_{x-} = -p_{x+}$ for a central difference. The perturbation parameter p_x must be small enough that the three points ($-p_x$, k_-), (0, k_0), and ($+p_x$, k_+) are in a line, but large enough that the numerator of Eq. (14) is statistically significant. The result can be compared with the result of Eq. (10), which uses the MCNP5 perturbation capability, but which is independent of the size of p_x.

Direct calculations were done with p_x = 5% and a different random number seed for each run. For ^{1}H, ^{235}U, and ^{238}U, the calculations used 120,000 neutrons per cycle, 20 settle cycles, and 680 active cycles; for C and ^{19}F, the calculations used 240,000 neutrons per cycle, 20 settle cycles, and 1360 active cycles. The perturbation calculations were done in a single run with 60,000 neutrons per cycle, 20 settle cycles, and 340 active cycles.

Results are shown in Table VI. The difference is the average,

$$\text{Difference} = \frac{S_1 - S_2}{\frac{1}{2}(S_1 + S_2)}, \tag{15}$$

with S_1 as the perturbation estimate and S_2 as the direct calculation. In addition, *Ns* is the difference represented as the number of standard deviations apart the results are, calculated by equating

$$S_1 \pm N s_1 = S_2 \mp N s_2 \tag{16}$$

and solving for *N* to find

$$N = \frac{|S_1 - S_2|}{s_1 + s_2}. \quad (17)$$

In the direct calculations, the least-squares best-fit lines through the three points had correlation coefficients greater than 0.9996 (in magnitude) except for ^{19}F, which was 0.9987.

Table VI. Energy-Integrated Total Sensitivities from MCNP5

Isotope	Direct	PERT	Difference	*Ns*
^{1}H	2.310E-01 ± 0.771%	2.215E-01 ± 0.811%	–4.210%	2.662
C	2.506E-02 ± 3.487%	1.981E-02 ± 2.644%	–23.401%	3.757
^{19}F	3.937E-02 ± 2.198%	3.432E-02 ± 1.931%	–13.716%	3.307
^{235}U	2.536E-01 ± 0.724%	2.559E-01 ± 0.074%	0.922%	1.159
^{238}U	–2.110E-01 ± 0.846%	–2.130E-01 ± 0.245%	0.933%	0.857

The results of Table VI suggest that the MCNP5 perturbation method should be accurate, in this test problem, for the uranium isotopes. The accuracy will probably not be high for C or ^{19}F. Results for ^{1}H are more ambiguous. The relative difference is only ~4%, but it is outside two standard deviations.

IV.C.2. Reaction Sensitivities

TSUNAMI-3D results for this problem were provided by B. T. Rearden (Oak Ridge National Laboratory). It is the same problem whose results appear in Table IV in Ref. 9. Dr. Rearden provided new results using 238 energy groups, ENDF-VI cross sections, and a light water scattering kernel; thus, there are differences from Ref. 9, which used 44 energy groups, ENDF-V cross sections, and a polyethylene scattering kernel. These changes resulted in a change in k_{eff} from 1.00416 ± 0.00037 (Ref. 9) to 1.00782 ± 0.00099.

MCNP5 perturbation estimates of the energy-integrated k_{eff} sensitivities are compared with TSUNAMI-3D results in Table VII. Differences were computed using Eq. (15) with S_1 as the MCNP5 result and S_2 as the TSUNAMI-3D result. The number of standard deviations separating the results, *Ns*, was computed using Eq. (17). Rows with differences greater (in magnitude) than 10% but less than 20% are blue. Rows with differences greater than 20% are red.

For hydrogen, the MCNP5 and TSUNAMI-3D results agree to within 1%, but the sensitivities to capture are far outside one standard deviation of each other. For the other isotopes, the sensitivities to capture and fission are within 2.7%, but in terms of standard deviations the differences are huge. This reflects the fact that the results are well converged but the calculations are fundamentally different (continuous-energy vs. multigroup, etc.).

For all isotopes except hydrogen, the differences in the sensitivities to total scattering and elastic scattering are very large, none smaller than 15%. These differences are responsible for almost all of the differences in the sensitivities to the total reaction cross sections. Thus, there seems to be a difference in the way MCNP5 and TSUNAMI-3D treat scattering in isotopes other than hydrogen. There is not an obvious bias. The MCNP5 estimated sensitivity to scattering in ^{235}U is larger than the TSUNAMI-3D value, but the other MCNP5 values are smaller then the corresponding TSUNAMI-3D values. Why are the scattering results so different? This is an issue that needs more study.

These code-to-code comparisons are fraught with ambiguity. It would be wrong to declare a priori that the TSUNAMI-3D sensitivities are correct. They may be so for the group structure, cross-section data, and other parameters used in the KENO calculation, but the MCNP5 calculation uses different data and methods and there is no completely fair way to compare.

However, it has already been shown (Table VI) that the differential operator method is expected to have some trouble with the carbon and fluorine in this problem. The comparison with TSUNAMI-3D (Table VII) suggests that the trouble is in the scattering reactions.

Table VII. Energy-Integrated Sensitivities

Isotope	Reaction	MCNP5			TSUNAMI-3D			Difference	*Ns*
^{1}H	Total	2.215E-01	±	0.81%	2.203E-01	±	0.09%	0.527%	0.58
	Scatter	3.223E-01	±	0.56%	3.220E-01	±	0.06%	0.073%	0.12
	Elastic	3.223E-01	±	0.56%	3.220E-01	±	0.06%	0.073%	0.12
	Capture	–1.008E-01	±	0.05%	–1.017E-01	±	0.01%	–0.918%	13.59
	n,γ	–1.008E-01	±	0.05%	–1.017E-01	±	0.01%	–0.918%	13.59
C	Total	1.981E-02	±	2.64%	2.416E-02	±	0.06%	–19.760%	8.07
	Scatter	2.048E-02	±	2.56%	2.484E-02	±	0.06%	–19.248%	8.11
	Elastic	2.028E-02	±	2.59%	2.462E-02	±	0.06%	–19.301%	8.04
	n,n′	1.963E-04	±	6.87%	2.250E-04	±	0.07%	–13.618%	2.10
	n,2n	–5.743E-10	±	68.56%	N/A[a]	±	N/A[a]	200%	1.46
	Capture	–6.681E-04	±	0.12%	–6.855E-04	±	0.01%	–2.570%	18.97
	n,γ	–4.943E-04	±	0.06%	–4.996E-04	±	0.01%	–1.053%	15.63
	n,p	–5.963E-08	±	9.41%	–2.975E-08	±	0.83%	66.877%	5.10
	n,d	–1.595E-07	±	11.19%	–5.932E-08	±	1.17%	91.542%	5.40
	n,α	–1.735E-04	±	0.45%	–1.858E-04	±	0.03%	–6.843%	14.75
^{19}F	Total	3.432E-02	±	1.93%	4.139E-02	±	0.05%	–18.680%	10.36
	Scatter	3.983E-02	±	1.67%	4.698E-02	±	0.04%	–16.472%	10.45
	Elastic	2.564E-02	±	2.43%	2.980E-02	±	0.06%	–15.002%	6.49
	n,n′	1.419E-02	±	1.35%	1.612E-02	±	0.03%	–12.699%	9.76
	n,2n	0.000E+00	±	0.000%	2.779E-06	±	0.13%	–200%	771.95
	Capture	–5.609E-03	±	0.08%	–5.592E-03	±	0.01%	0.298%	3.13
	n,γ	–2.361E-03	±	0.05%	–2.391E-03	±	0.01%	–1.274%	19.65
	n,p	–2.332E-04	±	0.22%	–2.380E-04	±	0.03%	–2.018%	8.41
	n,d	–1.114E-05	±	0.58%	–1.256E-05	±	0.04%	–12.056%	20.67
	n,t	–2.052E-06	±	1.27%	–2.625E-06	±	0.06%	–24.514%	20.80
	n,α	–3.002E-03	±	0.13%	–2.948E-03	±	0.02%	1.804%	12.06
^{235}U	Total	2.559E-01	±	0.07%	2.504E-01	±	0.02%	2.165%	23.43
	Scatter	5.524E-04	±	10.91%	4.421E-04	±	0.03%	22.188%	1.83
	Elastic	3.255E-04	±	17.42%	2.052E-04	±	0.05%	45.351%	2.12
	n,n′	2.118E-04	±	7.96%	2.196E-04	±	0.02%	–3.607%	0.46
	n,2n	1.506E-05	±	11.37%	1.727E-05	±	0.03%	–13.664%	1.29
	Fission	3.657E-01	±	0.05%	3.629E-01	±	0.01%	0.777%	12.82
	Capture	–1.103E-01	±	0.05%	–1.129E-01	±	0.01%	–2.274%	35.22
	n,γ	–1.103E-01	±	0.05%	–1.129E-01	±	0.01%	–2.274%	35.22
^{238}U	Total	–2.130E-01	±	0.25%	–2.049E-01	±	0.01%	3.859%	14.75
	Scatter	3.522E-02	±	1.39%	4.885E-02	±	0.01%	–32.422%	27.46
	Elastic	2.315E-02	±	2.00%	3.488E-02	±	0.01%	–40.424%	25.02
	n,n′	1.109E-02	±	1.25%	1.293E-02	±	0.02%	–15.318%	12.98
	n,2n	9.833E-04	±	1.48%	1.032E-03	±	0.03%	–4.806%	3.25
	Fission	3.441E-02	±	0.05%	3.350E-02	±	0.02%	2.685%	40.44
	Capture	–2.826E-01	±	0.05%	–2.873E-01	±	0.01%	–1.625%	28.50
	n,γ	–2.826E-01	±	0.05%	–2.873E-01	±	0.01%	–1.625%	28.50

[a] Not reported in TSUNAMI-3D output file.

Another fruitful way to analyze the results is to compare the total sensitivities computed directly with MCNP5 (shown in Table VI) with the TSUNAMI-3D results for the total cross section (shown in Table VII). This is done in Table VIII. The direct MCNP5 results and the TSUNAMI-3D results are all within 5% of each other. Table VIII shows that if the MCNP5 perturbation sensitivities to the total cross sections were accurate, they would be within a few percent of the TSUNAMI-3D sensitivities. This does not prove that the TSUNAMI-3D results are correct for all reactions in all isotopes, but it does suggest as much for the major reactions.

Table VIII. Energy-Integrated Total Sensitivities

Isotope	Direct MCNP5	TSUNAMI-3D	Difference	*Ns*
^{1}H	2.310E-01 ± 0.771%	2.203E–01 ± 0.091%	–4.736%	5.394
C	2.506E-02 ± 3.487%	2.416E–02 ± 0.059%	–3.684%	1.021
^{19}F	3.937E-02 ± 2.198%	4.139E–02 ± 0.048%	4.996%	2.278
^{235}U	2.536E-01 ± 0.724%	2.504E–01 ± 0.017%	–1.243%	1.666
^{238}U	–2.110E-01 ± 0.846%	–2.049E–01 ± 0.012%	–2.927%	3.366

In summary, k_{eff} sensitivities to scattering estimated with MCNP5 and TSUNAMI-3D do not agree except for ^{1}H. The direct evidence is that the MCNP5 perturbation sensitivities should match the TSUNAMI-3D sensitivities for the total reactions in Table VII. The circumstantial evidence is that the sensitivities should match for the other reactions as well. Differences are likely due to the effect of spatial and spectral fission source shifts induced by the perturbation, which are neglected by the differential operator method but accounted for (to first order) by the use of the adjoint flux in TSUNAMI-3D.

Hydrogen is a special case. The MCNP5 and TSUNAMI-3D results for the total cross section agree to within ~½% on Table VII, but Table VI shows that the MCNP5 perturbation result for the total cross section is actually in error by ~4%. Thus the MCNP5 and TSUNAMI-3D agreement for ^{1}H on Table VII should not be construed to suggest that the MCNP5 perturbation results are more correct for ^{1}H than for the other isotopes. Such are the difficulties of code-to-code comparisons.

IV. SUMMARY AND CONCLUSIONS

This paper has laid out some useful tools for using the MCNP5 perturbation feature for cross-section sensitivity analysis. The formula to convert the first-order Taylor term (METHOD=2) to a sensitivity has been given. The sensitivity is independent of the size of the perturbation. This makes the method of this paper more appealing than that of Ref. 5, in addition to the fact that the method of this paper more accurately gives the derivative needed in the definition of the sensitivity.

The accuracy of the perturbation estimate of the k_{eff} sensitivity to any isotopic total cross section can, in every case, be tested. These sensitivities can be calculated directly, in multiple MCNP runs with appropriately perturbed materials, using a central difference.

Appropriate reaction numbers for comparing MCNP5 results with TSUNAMI-3D results have been given.

The MCNP5 perturbation capability was tested in two problems. In a one-group fast reflected sphere, the sensitivities for the fuel cross sections were within 4% of the direct values, except for the sensitivity to the scattering cross section, which was in error by 12%. Sensitivities for the reflector cross sections were within only 13-17% of the direct values. A comparison with results of a fixed-source problem suggested that the errors were due to the MCNP5 approximation of the fission source distribution as unperturbed.

In a continuous-energy thermal homogeneous sphere, the k_{eff} sensitivities to the total isotopic cross sections were estimated directly using perturbed materials in MCNP5 calculations and a central-difference approximation for the derivatives. These direct results were compared with MCNP5 energy-integrated PERT results. It was clear that k_{eff} sensitivities to carbon and fluorine cross sections would be troublesome but that sensitivities to uranium cross sections would be well estimated with the perturbation capability. Then, MCNP5 perturbation estimates of the sensitivities were compared with TSUNAMI-3D results. Sensitivities to reactions in hydrogen agreed well. Sensitivities to fission and the important capture reactions agreed well. Sensitivities to scattering reactions in isotopes other than hydrogen did not agree.

Comparing the direct MCNP5 results with the TSUNAMI-3D results led to the conclusion that the MCNP5 perturbation sensitivities should match the TSUNAMI-3D sensitivities for isotopes other than ^{1}H. Differences may be due to the effect of spatial and spectral fission source shifts induced by the perturbation, which are neglected by the differential operator method in MCNP5 but accounted for (to first order) by the use of the adjoint flux in TSUNAMI-3D. However, if this were the case, then it is unclear why MCNP5 and TSUNAMI-3D results actually do agree for scattering in hydrogen, which should have a bigger spectral effect than scattering in carbon or fluorine.

Thus, the MCNP5 perturbation capability can be used for sensitivity analysis, but with caution. A method of computing adjoint-weighted quantities in continuous-energy problems, currently in development,[16] may provide much more accuracy than the differential operator method for problems with perturbation-induced fission source shifts.

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