LA-UR-09-0499

Approved for public release;
distribution is unlimited.

Title:	Comparison of MCNP5 Perturbation Estimates of k-Eigenvalue Sensitivities with Exact Results for One-Group and 30-Group Problems (U)
Author(s):	Jeffrey A. Favorite, X-1-TA
Intended for:	Electronic distribution and archive

Form 836 (7/06)

This page intentionally left blank.

Los Alamos
NATIONAL LABORATORY

research note

Applied Physics Division
Applied Science & Methods Development

Group X-1, MS F699
Los Alamos, New Mexico 87545
505/667-7780
Fax: 505/665-6722

To/MS: Distribution
From/MS: Jeffrey A. Favorite / X-1-TA, MS P365
Phone/Email: 7-7941 / fave@lanl.gov
Symbol: X-1–RN(U)09–03 (LA–UR–09–0499)
Date: January 26, 2009

SUBJECT: Comparison of MCNP5 Perturbation Estimates of *k*-Eigenvalue Sensitivities with Exact Results for One-Group and 30-Group Problems (U)

Abstract

The MCNP5 perturbation capability is used to estimate k_{eff} sensitivities to cross-section data for comparison with exact (calculated) results for two problems. One is a homogeneous k_∞ problem and the other is a two-region (spherical fuel and reflector) k_{eff} problem that is done using one and 30 groups. It is shown that sensitivities should be calculated using only the first-order Taylor term (METHOD=2 on the PERT card) and that calculated sensitivities are independent of the size of the perturbation. For the k_∞ problem, sensitivities are very accurately estimated with the MCNP perturbation capability (and, incidentally, the second-order Taylor term is also very accurately estimated). For the one-group k_{eff} problem, perturbation estimates of all sensitivities are compared with the results of direct MCNP calculations and errors of ~3% for k_{eff} sensitivities to fuel cross sections and ~15% for k_{eff} sensitivities to reflector cross sections are shown to be due to the code's lack of ability to account for the perturbed fission source distribution. For the 30-group k_{eff} problem, perturbation estimates of the sensitivities to groupwise scattering cross sections are compared with the results of direct MCNP calculations and direct PARTISN calculations, and there are large differences. It is suggested that an analysis using isotopic densities, which does not require direct perturbations of cross-section data, may allow users to assess the range of applicability of the MCNP perturbation capability for specific problems. Several recommendations are made for MCNP development and documentation, the most important of which are that the ability to perturb the number of neutrons per fission be implemented and that an existing rudimentary capability for accounting for the perturbed fission source distribution be developed for general use and released.

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]

The goal of this paper is to compare MCNP perturbation estimates of k_{eff} sensitivities to cross-section data with exact results in two problems in which exact sensitivities can be obtained. In realistic problems, exact sensitivities are difficult to obtain. Density perturbations are related to perturbations of the total cross section, so exact energy-integrated total cross-section sensitivities can be obtained simply.[6] For specific reactions (i.e., other cross sections), the data tables must be manipulated to produce exact sensitivities. If that were easy to do there would be little need for sensitivity techniques. The test problems of this paper are simple, but it is only through such problems that the comparisons with known results are possible. Code-to-code comparisons have their difficulties, but they will be the subject of a future paper.

One problem in this paper is an analytic homogeneous one-group k_∞ problem. The other is a two-region (spherical fuel and reflector) k_{eff} problem that is done using one and 30 groups. In the k_{eff} problem, exact results are obtained by directly perturbing the cross section tables. First, though, we briefly revisit the principles of sensitivity theory and show how the MCNP perturbation capability relates.

The next section of this paper discusses the Taylor series expansion of a perturbation, k_{eff} sensitivities, and the MCNP perturbation capability. In Sec. III, MCNP perturbation results are compared with analytic results in the one-region k_∞ problem. In Sec. IV, MCNP perturbation results are compared with exact results in the two-region k_{eff} problem using one energy group, and in Secs. V and VI, using 30 groups. Recommendations for MCNP development and documentation to support its use in sensitivity analysis are given in Sec. VII.

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

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

where $\sigma_{x,0}$ is the reference value of the cross section 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 base 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 MCNP perturbation capability, invoked with the PERT card, uses a two-term Taylor expansion.

Defining the relative cross-section perturbation p as

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

the first-order Taylor term is

$$\left[\Delta k(\Delta\sigma_x)\right]_{\text{1st}} = p\sigma_{x,0}\frac{dk}{d\sigma_x}. \tag{7}$$

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

$$S_{k,\sigma_x} \equiv \frac{\sigma_{x,0}}{k_0}\frac{dk}{d\sigma_x}, \tag{8}$$

where $k_0 = k(\sigma_{x,0})$ is the reference value of the response. The sensitivity is related to the first-order Taylor term of Eq. (7):

$$S_{k,\sigma_x} = \frac{1}{k_0\, p}\left[\Delta k(\Delta\sigma_x)\right]_{\text{1st}}. \tag{9}$$

Equation (9) provides a prescription for computing k_{eff} sensitivities to cross sections using the MCNP perturbation capability. Only the first-order term should be used (METHOD=2 on the PERT card). At one time this fact was well known,[1] but it seems to have been forgotten.[3,5] The computed sensitivity is independent of the size of the perturbation p; 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 to populate as many digits of the FORTRAN F17.5 format as desired. It is recommended that future versions of MCNP print more digits for both the result and the standard deviation in the "predicted changes in keff" output. It is further recommended that, in addition to or instead of the perturbation index, the user number of each perturbation be printed in the "predicted changes in keff" output as is presently done for perturbed tallies.

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. 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 about comparing the second- and first-order terms to diagnose the accuracy of the second-order Taylor expansion does not apply to sensitivity analysis since only the first-order term is of interest.

The third source of error in MCNP k_{eff} perturbation calculations is that the fission source is approximated as unperturbed. This approximation could lead to serious errors in sensitivity results. In the next section, a homogeneous k_∞ example problem will be used to avoid that issue. A more realistic two-region problem with leakage is examined in Secs. IV-VI.

Using Eqs. (2) and (6),

$$\sigma_x = \sigma_{x,0}(1+p) \tag{10}$$

and using this in Eq. (8) yields

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

In Eq. (11) p is given subscript x to emphasize that the derivative only applies to reaction x. Equation (11) suggests that sensitivities are additive. If

$$\sigma_x = \sum_{i=1}^{I}\sigma_i, \tag{12}$$

where I is the number of reactions included in reaction x, then

$$S_{k,\sigma_x} = \sum_{i=1}^{I} S_{k,\sigma_i}. \tag{13}$$

However, the second-order terms in the Taylor series are not additive in this way.

III. k_∞ Test Problem

The isotopes used in the example problem are listed in Table I. The cross sections are one-group macroscopic cross sections from Ref. 7. In this paper they are treated as microscopic cross sections and the isotopic densities in the homogeneous material are $N_1 = 0.6$ at/bn·cm and $N_2 = 0.4$ at/bn·cm so that the total material atom density $N_1 + N_2$ is 1 at/bn·cm. Nevertheless, we stress that N_1 and N_2 are atom densities, not atom fractions, and N_1 will vary but N_2 will not. These one-group data were put into a continuous-energy format suitable for use by MCNP using the MAKECE code provided by Bob Little (X-1-NAD).

Table I. Isotopes Used in the k_∞ Problem.

Index	ν	σ_f (cm^2)	σ_c (cm^2)	σ_s (cm^2)	σ_t (cm^2)
1[a]	3.24	0.081600	0.019584	0.225216	0.32640
2[b]	2.70	0.065280	0.013056	0.248064	0.32640

[a] Pu-239 (a), Table 2, Ref. 7.
[b] U-235 (a), Table 9, Ref. 7.

The analytic k_∞ is 2.4389362 [Eq. (14) below]. Using a 10-cm sphere of the material with a reflecting boundary and 5×10^5 neutrons per cycle, 30 settle cycles, 500 active cycles, and an initial guess of 1, the MCNP track-length estimate of k_∞ was 2.48947 ± 0.00008, having an error of 0.004% or 1.35 standard deviations. When sensitivities are calculated with MCNP, this is the value of k_0 that will be used in Eq. (9).

III.A. k_∞ *and Its Derivatives*

In a homogenous system from which there is no neutron leakage, the energy-integrated or one-group k-eigenvalue is[8]

$$k_\infty = \frac{\nu\Sigma_f}{\Sigma_f + \Sigma_c}, \tag{14}$$

where the notation is standard. Outside the MCNP manual, the denominator is referred to as the absorption cross section, Σ_a, but for some reason MCNP refers to capture as absorption. In Eq. (14) the capture cross section Σ_c is MCNP's absorption cross section. The total interaction cross section Σ_t is

$$\Sigma_t = \Sigma_f + \Sigma_c + \Sigma_s, \tag{15}$$

and Σ_s is the isotropic scattering cross section.

If the material is made of two isotopes with atom densities N_1 and N_2 such that $\Sigma_x = N_1\sigma_{x,1} + N_2\sigma_{x,2}$, Eq. (14) becomes

$$k_\infty = \frac{N_1\nu_1\sigma_{f,1} + N_2\nu_2\sigma_{f,2}}{N_1(\sigma_{f,1} + \sigma_{c,1}) + N_2(\sigma_{f,2} + \sigma_{c,2})}. \tag{16}$$

For comparison with MCNP perturbation results, we will examine derivatives of k_∞ with respect to each of the cross sections of material 1. The derivatives are

$$\frac{dk_\infty}{d\sigma_{t,1}} = \left(\frac{N_1}{\sigma_{t,1}}\right)\frac{dk_\infty}{dN_1} = \frac{\left(\nu_1\sigma_{f,1} - k_\infty(\sigma_{f,1} + \sigma_{c,1})\right)}{(\Sigma_f + \Sigma_c)}\left(\frac{N_1}{\sigma_{t,1}}\right), \tag{17}$$

$$\frac{d^2k_\infty}{d\sigma_{t,1}^2} = \left(\frac{N_1}{\sigma_{t,1}}\right)^2\frac{d^2k_\infty}{dN_1^2} = \frac{-2\left(\nu_1\sigma_{f,1}(\sigma_{f,1} + \sigma_{c,1}) - k_\infty(\sigma_{f,1} + \sigma_{c,1})^2\right)}{(\Sigma_f + \Sigma_c)^2}\left(\frac{N_1}{\sigma_{t,1}}\right)^2, \tag{18}$$

$$\frac{d^nk_\infty}{d\sigma_{t,1}^n} = \left(\frac{N_1}{\sigma_{t,1}}\right)^n\frac{d^nk_\infty}{dN_1^n} = \frac{(-1)^{n-1}n!\left(\nu_1\sigma_{f,1}(\sigma_{f,1} + \sigma_{c,1})^{n-1} - k_\infty(\sigma_{f,1} + \sigma_{c,1})^n\right)}{(\Sigma_f + \Sigma_c)^n}\left(\frac{N_1}{\sigma_{t,1}}\right)^n, \tag{19}$$

$$\frac{dk_\infty}{d\sigma_{f,1}} = \frac{N_1(\nu_1 - k_\infty)}{\Sigma_f + \Sigma_c}, \tag{20}$$

$$\frac{d^2k_\infty}{d\sigma_{f,1}^2} = \frac{-2N_1^2(\nu_1 - k_\infty)}{(\Sigma_f + \Sigma_c)^2}, \tag{21}$$

$$\frac{d^nk_\infty}{d\sigma_{f,1}^n} = \frac{(-1)^{n-1}n!\,N_1^n(\nu_1 - k_\infty)}{(\Sigma_f + \Sigma_c)^n}, \tag{22}$$

$$\frac{dk_\infty}{d\sigma_{c,1}} = \frac{-N_1k_\infty}{\Sigma_f + \Sigma_c}, \tag{23}$$

$$\frac{d^2k_\infty}{d\sigma_{c,1}^2} = \frac{2N_1^2k_\infty}{(\Sigma_f + \Sigma_c)^2}, \tag{24}$$

$$\frac{d^nk_\infty}{d\sigma_{c,1}^n} = \frac{(-1)^n n!N_1^nk_\infty}{(\Sigma_f + \Sigma_c)^n}, \tag{25}$$

and

$$\frac{dk_\infty}{d\sigma_{s,1}} = \frac{d^2k_\infty}{d\sigma_{s,1}^2} = \frac{d^nk_\infty}{d\sigma_{s,1}^n} = 0. \tag{26}$$

The derivatives with respect to ν_1 are not used because MCNP cannot perturb ν. It is recommended that this capability be added in a future version.

III.B. Total Cross Section

Perturbing the total cross section of an isotope by p is equivalent to perturbing all of the cross sections by p and also equivalent to perturbing the atom density of the isotope by p. Table II shows the results of a +30% perturbation in $\sigma_{t,1}$ (p = 0.30). The sensitivity, of course, does not depend on the size of the perturbation.

Table II. Results for the Total Cross Section.

			Difference	
	Analytic	PERT Estimate	Rel. to Analytic	Num. Std. Devs.
Δk_∞, 1st-order term	0.02445	0.02445 ± 0.276%	0.028%	0.10
Δk_∞, 2nd-order term	–0.00484	–0.00481 ± 0.667%	0.491%	0.74
Δk_∞, Sum of terms	0.01961	0.01964 ± 0.290%	0.156%	0.54
Δk_∞, Total pert.	0.02041	0.01964 ± 0.290%	3.766%	13.48
$S_{k_\infty,\sigma_{t,1}}$	0.03273	0.03274 ± 0.276%	0.024%	0.09

The MCNP perturbation capability does an excellent job estimating the first- and second-order Taylor terms of Δk_∞, as well as the sum of the terms. The 3.8% error in the MCNP perturbation estimate of the total Δk_∞ is made because the two terms in the expansion are not quite enough. This can be shown using the higher-order derivatives of Eq. (19) in the Taylor series of Eq. (1); using 12 terms, the Taylor series converges to within 10^{-6}% of the analytic result. The table also demonstrates the well-known fact that the smallness of the Monte Carlo statistical uncertainty is not always an indicator of the accuracy of the tally.

III.C. Fission Cross Section

Table III shows the results of a +30% perturbation in $\sigma_{f,1}$. The sensitivity, of course, does not depend on the size of the perturbation.

Table III. Results for the Fission Cross Section.

			Difference	
	Analytic	PERT Estimate	Rel. to Analytic	Num. Std. Devs.
Δk_∞, 1st-order term	0.11978	0.11977 ± 0.016%	0.009%	0.57
Δk_∞, 2nd-order term	–0.01911	–0.01912 ± 0.026%	0.012%	0.44
Δk_∞, Sum of terms	0.10067	0.10066 ± 0.015%	0.013%	0.89
Δk_∞, Total pert.	0.10330	0.10066 ± 0.015%	2.559%	175.17
$S_{k_\infty,\sigma_{t,1}}$	0.16039	0.16037 ± 0.016%	–0.013%	0.83

Again, the two Taylor terms are individually well estimated by MCNP, and the 2.6% error in the total MCNP perturbation estimate is because two terms are not enough. This can be shown using the higher-order derivatives of Eq. (22); using 11 terms, the Taylor series of Eq. (1) converges to within 10^{-6}% of the analytic result.

A question that many have about the MCNP perturbation capability is whether the code accounts for the correlation between the total cross section and the cross section specified on the RXN keyword. For example, if the fission cross section is perturbed by $\Delta\sigma_f$, then the total cross section of the isotope is perturbed by $\Delta\sigma_f$, and the total cross section of the material is perturbed by $N\Delta\sigma_f$, but without perturbing all the other cross sections as was done in Sec. III.B. The neutron mean free path in the material changes, as does the probability of having an interaction in isotope 1 versus 2, as does the probability of that interaction being a fission. The answer is that the differential operator method automatically accounts for all of these effects.

III.D. Capture Cross Section

Table IV shows the results of a +30% perturbation in $\sigma_{c,1}$. The sensitivity, of course, does not depend on the size of the perturbation.

Table IV. Results for the Capture Cross Section.

			Difference	
	Analytic	PERT Estimate	Rel. to Analytic	Num. Std. Devs.
Δk_∞, 1st-order term	–0.09534	–0.09535 ± 0.008%	0.009%	1.04
Δk_∞, 2nd-order term	0.00365	0.00365 ± 0.016%	0.008%	0.46
Δk_∞, Sum of terms	–0.09169	–0.09169 ± 0.008%	0.009%	1.08
Δk_∞, Total pert.	–0.09182	–0.09169 ± 0.008%	0.138%	17.43
$S_{k_\infty,\sigma_{t,1}}$	–0.12766	–0.12766 ± 0.009%	0.004%	0.48

Again, the two Taylor terms are individually well estimated by MCNP. In this case two Taylor terms represent the exact perturbation very well. Using six terms [the higher derivatives of Eq. (25)], the Taylor series of Eq. (1) converges to within 10^{-6}% of the analytic result.

III.E. Scattering Cross Section

Table V shows the results of a +30% perturbation in $\sigma_{s,1}$. The sensitivity, of course, does not depend on the size of the perturbation.

Table V. Results for the Scattering Cross Section.

			Difference	
	Analytic	PERT Estimate	Rel. to Analytic	Num. Std. Devs.
Δk_∞, 1st-order term	0.00000	0.00003 ± 233%	N/A[a]	0.43
Δk_∞, 2nd-order term	0.00000	0.00002 ± 104%	N/A[a]	0.97
Δk_∞, Sum of terms	0.00000	0.00005 ± 132%	N/A[a]	0.75
Δk_∞, Total pert.	0.00000	0.00005 ± 132%	N/A[a]	0.75
$S_{k_\infty,\sigma_{t,1}}$	0.00000	0.00003 ± 233%	N/A[a]	0.43

[a] Not applicable due to division by 0.

This problem is interesting because it has MCNP trying to compute a zero perturbation and sensitivity. In fact, the results are accurate, in the sense of being within one standard deviation of the exact answer, but not necessarily useful. We are taught to doubt results with such a large uncertainty. When faced with first-order perturbation and sensitivity results like those of Table V, what is a user to do? This question will be addressed in a future paper.

III.F. Total Cross Section Revisited

Since sensitivities are additive, the k_∞ sensitivity to the total cross section can be recovered by adding the sensitivities to fission, capture, and scattering cross sections as in Eq. (13). Table VI shows the results of this operation. In the table, the first-order Taylor term is recovered because all of the perturbations used the same p, but that consistency is not necessary to add the sensitivities. This property will be used to analyze scattering sensitivities in Secs. V and VI.

Table VI. Results for the Total Cross Section.

		PERT Estimate,	Difference	
	Analytic	Sum[a]	Rel. to Analytic	Num. Std. Devs.
Δk_∞, 1st-order term	0.02445	0.02445 ± 0.261%	0.029%	0.11
$S_{k_\infty,\sigma_{t,1}}$	0.03273	0.03274 ± 0.262%	0.025%	0.09

[a] Sum of $S_{k_\infty,\sigma_{f,1}}$, $S_{k_\infty,\sigma_{c,1}}$, and $S_{k_\infty,\sigma_{s,1}}$.

IV. One-Group k_{eff} Test Problem

The 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. 7. The macroscopic cross sections are listed in Table VII. Scattering is isotropic. These one-group data were put into a continuous-energy format suitable for use by MCNP using the MAKECE code provided by Bob Little (X-1-NAD).

Table VII. 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. 7.
[b] H_2O (refl), Table 9, Ref. 7.

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 MCNP track-length estimate of k_{eff} was $0.999916 \pm 6.74338 \times 10^{-5}$, having an error of –0.008% or 1.25 standard deviations. (Note that MCNP5 was modified to print more digits for the track-length k_{eff} estimator and its standard deviation.)

Unfortunately, the derivation of the continuous-angle critical parameters is too complicated to allow the analytic derivatives of k_{eff} that were derived for the k_∞ problem. Thus, 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%;

Table VIII. k_{eff} Eigenvalue Sensitivities.

		Direct	PERT Estimate	Difference Rel. to Exact
Fuel	S_{k_{eff},σ_t}	0.75801 ± 0.040%	0.73178 ± 0.088%	–3.460%
	S_{k_{eff},σ_f}	0.68296 ± 0.044%	0.67463 ± 0.024%	–1.219%
	S_{k_{eff},σ_c}	–0.06416 ± 0.461%	–0.06507 ± 0.063%	1.417%
	S_{k_{eff},σ_s}	0.13917 ± 0.213%	0.12222 ± 0.516%	–12.178%
	S_{k_{eff},σ_t}, sum	0.75797 ± 0.068%	0.73178 ± 0.089%	–3.455%
Refl.	S_{k_{eff},σ_t}	0.10891 ± 0.275%	0.12381 ± 0.165%	13.676%
	S_{k_{eff},σ_c}	–0.01825 ± 1.641%	–0.02137 ± 0.155%	17.076%
	S_{k_{eff},σ_s}	0.12742 ± 0.229%	0.14517 ± 0.150%	13.931%
	S_{k_{eff},σ_t}, sum	0.10917 ± 0.383%	0.12381 ± 0.178%	13.405%

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 $p = 0$ is the required derivative in Eq. (11). A χ^2 minimization (the Marquardt method[9]) 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 VIII. 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[10] and in reactivity worth calculations.[11] References 10 and 11 both dealt with 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 quantity of interest k is

$$k = \int dV\, \nu\Sigma_f(r)\phi(r), \tag{27}$$

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 MCNP 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 MCNP perturbation estimates in Table IX. 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.

Table IX. k Response Sensitivities.

		Direct	PERT Estimate	Difference Rel. to Exact
Fuel	S_{k,σ_t}	0.73216 ± 0.124%	0.73162 ± 0.213%	–0.381%
	S_{k,σ_f}	0.67584 ± 0.134%	0.67561 ± 0.100%	–0.318%
	S_{k,σ_c}	–0.06498 ± 1.387%	–0.06518 ± 0.161%	0.312%
	S_{k,σ_s}	0.12117 ± 0.744%	0.12119 ± 1.128%	–0.002%
	S_{k,σ_t}, sum	0.73203 ± 0.213%	0.73162 ± 0.209%	–0.321%
Refl.	S_{k,σ_t}	0.12433 ± 0.723%	0.12330 ± 0.412%	–0.866%
	S_{k,σ_c}	–0.02133 ± 4.439%	–0.02128 ± 0.354%	5.029%
	S_{k,σ_s}	0.14524 ± 0.619%	0.14458 ± 0.379%	–0.467%
	S_{k,σ_t}, sum	0.12391 ± 1.018%	0.12330 ± 0.448%	–1.358%

In the MCNP perturbation k_{eff}-eigenvalue sensitivity results of Table VIII, 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 IX.

Thus, assuming that the fission source distribution is unaffected by the perturbation is the cause of the MCNP perturbation errors in Table VIII. 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,[12] 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. This feature should be brought up to date in MCNP and generalized so that it works for any cross-section perturbation.

The implicit effects of perturbed isotope self-shielding[6] were not accounted for in this analysis.

V. 30-Group k_{eff} Test Problem

It may be argued that a one-group problem is too simplistic to be meaningful. The problem of Sec. IV was also done using 30 energy groups. Again, it is a spherical fuel region (radius 6.12745 cm) surrounded by a spherical reflector shell (thickness 3.063725 cm). The materials and their properties are listed in Table X. Scattering is isotropic.

Table X. Materials Used in the 30-Group k_{eff} Problem.

Material	Composition (wgt. frac.)	Density (g/cm^3)	Composition (atom frac.)	Density (at/bn·cm)	Library
Fuel	^{235}U, 1.	16.9	^{235}U, 1.	0.04329931	690nm
Water	^{1}H, 0.111915; ^{16}O, 0.888085	1.0	^{1}H, 0.666611; ^{16}O, 0.333389	0.10031948	601nm

To use this cross section data in MCNP, the problem was run using the PARTISN multigroup deterministic code.[13] The material macroscopic cross sections and fission spectra were then read from the output MACRXS file and used as input for the MAKEMG code, provided by Bob Little (X-1-NAD). First, however, the capture cross section (MCNP's absorption cross section) for each group was recovered using

$$\Sigma_c = \Sigma_a - \nu\Sigma_f / \nu \tag{28}$$

[the groupwise values for ν were obtained directly from the nuclear data using the NDICL tool provided by Morgan White (X-1-NAD)]. If the group-*g* capture cross section calculated this way was negative [presumably because of (n,2n) reaction data leading to a non-balancing absorption cross section[13]], it was set to 0.0001 cm^{-1} and the group-*g* total cross section was readjusted. This occurred in groups 1 through 7 in the ^{235}U. This slightly modified data library was used in a subsequent PARTISN calculation (S_{64}, isotropic scattering) and the result was k_{eff} = 0.99972692.

Using 3×10^5 neutrons per cycle, 20 settle cycles, 1500 active cycles, and an initial guess of 1, the MCNP track-length estimate of k_{eff} was $0.999690 \pm 4.05689 \times 10^{-5}$, within one standard deviation of the PARTISN result. We stress that the cross section tables contain macroscopic material cross sections, not isotopic microscopic cross sections, so the materials were each specified in MCNP with a single ZAID and given atom densities of 1 at/bn·cm.

V.A. Groupwise Scattering Cross Sections

In this section, only sensitivities to the scattering cross sections were examined. Data libraries with perturbed scattering (and total) cross sections were constructed as described in Sec. IV. For this purpose the scattering cross section for group *g*, Σ_s^g, is defined as self-scattering plus all outscattering. When Σ_s^g was perturbed by *p*%, each of these components was perturbed by *p*%. The group total cross section was adjusted consistently.

Scattering is not a reaction that can be easily tallied or perturbed with FM or PERT cards in multigroup MCNP. To obtain scattering cross-section sensitivities, the total, fission, and capture sensitivities were computed as discussed in Sec. II; the scattering cross-section sensitivity in group *g* is $S_{k_{eff},\sigma_s^g} = S_{k_{eff},\sigma_t^g} - S_{k_{eff},\sigma_c^g} - S_{k_{eff},\sigma_f^g}$ (obviously, $S_{k_{eff},\sigma_f^g} = 0$ in the reflector).

Results for the k_{eff} sensitivities to scattering cross sections in the fuel are shown in Table XI on the next page and results for the k_{eff} sensitivities to scattering cross sections in the reflector are shown in Table XII on page 10.

Table XI. k_{eff} Sensitivities to Fuel Scattering Cross Sections; Direct MCNP Results.

Group Index	Midpoint Energy (MeV)	Direct (MCNP)	PERT Estimate	Difference Rel. to Direct	Key to Direct[a]
30	7.6070E-08	–4.903E-05 ± 330.90%	–9.883E-05 ± 53.88%	101.57%	A
29	2.8300E-07	–6.304E-05 ± 258.30%	–3.254E-05 ± 49.07%	–48.37%	A
28	7.7200E-07	–1.303E-04 ± 124.24%	–1.004E-04 ± 18.38%	–22.95%	A
27	2.0950E-06	–1.461E-04 ± 111.02%	–1.160E-04 ± 11.37%	–20.59%	A
26	5.6900E-06	–5.279E-05 ± 309.33%	3.109E-05 ± 34.20%	–158.88%	A
25	1.5460E-05	8.071E-05 ± 203.00%	–4.089E-05 ± 35.89%	–150.66%	A
24	4.2000E-05	–9.681E-06 ± 1689.75%	–8.756E-05 ± 17.87%	804.41%	A
23	1.1420E-04	–2.959E-04 ± 54.95%	–1.927E-04 ± 8.21%	–34.87%	A
22	3.1050E-04	–4.665E-04 ± 35.09%	–3.463E-04 ± 4.83%	–25.76%	A
21	8.4450E-04	–9.337E-04 ± 17.38%	–5.416E-04 ± 3.05%	–41.99%	A
20	2.2925E-03	–1.409E-03 ± 13.57%	–7.669E-04 ± 2.05%	–45.58%	B
19	6.2350E-03	–2.019E-03 ± 9.54%	–1.154E-03 ± 1.46%	–42.86%	B
18	1.6960E-02	–1.675E-03 ± 11.66%	–1.024E-03 ± 1.78%	–38.88%	B
17	4.6200E-02	–1.766E-04 ± 92.76%	–2.201E-04 ± 10.75%	24.66%	A
16	1.2580E-01	5.819E-03 ± 5.48%	3.884E-03 ± 0.80%	–33.26%	C
15	2.4350E-01	8.247E-03 ± 3.74%	6.738E-03 ± 0.42%	–18.29%	C
14	4.0150E-01	1.263E-02 ± 2.44%	1.042E-02 ± 0.31%	–17.48%	C
13	6.6150E-01	2.039E-02 ± 1.53%	1.772E-02 ± 0.18%	–13.07%	C
12	1.0880E+00	2.185E-02 ± 1.47%	1.964E-02 ± 0.16%	–10.11%	C
11	1.5455E+00	1.274E-02 ± 2.44%	1.225E-02 ± 0.18%	–3.88%	C
10	1.9850E+00	1.326E-02 ± 2.40%	1.301E-02 ± 0.18%	–1.87%	C
9	2.5485E+00	1.407E-02 ± 2.18%	1.356E-02 ± 0.16%	–3.59%	C
8	3.2725E+00	1.159E-02 ± 2.69%	1.156E-02 ± 0.19%	–0.31%	C
7	4.8750E+00	1.508E-02 ± 2.10%	1.432E-02 ± 0.16%	–5.05%	C
6	6.9300E+00	1.351E-03 ± 14.20%	1.651E-03 ± 0.58%	22.21%	B
5	8.8950E+00	3.442E-04 ± 47.82%	3.027E-04 ± 1.88%	–12.06%	A
4	1.1000E+01	5.297E-05 ± 308.37%	3.886E-05 ± 6.62%	–26.63%	A
3	1.2750E+01	–2.715E-04 ± 60.22%	4.426E-06 ± 28.86%	–101.63%	A
2	1.4250E+01	–1.698E-05 ± 966.99%	1.740E-06 ± 44.37%	–110.25%	A
1	1.6000E+01	–2.969E-06 ± 3249.89%	3.508E-07 ± 150.70%	–111.82%	D
–	Total	1.310E-01 ± 0.24%	1.204E-01 ± 0.10%	–8.11%	C

[a] A: $p = \pm 10\%$ and $\pm 20\%$, 6×10^5 neutrons/cycle, 1200 active cycles; B: $p = \pm 10\%$ and $\pm 20\%$, 6×10^5 neutrons/cycle, 600 active cycles; C: $p = \pm 10\%$ and $\pm 20\%$, 3×10^5 neutrons/cycle, 300 active cycles; D: $p = \pm 20\%$ and $\pm 40\%$, 6×10^5 neutrons/cycle, 600 active cycles.

It was quite difficult to obtain direct results (as well as perturbation estimates) for many groups using MCNP even with very long runs. Values with uncertainties greater than 30% are shown in red on Tables XI and XII. The k_{eff} differences and therefore the slopes are simply too small to be accurately estimated with reasonable computing resources. (More could be done for this study.) Of course, this problem highlights the very need for a Monte Carlo perturbation theory!

For groups in which the uncertainty in both the direct calculation and perturbation estimate are small, the results are not impressive. As in the one-group version of this problem (Sec. IV, Table VIII), the differences are generally much larger than two standard deviations, although there are some groups in the fuel (groups 6-11) that have better agreement. The errors in the group total sensitivities are worse than in the one-group problem of Sec. IV. Large uncertainties in the direct Monte Carlo calculations make groupwise comparisons difficult.

Table XII. k_{eff} Sensitivities to Reflector Scattering Cross Sections; Direct MCNP Results.

Group Index	Midpoint Energy (MeV)	Direct (MCNP)	PERT Estimate	Difference Rel. to Direct	Key to Direct[a]
30	7.6070E-08	–1.177E-03 ± 13.89%	–1.875E-03 ± 3.89%	59.41%	A
29	2.8300E-07	–1.188E-04 ± 137.22%	–1.886E-05 ± 111.37%	–84.12%	A
28	7.7200E-07	–7.016E-04 ± 27.27%	–4.088E-04 ± 5.20%	–41.74%	B
27	2.0950E-06	6.684E-04 ± 28.97%	1.674E-03 ± 1.29%	150.46%	B
26	5.6900E-06	3.613E-03 ± 5.30%	5.032E-03 ± 0.42%	39.27%	B
25	1.5460E-05	2.486E-03 ± 7.64%	3.287E-03 ± 0.68%	32.22%	B
24	4.2000E-05	2.086E-03 ± 9.24%	2.592E-03 ± 0.91%	24.26%	B
23	1.1420E-04	1.542E-03 ± 12.60%	2.956E-03 ± 0.84%	91.67%	B
22	3.1050E-04	1.093E-03 ± 14.99%	2.591E-03 ± 0.98%	137.12%	A
21	8.4450E-04	1.336E-03 ± 14.25%	3.391E-03 ± 0.75%	153.82%	B
20	2.2925E-03	1.865E-03 ± 10.40%	4.749E-03 ± 0.57%	154.62%	B
19	6.2350E-03	2.488E-03 ± 7.66%	5.755E-03 ± 0.48%	131.29%	B
18	1.6960E-02	4.963E-03 ± 6.20%	8.844E-03 ± 0.32%	78.19%	C
17	4.6200E-02	9.950E-03 ± 2.97%	1.499E-02 ± 0.19%	50.61%	C
16	1.2580E-01	2.346E-02 ± 1.37%	3.001E-02 ± 0.09%	27.96%	C
15	2.4350E-01	2.284E-02 ± 1.40%	2.755E-02 ± 0.07%	20.61%	C
14	4.0150E-01	3.106E-02 ± 0.96%	3.730E-02 ± 0.06%	20.11%	C
13	6.6150E-01	4.113E-02 ± 0.77%	4.839E-02 ± 0.04%	17.64%	C
12	1.0880E+00	4.079E-02 ± 0.78%	4.756E-02 ± 0.04%	16.60%	C
11	1.5455E+00	1.882E-02 ± 1.66%	2.220E-02 ± 0.05%	17.97%	C
10	1.9850E+00	1.731E-02 ± 1.83%	1.931E-02 ± 0.05%	11.58%	C
9	2.5485E+00	1.388E-02 ± 2.26%	1.558E-02 ± 0.05%	12.23%	C
8	3.2725E+00	1.145E-02 ± 2.70%	1.256E-02 ± 0.06%	9.73%	C
7	4.8750E+00	1.050E-02 ± 2.90%	1.164E-02 ± 0.06%	10.83%	C
6	6.9300E+00	1.234E-03 ± 15.65%	1.352E-03 ± 0.16%	9.53%	B
5	8.8950E+00	3.968E-04 ± 41.03%	3.716E-04 ± 0.31%	–6.36%	A
4	1.1000E+01	1.724E-04 ± 95.22%	6.331E-05 ± 0.74%	–63.27%	A
3	1.2750E+01	7.216E-05 ± 226.48%	1.210E-05 ± 1.76%	–83.24%	A
2	1.4250E+01	–2.663E-05 ± 613.75%	3.826E-06 ± 3.23%	–114.37%	A
1	1.6000E+01	1.543E-04 ± 62.83%	1.566E-06 ± 5.11%	–98.99%	D
–	Total	2.570E-01 ± 0.12%	3.275E-01 ± 0.04%	27.41%	C

[a] A: $p = \pm 10\%$ and $\pm 20\%$, 6×10^5 neutrons/cycle, 1200 active cycles; B: $p = \pm 10\%$ and $\pm 20\%$, 6×10^5 neutrons/cycle, 600 active cycles; C: $p = \pm 10\%$ and $\pm 20\%$, 3×10^5 neutrons/cycle, 300 active cycles; D: $p = \pm 20\%$ and $\pm 40\%$, 6×10^5 neutrons/cycle, 600 active cycles.

In order to more thoroughly test the MCNP perturbation capability for sensitivities, more accurate direct values are required. The direct perturbation calculations were done using PARTISN in one spatial dimension with S_{64} quadrature, 10^{-12} convergence, and the same cross section data that were used in the MCNP calculations. Such a calculation provided an excellent match with multigroup MCNP for k_{eff} of the unperturbed problem (Sec. V on p. 8). Since the multigroup cross sections themselves – not just the evaluation – were the same in each code, a high-quadrature discrete-ordinates calculation should match the continuous-angle Monte Carlo calculation, especially in one spatial dimension, and because a global response is the only quantity of interest.

For the χ^2 minimization of the linear fits, all standard deviations were set to 10^{-12}. This essentially turns the Marquardt method into a least-squares fitting algorithm. In this case no uncertainty estimate is available for the fit but the correlation coefficient r is a measure of the straightness of the line.

Results are given in Table XIII for k_{eff} sensitivities to fuel scattering cross sections and Table XIV for reflector scattering cross sections. The direct results are given with the linear correlation coefficients of the fits, which are all greater than 0.95 (in magnitude).

When the PARTISN sensitivities are compared with the direct MCNP sensitivities of Tables XI and XII for the 60 problems (not counting the energy-group sums), 71.7% of the PARTISN results were within one standard deviation of the MCNP results, 93.3% were within two standard deviations, 95.0% were within three standard deviations, and all were within four standard deviations. Thus, the PARTISN sensitivities are in agreement with the direct MCNP sensitivities, but the absence of statistical noise makes them much more useful.

Table XIII. k_{eff} Sensitivities to Fuel Scattering Cross Sections; Direct PARTISN Results.

Group Index	Midpoint Energy (MeV)	Direct (PARTISN); (r)	PERT Estimate	Difference Rel. to Direct	Key to Direct[a]
30	7.6070E-08	–7.910E-05 ; (–1.000)	–9.883E-05 ± 53.88%	24.94%	A
29	2.8300E-07	–2.716E-05 ; (–1.000)	–3.254E-05 ± 49.07%	19.84%	A
28	7.7200E-07	–1.067E-04 ; (–1.000)	–1.004E-04 ± 18.38%	-5.94%	A
27	2.0950E-06	–2.240E-04 ; (–1.000)	–1.160E-04 ± 11.37%	-48.22%	A
26	5.6900E-06	–3.042E-05 ; (–1.000)	3.109E-05 ± 34.20%	–202.20%	A
25	1.5460E-05	–4.513E-05 ; (–1.000)	–4.089E-05 ± 35.89%	–9.40%	A
24	4.2000E-05	–1.068E-04 ; (–1.000)	–8.756E-05 ± 17.87%	–17.99%	A
23	1.1420E-04	–2.948E-04 ; (–1.000)	–1.927E-04 ± 8.21%	–34.63%	A
22	3.1050E-04	–5.407E-04 ; (–1.000)	–3.463E-04 ± 4.83%	–35.95%	A
21	8.4450E-04	–9.224E-04 ; (–0.999)	–5.416E-04 ± 3.05%	–41.28%	A
20	2.2925E-03	–1.382E-03 ; (–0.999)	–7.669E-04 ± 2.05%	–44.50%	A
19	6.2350E-03	–1.888E-03 ; (–0.999)	–1.154E-03 ± 1.46%	–38.90%	A
18	1.6960E-02	–1.676E-03 ; (–0.999)	–1.024E-03 ± 1.78%	–38.89%	A
17	4.6200E-02	–2.537E-04 ; (–1.000)	–2.201E-04 ± 10.75%	–13.25%	A
16	1.2580E-01	5.579E-03 ; (0.999)	3.884E-03 ± 0.80%	–30.39%	A
15	2.4350E-01	8.682E-03 ; (0.999)	6.738E-03 ± 0.42%	–22.38%	A
14	4.0150E-01	1.313E-02 ; (0.999)	1.042E-02 ± 0.31%	–20.63%	A
13	6.6150E-01	2.036E-02 ; (0.999)	1.772E-02 ± 0.18%	–12.96%	A
12	1.0880E+00	2.194E-02 ; (0.999)	1.964E-02 ± 0.16%	–10.47%	A
11	1.5455E+00	1.304E-02 ; (0.999)	1.225E-02 ± 0.18%	–6.09%	A
10	1.9850E+00	1.367E-02 ; (0.999)	1.301E-02 ± 0.18%	–4.85%	A
9	2.5485E+00	1.406E-02 ; (0.998)	1.356E-02 ± 0.16%	–3.54%	A
8	3.2725E+00	1.194E-02 ; (0.998)	1.156E-02 ± 0.19%	–3.24%	A
7	4.8750E+00	1.469E-02 ; (0.998)	1.432E-02 ± 0.16%	–2.56%	A
6	6.9300E+00	1.675E-03 ; (0.998)	1.651E-03 ± 0.58%	–1.44%	A
5	8.8950E+00	2.956E-04 ; (0.995)	3.027E-04 ± 1.88%	2.38%	A
4	1.1000E+01	3.671E-05 ; (0.991)	3.886E-05 ± 6.62%	5.86%	A
3	1.2750E+01	5.542E-06 ; (0.988)	4.426E-06 ± 28.86%	–20.13%	A
2	1.4250E+01	1.470E-06 ; (0.984)	1.740E-06 ± 44.37%	18.33%	A
1	1.6000E+01	3.251E-07 ; (0.955)	3.508E-07 ± 150.70%	7.90%	C
–	Total	1.312E-01 ; (1.000)	1.204E-01 ± 0.10%	–8.23%	A

[a] A: p = ±10% and ±20%; B: p = ±10%;C: p = ±20%; D: p = ±20% and ±40%.

Unfortunately, the MCNP perturbation estimates of the sensitivities are not in agreement with the direct PARTISN sensitivities. In a few places (groups 3-5 in the fuel, group 1 in the reflector) the agreement is within one or two standard deviations. Generally, the perturbation estimates are poor.

Table XIV. k_{eff} Sensitivities to Reflector Scattering Cross Sections; Direct PARTISN Results.

Group Index	Midpoint Energy (MeV)	Direct (PARTISN); (r)	PERT Estimate	Difference Rel. to Direct	Key to Direct[a]
30	7.6070E-08	–1.219E-03 ; (–0.964)	–1.875E-03 ± 3.89%	53.88%	A
29	2.8300E-07	–7.477E-05 ; (–0.962)	–1.886E-05 ± 111.37%	–74.77%	B
28	7.7200E-07	–6.000E-04 ; (–1.000)	–4.088E-04 ± 5.20%	–31.87%	A
27	2.0950E-06	5.962E-04 ; (0.968)	1.674E-03 ± 1.29%	180.81%	A
26	5.6900E-06	3.373E-03 ; (0.992)	5.032E-03 ± 0.42%	49.20%	A
25	1.5460E-05	2.268E-03 ; (0.989)	3.287E-03 ± 0.68%	44.91%	A
24	4.2000E-05	1.681E-03 ; (0.985)	2.592E-03 ± 0.91%	54.17%	A
23	1.1420E-04	1.584E-03 ; (0.982)	2.956E-03 ± 0.84%	86.54%	A
22	3.1050E-04	1.049E-03 ; (0.965)	2.591E-03 ± 0.98%	147.08%	A
21	8.4450E-04	1.238E-03 ; (0.962)	3.391E-03 ± 0.75%	173.94%	A
20	2.2925E-03	1.914E-03 ; (0.970)	4.749E-03 ± 0.57%	148.11%	A
19	6.2350E-03	2.405E-03 ; (0.968)	5.755E-03 ± 0.48%	139.31%	A
18	1.6960E-02	5.024E-03 ; (0.982)	8.844E-03 ± 0.32%	76.02%	A
17	4.6200E-02	1.028E-02 ; (0.989)	1.499E-02 ± 0.19%	45.79%	A
16	1.2580E-01	2.328E-02 ; (0.993)	3.001E-02 ± 0.09%	28.92%	A
15	2.4350E-01	2.246E-02 ; (0.995)	2.755E-02 ± 0.07%	22.67%	A
14	4.0150E-01	3.120E-02 ; (0.996)	3.730E-02 ± 0.06%	19.57%	A
13	6.6150E-01	4.089E-02 ; (0.998)	4.839E-02 ± 0.04%	18.33%	A
12	1.0880E+00	4.097E-02 ; (0.998)	4.756E-02 ± 0.04%	16.07%	A
11	1.5455E+00	1.931E-02 ; (0.999)	2.220E-02 ± 0.05%	14.94%	A
10	1.9850E+00	1.694E-02 ; (0.999)	1.931E-02 ± 0.05%	14.03%	A
9	2.5485E+00	1.371E-02 ; (0.999)	1.558E-02 ± 0.05%	13.63%	A
8	3.2725E+00	1.120E-02 ; (0.999)	1.256E-02 ± 0.06%	12.11%	A
7	4.8750E+00	1.049E-02 ; (1.000)	1.164E-02 ± 0.06%	10.99%	A
6	6.9300E+00	1.232E-03 ; (1.000)	1.352E-03 ± 0.16%	9.70%	A
5	8.8950E+00	3.411E-04 ; (1.000)	3.716E-04 ± 0.31%	8.96%	A
4	1.1000E+01	5.851E-05 ; (1.000)	6.331E-05 ± 0.74%	8.20%	A
3	1.2750E+01	1.107E-05 ; (1.000)	1.210E-05 ± 1.76%	9.25%	A
2	1.4250E+01	3.471E-06 ; (1.000)	3.826E-06 ± 3.23%	10.22%	A
1	1.6000E+01	1.475E-06 ; (1.000)	1.566E-06 ± 5.11%	6.12%	D
–	Total	2.565E-01 ; (1.000)	3.275E-01 ± 0.04%	27.66%	A

[a] A: p = ±10% and ±20%; B: p = ±10%;C: p = ±20%; D: p = ±20% and ±40%.

V.B. Energy-Integrated Total Cross Section

In this section, the energy-integrated k_{eff} sensitivities to fuel and reflector total cross sections are examined. The k_{eff} vs. p_t curves were computed in MCNP by modifying the material atom densities on the cell cards by ±20% and ±10% and using 3×10^5 neutrons/cycle, 20 settle cycles, and 300 active cycles. Each calculation used a different random number seed. Results are shown in Table XV. (Reference 6 contains similar comparisons.)

Table XV. k_{eff} Total Sensitivities.

Material	Direct	PERT Estimate	Difference Rel. to Direct
S_{k,σ_t}, Fuel	0.6102 ± 0.052%	0.5594 ± 0.020%	–8.33%
S_{k,σ_t}, Refl.	0.2485 ± 0.125%	0.3157 ± 0.041%	27.05%

This type of study is accessible to any user; it does not require the manipulation of cross-section libraries. The results indicate qualitatively the effect of the fission source distribution on the perturbation. If the differential operator method approximating the fission source as unperturbed (that is, the MCNP perturbation capability) accurately estimates the total cross section sensitivity of a particular region, then evidently the fission source shift has only a small effect.

This technique may also be used to estimate the effect of fission source distribution shifts as a function of isotopic density, which would be important for determining isotopic sensitivities in a mixture. An example will be given in Sec. VI.

Naturally, this simple analysis ignores energy dependencies – as seen in Sec. V.A, some group sensitivities may be well estimated when others are not. However, it may be a useful means of identifying the regions of applicability of the MCNP perturbation capability for sensitivity analysis. This idea will be explored further using continuous-energy problems in a subsequent paper.

VI. 30-Group k_{eff} Test Problem with Reflector Isotopics

It may yet be argued that the reflector perturbations of Sec. V are still too unrealistic because the bulk material cross sections were perturbed rather than the isotopic cross sections. The final test problem of this paper was the same one used in Sec. V, but this time the elemental composition of the water reflector was explicitly represented and ^{1}H and ^{16}O sensitivities were calculated. The composition of the water is given in Table X of Sec. V. Scattering is isotropic. A similar procedure to that discussed in Sec. V was used to create input to the MAKEMG code. When the microscopic ^{235}U capture cross section was negative after applying Eq. (28) (groups 1 through 7), it was reset to 0.002 cm^2. The capture cross section for ^{16}O is very slightly negative in the 601nm library in groups 9, 10, 12, 13, 14, 18, 22, and 23; it was reset to 10^{-6} cm^2 in these groups. This slightly modified data library was used in a subsequent PARTISN calculation (S_{64}, isotropic scattering) and the result was $k_{eff} = 0.99973273$.

Using 3×10^5 neutrons per cycle, 20 settle cycles, 1500 active cycles, and an initial guess of 1, the MCNP track-length estimate of k_{eff} was $0.999647 \pm 4.07993 \times 10^{-5}$, which is 2.10 standard deviations away from the PARTISN result. (This problem used a different random number seed than the unperturbed problem of Sec. V.)

VI.A. Energy-Integrated Total Cross Section

In this section, the energy-integrated k_{eff} sensitivities to hydrogen and oxygen total cross sections are examined. The k_{eff} vs. p_t curves were computed in MCNP by modifying the material atom densities on the water material card by ±20% and ±10% for each isotope separately and modifying the cell atom density appropriately and using 3×10^5 neutrons/cycle, 20 settle cycles, and 300 active cycles. Each calculation used a different random number seed. Results are shown in Table XVI.

Table XVI. k_{eff} Sensitivities to Hydrogen and Oxygen.

Material	Direct	PERT Estimate	Difference Rel. to Direct
S_{k,σ_t}, ^{1}H	0.1965 ± 0.155%	0.2575 ± 0.050%	31.05%
S_{k,σ_t}, ^{16}O	0.0516 ± 0.609%	0.0583 ± 0.076%	12.93%

Based on these results, it was predicted that the MCNP perturbation capability would estimate k_{eff} sensitivities to oxygen more accurately than it would sensitivities to hydrogen, but that the sensitivities to oxygen would not be very accurately estimated. This prediction will be tested in the next section.

Note that the linearity of sensitivities is displayed here. The sum of the k_{eff} sensitivities to hydrogen and oxygen of Table XVI is (within the statistical uncertainties) equal to the total sensitivity to the reflector of Table XV.

VI.B. Groupwise Scattering Cross Section

The k_{eff} sensitivities to scattering in hydrogen and oxygen were estimated using the MCNP perturbation capability (for the total and capture sensitivities, as explained in Sec. V.A) and computed directly by perturbing the cross-section data in the libraries, running PARTISN calculations, and fitting the results to a line. The results are shown, with the linear correlation coefficients of the fits, in Table XVII for hydrogen and Table XVIII for oxygen. Perturbation estimates with uncertainties greater than 10% are printed in red. The correlation coefficients are all greater (in magnitude) than 0.96.

As in Sec. V, agreement is poor, particularly for hydrogen, as predicted.

Table XVII. k_{eff} Sensitivities to Hydrogen Scattering.

Group Index	Midpoint Energy (MeV)	Direct (PARTISN); (r)	PERT Estimate	Difference Rel. to Direct	Key to Direct[a]
30	7.6070E-08	–1.153E-03 ; (–0.969)	–1.778E-03 ± 4.18%	54.23%	A
29	2.8300E-07	–8.800E-05 ; (–0.983)	2.878E-05 ± 66.34%	–132.70%	B
28	7.7200E-07	–6.123E-04 ; (–1.000)	–4.629E-04 ± 4.38%	–24.41%	A
27	2.0950E-06	5.300E-04 ; (0.971)	1.629E-03 ± 1.23%	207.45%	A
26	5.6900E-06	3.216E-03 ; (0.992)	4.875E-03 ± 0.41%	51.60%	A
25	1.5460E-05	2.153E-03 ; (0.990)	3.097E-03 ± 0.67%	43.82%	A
24	4.2000E-05	1.567E-03 ; (0.987)	2.420E-03 ± 0.90%	54.39%	A
23	1.1420E-04	1.454E-03 ; (0.984)	2.832E-03 ± 0.81%	94.76%	A
22	3.1050E-04	9.119E-04 ; (0.968)	2.427E-03 ± 1.00%	166.21%	A
21	8.4450E-04	1.059E-03 ; (0.965)	3.128E-03 ± 0.83%	195.28%	A
20	2.2925E-03	1.664E-03 ; (0.973)	4.440E-03 ± 0.59%	166.83%	A
19	6.2350E-03	2.055E-03 ; (0.971)	5.288E-03 ± 0.51%	157.32%	A
18	1.6960E-02	4.455E-03 ; (0.984)	8.263E-03 ± 0.33%	85.48%	A
17	4.6200E-02	9.194E-03 ; (0.990)	1.375E-02 ± 0.20%	49.58%	A
16	1.2580E-01	2.055E-02 ; (0.994)	2.702E-02 ± 0.10%	31.50%	A
15	2.4350E-01	1.921E-02 ; (0.996)	2.399E-02 ± 0.08%	24.91%	A
14	4.0150E-01	2.204E-02 ; (0.998)	2.741E-02 ± 0.07%	24.37%	A
13	6.6150E-01	3.337E-02 ; (0.998)	4.017E-02 ± 0.04%	20.38%	A
12	1.0880E+00	2.904E-02 ; (0.999)	3.454E-02 ± 0.05%	18.92%	A
11	1.5455E+00	1.523E-02 ; (0.999)	1.777E-02 ± 0.06%	16.69%	A
10	1.9850E+00	1.363E-02 ; (0.999)	1.574E-02 ± 0.06%	15.52%	A
9	2.5485E+00	1.207E-02 ; (1.000)	1.380E-02 ± 0.06%	14.36%	A
8	3.2725E+00	7.990E-03 ; (1.000)	9.102E-03 ± 0.07%	13.91%	A
7	4.8750E+00	7.463E-03 ; (1.000)	8.398E-03 ± 0.07%	12.53%	A
6	6.9300E+00	9.257E-04 ; (1.000)	1.024E-03 ± 0.20%	10.57%	A
5	8.8950E+00	2.282E-04 ; (1.000)	2.494E-04 ± 0.40%	9.32%	A
4	1.1000E+01	3.348E-05 ; (1.000)	3.693E-05 ± 1.08%	10.31%	A
3	1.2750E+01	5.622E-06 ; (1.000)	5.986E-06 ± 2.71%	6.48%	A
2	1.4250E+01	1.600E-06 ; (1.000)	1.870E-06 ± 4.95%	16.82%	A
1	1.6000E+01	1.250E-06 ; (1.000)	5.960E-07 ± 8.86%	–52.33%	A
–	Total	2.047E-01 ; (1.000)	2.692E-01 ± 0.05%	31.52%	A

[a] A: p = ±10% and ±20%; B: p = ±10%.

Table XVIII. k_{eff} Sensitivities to Oxygen Scattering.

Group Index	Midpoint Energy (MeV)	Direct (PARTISN); (r)	PERT Estimate	Difference Rel. to Direct	Key to Direct[a]
30	7.6070E-08	–8.417E-05 ; (–1.000)	–1.226E-04 ± 15.32%	45.70%	A
29	2.8300E-07	1.132E-05 ; (0.999)	2.046E-05 ± 28.84%	80.68%	A
28	7.7200E-07	3.791E-06 ; (0.992)	1.265E-05 ± 50.04%	233.65%	A
27	2.0950E-06	5.385E-05 ; (1.000)	1.077E-04 ± 6.01%	99.93%	A
26	5.6900E-06	1.412E-04 ; (1.000)	2.291E-04 ± 2.92%	62.28%	A
25	1.5460E-05	9.971E-05 ; (1.000)	1.400E-04 ± 4.96%	40.45%	A
24	4.2000E-05	9.697E-05 ; (1.000)	1.502E-04 ± 4.81%	54.88%	A
23	1.1420E-04	1.109E-04 ; (1.000)	1.865E-04 ± 4.03%	68.08%	A
22	3.1050E-04	1.138E-04 ; (1.000)	1.816E-04 ± 4.23%	59.60%	A
21	8.4450E-04	1.501E-04 ; (1.000)	2.522E-04 ± 3.11%	68.06%	A
20	2.2925E-03	2.134E-04 ; (1.000)	3.327E-04 ± 2.46%	55.89%	A
19	6.2350E-03	3.011E-04 ; (1.000)	4.234E-04 ± 2.09%	40.63%	A
18	1.6960E-02	5.031E-04 ; (1.000)	6.535E-04 ± 1.44%	29.89%	A
17	4.6200E-02	9.867E-04 ; (1.000)	1.196E-03 ± 0.82%	21.25%	A
16	1.2580E-01	2.576E-03 ; (1.000)	2.987E-03 ± 0.38%	15.97%	A
15	2.4350E-01	3.114E-03 ; (1.000)	3.573E-03 ± 0.26%	14.74%	A
14	4.0150E-01	8.907E-03 ; (1.000)	9.909E-03 ± 0.15%	11.25%	A
13	6.6150E-01	7.418E-03 ; (1.000)	8.209E-03 ± 0.12%	10.66%	A
12	1.0880E+00	1.181E-02 ; (1.000)	1.299E-02 ± 0.09%	9.99%	A
11	1.5455E+00	4.053E-03 ; (1.000)	4.447E-03 ± 0.14%	9.71%	A
10	1.9850E+00	3.294E-03 ; (1.000)	3.581E-03 ± 0.14%	8.70%	A
9	2.5485E+00	1.642E-03 ; (1.000)	1.775E-03 ± 0.19%	8.11%	A
8	3.2725E+00	3.205E-03 ; (1.000)	3.437E-03 ± 0.14%	7.23%	A
7	4.8750E+00	3.026E-03 ; (1.000)	3.236E-03 ± 0.13%	6.94%	A
6	6.9300E+00	3.064E-04 ; (1.000)	3.312E-04 ± 0.35%	8.08%	A
5	8.8950E+00	1.128E-04 ; (1.000)	1.212E-04 ± 0.58%	7.45%	A
4	1.1000E+01	2.504E-05 ; (1.000)	2.672E-05 ± 1.15%	6.71%	A
3	1.2750E+01	5.431E-06 ; (1.000)	5.759E-06 ± 2.71%	6.04%	A
2	1.4250E+01	1.850E-06 ; (1.000)	2.001E-06 ± 4.73%	8.13%	A
1	1.6000E+01	1.700E-06 ; (1.000)	8.158E-07 ± 7.32%	–52.03%	A
–	Total	5.218E-02 ; (1.000)	5.839E-02 ± 0.08%	11.91%	A

[a] A: p = ±10% and ±20%.

VII.Summary and Recommendations

In this paper, use of the MCNP perturbation capability to estimate k_{eff} sensitivities to cross sections was tested in problems for which exact sensitivities could be computed. Two problems were used, a two-isotope homogenous-material k_∞ problem and a two-region spherical fuel/reflector system. The second problem was done in one and 30 energy groups and the sensitivities to different components in the fuel and reflector were studied.

All results indicate that the MCNP perturbation feature must be used with great caution on k-eigenvalue problems. The assumption of an unperturbed fission source distribution severely limits the accuracy of the differential operator method.[10–12] When there is no fission source shift, as in the k_∞ problem, the MCNP perturbation results are very accurate for sensitivities. Note that only the first-order Taylor term is needed in sensitivity analysis. There is every indication (e.g., Sec. IV) that the perturbation feature is very accurate for sensitivities in fixed-source problems.

Users might think that by using a miniscule parameter p for the perturbations, they will be minimizing the effect of the perturbed fission source distribution. Such is not the case. The differential operator method works by estimating derivatives of the response with respect to the perturbed parameter, then multiplying the derivatives by the perturbation. Sensitivity analysis needs only the first derivative, whose value is independent of the size of the perturbation. This result was simply derived in Sec. II of this paper.

While there are clearly many problems for which the application of the current MCNP perturbation capability is inappropriate, there must be others for which it works well. It would be helpful to find a means of deciding in advance which types of problems were in which category. One suggestion is that the comparison of the perturbation estimate with a direct calculation for an isotopic density (total cross section) perturbation might be useful. This can be done without manipulating data tables.

This study will be followed with more geometrically realistic multigroup problems for which direct results may be obtained for comparison. Continuous-energy problems are planned, but there it is difficult to directly compute the right answer. In future studies, code-to-code comparisons will be done with the Oak Ridge TSUNAMI code.[6]

We make the following six recommendations regarding documentation and development in support of the use of MCNP for sensitivity analysis:

1. The manual[3] should be modified. Chapter 2, Sec. XII (beginning on p. 2-192 in the 10/3/05 version) should somewhere include Eq. (9) and its derivation, and the end of Sec. XII.C (p. 2-200) should include a reminder that only the first-order term is normally needed for sensitivity analysis. In Chap. 3, Sec. IV.J.10 (on the PERT card), under the METHOD keyword (p. 3-153), a note should be made that METHOD=2 should be used for sensitivity analysis and the PERT cards in Example 4 (p. 3-155) should be changed to use METHOD=2. The discussion of that example should include a brief statement of why METHOD=2 is used.

2. Future versions of MCNP should print more digits for both the result and the standard deviation in the "predicted changes in keff" output. This will facilitate comparison with other codes, namely TSUNAMI, which apparently uses a FORTRAN 1PE12.4 format for both the sensitivity and its standard deviation.

3. In addition to or instead of the perturbation index, the user number of each perturbation should be printed in the "predicted changes in keff" output as is presently done for perturbed tallies.

4. The ability to perturb ν, the number of neutrons produced per fission, should be added.

5. Nagaya's method[12] for estimating the effect of fission source distribution perturbations on the change in k_{eff} should be extended to general reactions and made available as a standard feature. Its present implementation in MCNP6 is only for the total cross section, but it does not work at all in the MCNP6 version available on LANL's yellow network.

6. In the short term, methods should be developed to assist users in applying the current RSICC release of MCNP5 to sensitivity analysis. It should be possible to predict the areas of applicability of the MCNP perturbation capability, perhaps using novel post-processing of standard MCNP output.[11]

References

1. M. C. G. Hall, "Cross-Section Adjustment with Monte Carlo Sensitivities: Application to the Winfrith Iron Benchmark," *Nucl. Sci. Eng.*, **81**, 423-431 (1982).

2. G. McKinney, "A Monte Carlo (MCNP) Sensitivity Code Development and Application," M. S. Thesis, University of Washington (1984).

3. X-5 Monte Carlo Team, "MCNP–A General Monte Carlo N-Particle Transport Code, Version 5," Vol. I, LA–UR–03–1987, and Vol. II, LA–CP–03–0245, Los Alamos National Laboratory (April 24, 2003; Rev. October 3, 2005).

4. H. Rief, "Generalized Monte Carlo Perturbation Algorithms for Correlated Sampling and a Second-Order Taylor Series Approach," *Annals of Nuclear Energy*, **11**, *9*, 455-476 (1984).

5. A. Hogenbirk, "An Easy Way to Carry Out 3D Uncertainty Analysis," Proceedings of the Joint International Topical Meeting on Mathematics & Computation and Supercomputing in Nuclear Applications (M&C + SNA 2007), Monterey, California, April 15-19, 2007, on CD-ROM (2007).

6. B. T. Rearden, "Perturbation Theory Eigenvalue Sensitivity Analysis with Monte Carlo Techniques," *Nucl. Sci. Eng.*, **146**, 367-382 (2004).

7. Avneet Sood, R. Arthur Forster, and D. Kent Parsons, "Analytical Benchmark Test Set For Criticality Code Verification," *Progress in Nuclear Energy*, **42**, *1*, 55-106 (2003).

8. James J. Duderstadt and Louis J. Hamilton, *Nuclear Reactor Analysis*, Chap. 3, John Wiley & Sons, New York, New York (1976).

9. William H. Press, Saul A. Teukolsky, William T. Vetterling, and Brian P. Flannery, *Numerical Recipes in FORTRAN: The Art of Scientific Computing*, 2nd Ed. (reprinted with corrections), Chap. 15, Cambridge University Press (1994).

10. B. T. Rearden and D. E. Peplow, "Comparison of Sensitivity Analysis Techniques in Monte Carlo Codes for Multi-Region Criticality Calculations," *Trans. Am. Nucl. Soc.*, **85**, 163-165 (2001).

11. J. A. Favorite, "An Alternative Implementation of the Differential Operator (Taylor Series) Perturbation Method for Monte Carlo Criticality Problems," *Nucl. Sci. Eng.*, **142**, 327-341 (2002).

12. Yasunobu Nagaya and Forrest B. Brown, "Estimation of Change in k_{eff} Due to Perturbed Fission Source Distribution in MCNP," *Proceedings of the International Topical Meeting on Nuclear Mathematical and Computational Sciences (M&C'03)*, Gatlinburg, Tennessee, April 16-11, 2003, on CD-ROM (2003).

13. Ray E. Alcouffe, Randal S. Baker, Jon A. Dahl, Scott A. Turner, and Robert C. Ward, "PARTISN: A Time-Dependent, Parallel Neutral Particle Transport Code System," LA–UR–05-3925, UC–705, Version 5.74, Los Alamos National Laboratory (May 2005).

JAF:jaf

Distribution:
M. P. Bernardin, X-DO, MS B218, mpb@lanl.gov
S. M. Sterbenz, X-1, MS F699, sterbenz@lanl.gov
J. S. Sarracino, X-1-TA, MS F663, jxs@lanl.gov
F. B. Brown, X-3-MCC, MS A143, fbrown@lanl.gov
J. T. Goorley, X-3-MCC, MS A143, jgoorley@lanl.gov
J. S. Hendricks, X-3-MCC, MS A143, jxh@lanl.gov
B. C. Kiedrowski, X-3-MCC, MS P365, bckiedro@lanl.gov
G. W. McKinney, X-3-MCC, MS K575, gwm@lanl.gov
R. C. Little, X-1-NAD, MS F663, rcl@lanl.gov
D. K. Parsons, X-1-NAD, MS F663, dkp@lanl.gov
M. C. White, X-1-NAD, MS F663, morgan@lanl.gov
K. C. Bledsoe, X-1-TA, MS P365, kbledsoe@lanl.gov
J. A. Favorite, X-1-TA, MS P365, fave@lanl.gov
X-Archive, x-wellnitz@lanl.gov
X-DO File
X-1 File