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Title: Analytic One-Group Two-Isotope k-infinity Reaction-Rate Taylor Series Perturbations (U)

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SUBJECT: Analytic One-Group Two-Isotope k_∞ Reaction-Rate Taylor Series Perturbations (U)

Abstract

The MCNP perturbation capability was again tested against analytic results. The test problem was a one-group, two-isotope k_∞ problem done in continuous energy. Quantities compared were first- and second-order Taylor series terms for the change in capture, fission, scattering, and total reaction rates due to (independent) changes in capture, fission, scattering, and total cross sections for one isotope. The MCNP Taylor series terms were extremely accurate in most cases, but two bugs were found: 1) for fission and capture cross-section perturbations, the change in the total reaction rate was not equal to the sum of the changes in the fission, capture, and scattering reaction rates (which were individually correct); and 2) for a scattering cross-section perturbation, the change in the scattering and total reaction rates were incorrect. These bugs have been fixed in a version of MCNP6.

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 perturbation capability in MCNP5 has recently undergone some verification efforts.[6–10] In particular, Ref. 6 included a one-group, two-isotope homogeneous analytic k_∞ problem that was used to test the two Taylor series terms for the change in k_∞ due to changes in the microscopic cross sections of one isotope. The Taylor series terms were found to be extremely accurate. However, in Ref. 8, the problem was used to help identify bugs in the MCNP perturbation capability (perturbed tally results depend on the presence or absence of other tallies in the problem, and nonzero Δk_{eff} results are sometimes obtained for fission reactions that do not exist).

In this paper, the same k_∞ problem is used to test the Taylor series terms for the change in reaction-rate tallies due to changes in the microscopic cross sections of one isotope. MCNP5 version 1.50 was used in this work.

The next section of this paper discusses the Taylor series expansion of a perturbation and the MCNP perturbation capability. In Sec. III, derivatives of reaction rates with respect to the cross sections of one isotope are derived. MCNP perturbation results are compared with analytic results in Sec. IV. The paper is summarized in Sec. V. The input file and cross section files are given in an attachment.

II. Taylor Series 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

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

Define the first- and second-order Taylor series terms as

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

and

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

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

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

The subscript PERT is used because, at present, the MCNP perturbation capability, invoked with the PERT card, uses a two-term Taylor expansion with no cross terms.[11]

III. k_∞ Test Problem

In a homogenous system from which there is no neutron leakage, the energy-integrated or one-group k-eigenvalue is[12]

$$k_\infty = \frac{\nu\Sigma_f}{\Sigma_f + \Sigma_c}, \tag{6}$$

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. (6) the capture cross section Σ_c is MCNP's absorption cross section. The total interaction cross section Σ_t is

$$\Sigma_t = \Sigma_f + \Sigma_c + \Sigma_s, \tag{7}$$

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. (6) becomes

$$k_\infty = \frac{N_1\nu_1\sigma_{f,1} + N_2\nu_2\sigma_{f,2}}{N_1(\sigma_{f,1}+\sigma_{c,1}) + N_2(\sigma_{f,2}+\sigma_{c,2})}. \tag{8}$$

In Ref. 6, derivatives of k_∞ with respect to the four cross sections of isotope 1 were given and used to verify the two Taylor series terms computed in the MCNP perturbation feature for the change in the k-eigenvalue, Δk_∞. In this paper, we attempt to verify the two Taylor series terms computed for the change in the four reaction rates (fission, capture, scattering, and total) for the k_∞ problem.

In MCNP k-eigenvalue calculations, the scalar flux is normalized such that

$$k_{eff} = \int_0^\infty dE \int dV\ \nu\Sigma_f(r,E)\phi(r,E). \tag{9}$$

In the one-group k_∞ problem, Eq. (9) is

$$k_\infty = \nu\Sigma_f\phi, \tag{10}$$

which can be rearranged using Eqs. (6) and (8) to yield an equation for the normalized scalar flux:

$$\phi = \frac{1}{\Sigma_f + \Sigma_c} = \frac{1}{N_1(\sigma_{f,1}+\sigma_{c,1}) + N_2(\sigma_{f,2}+\sigma_{c,2})}. \tag{11}$$

We will need derivatives of ϕ with respect to each of the cross sections of material 1. First, we take derivatives with respect to the atom density of material 1. The derivatives are

$$\frac{d\phi}{dN_1} = \frac{-(\sigma_{f,1} + \sigma_{c,1})}{(\Sigma_f + \Sigma_c)^2}, \tag{12}$$

$$\frac{d^2\phi}{dN_1^2} = \frac{2(\sigma_{f,1} + \sigma_{c,1})^2}{(\Sigma_f + \Sigma_c)^3}, \tag{13}$$

and

$$\frac{d^n\phi}{dN_1^n} = \frac{(-1)^n n!(\sigma_{f,1} + \sigma_{c,1})^n}{(\Sigma_f + \Sigma_c)^{n+1}}. \tag{14}$$

We assume that perturbing the total cross section of an isotope by $p = \Delta\sigma_{t,1}/\sigma_{t,1,0}$ is equivalent to perturbing all of the isotope's cross sections by *p* and also equivalent to perturbing the atom density of the isotope by *p*. Thus the ratio $N_1/\sigma_{t,1}$ is constant and, using the chain rule,

$$\frac{d^n\phi}{d\sigma_{t,1}^n} = \left(\frac{N_1}{\sigma_{t,1}}\right)^n \frac{d^n\phi}{dN_1^n}. \tag{15}$$

Derivatives of ϕ with respect to each of the other cross sections of material 1 are

$$\frac{d\phi}{d\sigma_{f,1}} = \frac{d\phi}{d\sigma_{c,1}} = \frac{-N_1}{(\Sigma_f + \Sigma_c)^2}, \tag{16}$$

$$\frac{d^2\phi}{d\sigma_{f,1}^2} = \frac{d^2\phi}{d\sigma_{c,1}^2} = \frac{2N_1^2}{(\Sigma_f + \Sigma_c)^3}, \tag{17}$$

$$\frac{d^n\phi}{d\sigma_{f,1}^n} = \frac{d^n\phi}{d\sigma_{f,1}^n} = \frac{(-1)^n n!\, N_1^n}{(\Sigma_f + \Sigma_c)^{n+1}}, \tag{18}$$

and

$$\frac{d\phi}{d\sigma_{s,1}} = \frac{d^2\phi}{d\sigma_{s,1}^2} = \frac{d^n\phi}{d\sigma_{s,1}^n} = 0. \tag{19}$$

Reaction rate *X*, where *X* = *C*, *F*, *S*, or *T* for capture, fission, scattering, or total, respectively, is

$$\begin{aligned} X &= \Sigma_x\phi \\ &= (N_1\sigma_{x,1} + N_2\sigma_{x,2})\phi. \end{aligned} \tag{20}$$

We now give the derivatives of each of the four reaction rates with respect to each of the four cross sections of isotope 1. Using the chain rule as above, the derivatives of reaction rate *X* (for *X* ≠ *T*) with respect to the total cross section of isotope 1 are

$$\frac{dX}{d\sigma_{t,1}} = \left(\frac{N_1}{\sigma_{t,1}}\right)\frac{dX}{dN_1} = \left(\Sigma_x \frac{d\phi}{dN_1} + \sigma_{x,1}\phi\right)\left(\frac{N_1}{\sigma_{t,1}}\right), \tag{21}$$

$$\frac{d^2X}{d\sigma_{t,1}^2} = \left(\frac{N_1}{\sigma_{t,1}}\right)^2 \frac{d^2X}{dN_1^2} = \left(\Sigma_x \frac{d^2\phi}{dN_1^2} + 2\sigma_{x,1}\frac{d\phi}{dN_1}\right)\left(\frac{N_1}{\sigma_{t,1}}\right)^2, \tag{22}$$

and

$$\frac{d^nX}{d\sigma_{t,1}^n} = \left(\frac{N_1}{\sigma_{t,1}}\right)^n \frac{d^nX}{dN_1^n} = \left(\Sigma_x \frac{d^n\phi}{dN_1^n} + n\sigma_{x,1}\frac{d^{n-1}\phi}{dN_1^{n-1}}\right)\left(\frac{N_1}{\sigma_{t,1}}\right)^n, \tag{23}$$

and the derivatives of the total reaction rate *T* with respect to the total cross section of isotope 1 are

$$\frac{d^nT}{d\sigma_{t,1}^n} = \frac{d^nC}{d\sigma_{t,1}^n} + \frac{d^nF}{d\sigma_{t,1}^n} + \frac{d^nS}{d\sigma_{t,1}^n}. \tag{24}$$

The derivatives of reaction rate *X* with respect to the capture cross section of isotope 1 are

$$\frac{dC}{d\sigma_{c,1}} = \Sigma_c \frac{d\phi}{d\sigma_{c,1}} + N_1\phi, \tag{25}$$

$$\frac{d^2C}{d\sigma_{c,1}^2} = \Sigma_c \frac{d^2\phi}{d\sigma_{c,1}^2} + 2N_1 \frac{d\phi}{d\sigma_{c,1}}, \tag{26}$$

$$\frac{d^nC}{d\sigma_{c,1}^n} = \Sigma_c \frac{d^n\phi}{d\sigma_{c,1}^n} + nN_1 \frac{d^{n-1}\phi}{d\sigma_{c,1}^{n-1}}, \tag{27}$$

$$\frac{d^nF}{d\sigma_{c,1}^n} = \Sigma_f \frac{d^n\phi}{d\sigma_{c,1}^n}, \tag{28}$$

$$\frac{d^nS}{d\sigma_{c,1}^n} = \Sigma_s \frac{d^n\phi}{d\sigma_{c,1}^n}, \tag{29}$$

and

$$\frac{d^nT}{d\sigma_{c,1}^n} = \frac{d^nC}{d\sigma_{c,1}^n} + \frac{d^nF}{d\sigma_{c,1}^n} + \frac{d^nS}{d\sigma_{c,1}^n}. \tag{30}$$

The derivatives of reaction rate X with respect to the fission cross section of isotope 1 are

$$\frac{dF}{d\sigma_{f,1}} = \Sigma_f \frac{d\phi}{d\sigma_{f,1}} + N_1\phi, \tag{31}$$

$$\frac{d^2F}{d\sigma_{f,1}^2} = \Sigma_f \frac{d^2\phi}{d\sigma_{f,1}^2} + 2N_1 \frac{d\phi}{d\sigma_{f,1}}, \tag{32}$$

$$\frac{d^nF}{d\sigma_{f,1}^n} = \Sigma_f \frac{d^n\phi}{d\sigma_{f,1}^n} + nN_1 \frac{d^{n-1}\phi}{d\sigma_{f,1}^{n-1}}, \tag{33}$$

$$\frac{d^nC}{d\sigma_{f,1}^n} = \Sigma_c \frac{d^n\phi}{d\sigma_{f,1}^n}, \tag{34}$$

$$\frac{d^nS}{d\sigma_{f,1}^n} = \Sigma_s \frac{d^n\phi}{d\sigma_{f,1}^n}, \tag{35}$$

and

$$\frac{d^nT}{d\sigma_{f,1}^n} = \frac{d^nC}{d\sigma_{f,1}^n} + \frac{d^nF}{d\sigma_{f,1}^n} + \frac{d^nS}{d\sigma_{f,1}^n}. \tag{36}$$

The derivatives of reaction rate X with respect to the scattering cross section of isotope 1 are

$$\frac{dS}{d\sigma_{s,1}} = N_1\phi, \tag{37}$$

$$\frac{d^nS}{d\sigma_{s,1}^n} = 0, n \geq 2, \tag{38}$$

$$\frac{d^nC}{d\sigma_{s,1}^n} = \frac{d^nF}{d\sigma_{s,1}^n} = 0, \tag{39}$$

and

$$\frac{d^nT}{d\sigma_{s,1}^n} = \frac{d^nS}{d\sigma_{s,1}^n}. \tag{40}$$

IV. Test Problem and Results

The isotopes used in the example problem are listed in Table I. The cross sections are one-group macroscopic cross sections from Ref. 13. In this paper, as in Ref. 6, 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 (T-DO).

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. 13.
[b] U-235 (a), Table 9, Ref. 13.

Using Eq. (8), the analytic k_∞ is 2.489362 (there was a typo in this value in Ref. 6). 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. The unperturbed reaction rates computed using Eq. (20) are compared with the results of MCNP track-length tallies in Table II.

Table II. Unperturbed Reaction Rates.

	Analytic	PERT Estimate	Difference: Rel. to Analytic	Difference: Num. Std. Devs.
Capture	1.84397E-01	1.84405E-01 ± 0.003%	0.004%	1.246
Fission	8.15603E-01	8.15639E-01 ± 0.003%	0.004%	1.300
Scattering	2.54610E+00	2.54621E+00 ± 0.003%	0.004%	1.275
Total	3.54610E+00	3.54626E+00 ± 0.003%	0.005%	1.329

In the following subsections, each cross section is increased by 30%, and the effect on each reaction rate is computed. Analytic Taylor series terms are computed using the derivatives given in Sec. III, and the analytic total reaction rate perturbations (“Total pert.” in the tables) are computed using

$$\Delta X = \Sigma_x' \phi' - \Sigma_x \phi, \tag{41}$$

where a prime indicates perturbed quantities and the unprimed quantities are the initial, unperturbed values. For the MCNP results, the total reaction rate perturbation is the sum of the first- and second-order Taylor series terms.

MCNP5 version 1.50 was used in this work. It was slightly modified to write tally relative errors in the same format as the tallies themselves. Relative errors of one standard deviation are given in all tables (including Table II above).

IV.A. Total Cross Section

Perturbing the total cross section of an isotope by a relative amount 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 III shows the results of a +30% perturbation in $\sigma_{t,1}$ (p = 0.30).

Table III. Effect of Perturbing the Total Cross Section.

		Analytic	PERT Estimate	Difference: Rel. to Analytic	Difference: Num. Std. Devs.
Effect on Capture, ΔC	1st-order term	1.81077E-03	1.81128E-03 ± 0.291%	0.028%	0.096
	2nd-order term	–3.58302E-04	–3.56544E-04 ± 0.694%	–0.491%	0.711
	Sum of terms	1.45247E-03	1.45473E-03 ± 0.292%	0.155%	0.531
	Total pert.	1.51166E-03	1.45473E-03 ± 0.292%	–3.766%	13.38
Effect on Fission, ΔF	1st-order term	–1.81077E-03	–1.80898E-03 ± 1.299%	–0.099%	0.076
	2nd-order term	3.58302E-04	3.66140E-04 ± 3.041%	2.188%	0.704
	Sum of terms	–1.45247E-03	–1.44284E-03 ± 1.299%	–0.663%	0.514
	Total pert.	–1.51166E-03	–1.44284E-03 ± 1.299%	–4.553%	3.67
Effect on Scattering, ΔS	1st-order term	–6.33771E-02	–6.33740E-02 ± 0.118%	–0.005%	0.041
	2nd-order term	1.25406E-02	1.25654E-02 ± 0.286%	0.198%	0.691
	Sum of terms	–5.08365E-02	–5.08086E-02 ± 0.114%	–0.055%	0.481
	Total pert.	–5.29081E-02	–5.08086E-02 ± 0.114%	–3.968%	36.19
Effect on Total, ΔT	1st-order term	–6.33771E-02	–6.33717E-02 ± 0.163%	–0.009%	0.052
	2nd-order term	1.25406E-02	1.25750E-02 ± 0.394%	0.275%	0.695
	Sum of terms	–5.08365E-02	–5.07967E-02 ± 0.159%	–0.078%	0.492
	Total pert.	–5.29081E-02	–5.07967E-02 ± 0.159%	–3.991%	26.07

The MCNP perturbation capability does an excellent job estimating the first- and second-order Taylor series terms of ΔC, ΔF, ΔS, and ΔT, as well as the sum of the Taylor series terms. The 3.8-4.5% errors in the MCNP perturbation estimates of the total reaction-rate perturbations are made because the two terms in the expansion are not quite enough.

IV.B. Fission Cross Section

Table IV shows the results of a +30% perturbation in $\sigma_{f,1}$.

Table IV. Effect of Perturbing the Fission Cross Section.

		Analytic	PERT Estimate	Difference Rel. to Analytic	Difference Num. Std. Devs.
Effect on Capture, ΔC	1st-order term	–2.94251E-02	–2.94276E-02 ± 0.009%	0.009%	0.992
	2nd-order term	4.69549E-03	4.69584E-03 ± 0.017%	0.007%	0.431
	Sum of terms	–2.47296E-02	–2.47317E-02 ± 0.007%	0.009%	1.160
	Total pert.	–2.53758E-02	–2.47317E-02 ± 0.007%	–2.538%	353.6
Effect on Fission, ΔF	1st-order term	2.94251E-02	2.94210E-02 ± 0.023%	–0.014%	0.606
	2nd-order term	–4.69549E-03	–4.69610E-03 ± 0.038%	0.013%	0.343
	Sum of terms	2.47296E-02	2.47249E-02 ± 0.022%	–0.019%	0.866
	Total pert.	2.53758E-02	2.47249E-02 ± 0.022%	–2.565%	120.2
Effect on Scattering, ΔS	1st-order term	–4.06292E-01	–4.06327E-01 ± 0.009%	0.009%	0.985
	2nd-order term	6.48339E-02	6.48388E-02 ± 0.017%	0.008%	0.438
	Sum of terms	–3.41459E-01	–3.41488E-01 ± 0.007%	0.009%	1.171
	Total pert.	–3.50381E-01	–3.41488E-01 ± 0.007%	–2.538%	353.6
Effect on Total, ΔT	1st-order term	–4.06292E-01	–5.65915E-01 ± 0.009%	39.29%	3268
	2nd-order term	6.48339E-02	9.03047E-02 ± 0.017%	39.29%	1636
	Sum of terms	–3.41459E-01	–4.75610E-01 ± 0.007%	39.29%	3830
	Total pert.	–3.50381E-01	–4.75610E-01 ± 0.007%	35.74%	3575

The two Taylor series terms (and their sum) of ΔC, ΔF, and ΔS are individually well estimated by MCNP, and the 2.6% error in the total MCNP perturbation estimate is because two terms are not enough. However, MCNP has trouble estimating the effect of a fission cross-section perturbation on the total reaction rate. There appears to be a bug in the code.

IV.C. Capture Cross Section

Table V shows the results of a +30% perturbation in $\sigma_{c,1}$.

Table V. Effect of Perturbing the Capture Cross Section.

		Analytic	PERT Estimate	Difference Rel. to Analytic	Difference Num. Std. Devs.
Effect on Capture, ΔC	1st-order term	3.12359E-02	3.12369E-02 ± 0.003%	0.003%	1.310
	2nd-order term	–1.19627E-03	–1.19637E-03 ± 0.007%	0.009%	1.207
	Sum of terms	3.00396E-02	3.00406E-02 ± 0.002%	0.003%	1.387
	Total pert.	3.00837E-02	3.00406E-02 ± 0.002%	–0.143%	59.01
Effect on Fission, ΔF	1st-order term	–3.12359E-02	–3.12385E-02 ± 0.009%	0.008%	0.982
	2nd-order term	1.19627E-03	1.19636E-03 ± 0.017%	0.008%	0.452
	Sum of terms	–3.00396E-02	–3.00422E-02 ± 0.008%	0.009%	1.042
	Total pert.	–3.00837E-02	–3.00422E-02 ± 0.008%	–0.138%	16.56
Effect on Scattering, ΔS	1st-order term	–9.75102E-02	–9.75185E-02 ± 0.009%	0.009%	0.988
	2nd-order term	3.73443E-03	3.73471E-03 ± 0.017%	0.007%	0.431
	Sum of terms	–9.37758E-02	–9.37838E-02 ± 0.008%	0.009%	1.028
	Total pert.	–9.39135E-02	–9.37838E-02 ± 0.008%	–0.138%	16.57
Effect on Total, ΔT	1st-order term	–9.75102E-02	–1.35820E-01 ± 0.009%	39.29%	3268
	2nd-order term	3.73443E-03	5.20155E-03 ± 0.017%	39.29%	1636
	Sum of terms	–9.37758E-02	–1.30618E-01 ± 0.008%	39.29%	3379
	Total pert.	–9.39135E-02	–1.30618E-01 ± 0.008%	39.08%	3367

Again, the two Taylor series terms (and their sum) of ΔC, ΔF, and ΔS are individually well estimated by MCNP. In this case two Taylor series terms represent the exact perturbation very well. However, MCNP has trouble estimating the effect of a capture cross-section perturbation on the total reaction rate. There appears to be a bug in the code.

IV.D. Scattering Cross Section

Table VI shows the results of a +30% perturbation in $\sigma_{s,1}$.

Table VI. Effect of Perturbing the Scattering Cross Section.

		Analytic	PERT Estimate	Difference Rel. to Analytic	Difference Num. Std. Devs.
Effect on Capture, ΔC	1st-order term	0.00000E+00	1.92417E-06 ± 100.0%	N/A[a]	1.0
	2nd-order term	0.00000E+00	1.52350E-06 ± 100.0%	N/A[a]	1.0
	Sum of terms	0.00000E+00	3.44767E-06 ± 100.0%	N/A[a]	1.0
	Total pert.	0.00000E+00	3.44767E-06 ± 100.0%	N/A[a]	1.0
Effect on Fission, ΔF	1st-order term	0.00000E+00	8.51073E-06 ± 100.0%	N/A[a]	1.0
	2nd-order term	0.00000E+00	6.73857E-06 ± 100.0%	N/A[a]	1.0
	Sum of terms	0.00000E+00	1.52493E-05 ± 100.0%	N/A[a]	1.0
	Total pert.	0.00000E+00	1.52493E-05 ± 100.0%	N/A[a]	1.0
Effect on Scattering, ΔS	1st-order term	4.40426E-01	2.65683E-05 ± 100.0%	–100.0%	16576
	2nd-order term	0.00000E+00	2.10361E-05 ± 100.0%	N/A[a]	1.0
	Sum of terms	4.40426E-01	4.76043E-05 ± 100.0%	–100.0%	9251
	Total pert.	4.40426E-01	4.76043E-05 ± 100.0%	–100.0%	9251
Effect on Total, ΔT	1st-order term	4.40426E-01	3.70032E-05 ± 100.0%	–100.0%	11901
	2nd-order term	0.00000E+00	2.92981E-05 ± 100.0%	N/A[a]	1.0
	Sum of terms	4.40426E-01	6.63013E-05 ± 100.0%	–100.0%	6642
	Total pert.	4.40426E-01	6.63013E-05 ± 100.0%	–100.0%	6642

[a] Not applicable due to division by zero.

For this problem, MCNP computed essentially zero for the effect of perturbing the scattering cross section on the scattering rate and on the total reaction rate. These values are wrong. There appears to be a bug in the code.

However, some of the zeroes are accurate, in the sense of being within one standard deviation of the exact answer. These results are 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 VI, what is a user to do? This question will be addressed in a future paper.

V. Summary and Conclusions

In this paper, the MCNP perturbation capability was used to estimate changes in reaction-rate tallies due to changes in cross sections in a k_∞ problem. MCNP results were compared with analytic results. Two bugs were found: 1) for fission and capture cross-section perturbations, the change in the total reaction rate was not equal to the sum of the changes in the fission, capture, and scattering reaction rates (which were individually correct); and 2) for a scattering cross-section perturbation, the change in the scattering and total reaction rates were incorrect.

Results from an older version of MCNP5 (version 1.50) are reported. It has been found that MCNP5_LANL version 1.51, MCNP6 version 6.1.61, and MCNPX version 2.7.a all have this bug as well.

Dr. Brian Kiedrowski (XCP-3) has already fixed this bug in a version of MCNP6 (6.1.67) which he has provided the author. Dr. Kiedrowski's version also fixes the bugs reported in Ref. 8. The new MCNP6 version gave the exact same results as MCNP5 for the one-group two-region k_{eff} and "k-response" problems of Ref. 6 (Sec. IV of that reference) and the U(2)F_4/paraffin problem of Ref. 7. The new MCNP6 version gave similar results (differences seem to be due to a particle tracking difference introduced in cycle 1000) for the 30-group two-region problem of Ref. 6 (Sec. V of that reference). Thus, the bugs in MCNP had nothing to do with the generally poor MCNP perturbation results for eigenvalue problems reported previously,[5–7,14] which are thought to be due to the inability to estimate the effect of the perturbed fission source distribution on the perturbed quantities of interest.[10]

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XCP-DO File
XCP-7 File

ATTACHMENT 1

INPUT FILE AND CROSS SECTION FILES

These files are available electronically from the author.

Input file for the k_∞ problem:

```
message: xsdir=xsdir1

pu239a and u235a, unpert
10  1    1.              -10    imp:n=1
99  0                     10    imp:n=0

*10  so  10.

mode n
idum 1
rand gen=2 seed=20000000001
kcode 500000   1.    30    530
prdmp j 100
sdef        pos=0. 0. 0. rad=d2
si2 0. 10.
sp2 -21 2
m1   90240.40c 0.6   90240.60c 0.4
m2   90240.40c 0.78  90240.60c 0.4
m3   90240.40c 0.42  90240.60c 0.4
m4   90240.40c 0.606 90240.60c 0.4
f004:n 10
fm004 (-1 1 1)
sd004 1.
f014:n 10
fm014 (-1 1 22)
sd014 1.
f024:n 10
fm024 (-1 1 18)
sd024 1.
f034:n 10
fm034 (-1 1 102)
sd034 1.
f054:n 10
fm054 (-1 1 -7 18)
sd054 1.
f064:n 10
fm064 (-1 1 -7 -6)
sd064 1.
c
f994:n 10
sd994 1.
C
pert101:n cell=10 rho=1.18 mat=2 rxn=1       method=1
pert111:n cell=10 rho=0.82 mat=3 rxn=1       method=1
pert102:n cell=10 rho=1.18 mat=2 rxn=18      method=1
pert112:n cell=10 rho=0.82 mat=3 rxn=18      method=1
pert103:n cell=10 rho=1.18 mat=2 rxn=102     method=1
pert113:n cell=10 rho=0.82 mat=3 rxn=102     method=1
pert104:n cell=10 rho=1.18 mat=2 rxn=22      method=1
pert114:n cell=10 rho=0.82 mat=3 rxn=22      method=1
pert105:n cell=10 rho=1.18 mat=2 rxn=18 102  method=1
pert115:n cell=10 rho=0.82 mat=3 rxn=18 102  method=1
pert106:n cell=10 rho=1.18 mat=2 rxn=18 22   method=1
pert116:n cell=10 rho=0.82 mat=3 rxn=18 22   method=1
pert201:n cell=10 rho=1.18 mat=2 rxn=1       method=2
pert211:n cell=10 rho=0.82 mat=3 rxn=1       method=2
pert202:n cell=10 rho=1.18 mat=2 rxn=18      method=2
pert212:n cell=10 rho=0.82 mat=3 rxn=18      method=2
pert203:n cell=10 rho=1.18 mat=2 rxn=102     method=2
pert213:n cell=10 rho=0.82 mat=3 rxn=102     method=2
pert204:n cell=10 rho=1.18 mat=2 rxn=22      method=2
pert214:n cell=10 rho=0.82 mat=3 rxn=22      method=2
```

```
pert205:n cell=10 rho=1.18 mat=2 rxn=18 102  method=2
pert215:n cell=10 rho=0.82 mat=3 rxn=18 102  method=2
pert206:n cell=10 rho=1.18 mat=2 rxn=18 22   method=2
pert216:n cell=10 rho=0.82 mat=3 rxn=18 22   method=2
pert301:n cell=10 rho=1.18 mat=2 rxn=1       method=3
pert311:n cell=10 rho=0.82 mat=3 rxn=1       method=3
pert302:n cell=10 rho=1.18 mat=2 rxn=18      method=3
pert312:n cell=10 rho=0.82 mat=3 rxn=18      method=3
pert303:n cell=10 rho=1.18 mat=2 rxn=102     method=3
pert313:n cell=10 rho=0.82 mat=3 rxn=102     method=3
pert304:n cell=10 rho=1.18 mat=2 rxn=22      method=3
pert314:n cell=10 rho=0.82 mat=3 rxn=22      method=3
pert305:n cell=10 rho=1.18 mat=2 rxn=18 102  method=3
pert315:n cell=10 rho=0.82 mat=3 rxn=18 102  method=3
pert306:n cell=10 rho=1.18 mat=2 rxn=18 22   method=3
pert316:n cell=10 rho=0.82 mat=3 rxn=18 22   method=3
c
print -30

end of input
```

Cross-section directory file xsdir1:

```
atomic weight ratios
 90240 2.40000E+02
directory
 90240.40c  2.40000E+02 xs01     0 1  1   82
 90240.60c  2.40000E+02 xs01     0 1 34   82
```

Cross-section file xs01:

```
90240.40c 2.40000E+02 0.00000E+00 11/02/97
pu239 a, table 2, unperturbed



      82    90240        2        3        2        0        0        0
       0        0        0        0        0        0        0        0
       1       11       18       21       24       27       30       42
      45       45       47        0        0        0        0        0
       0        0        0        0        0       82        0        0
       0        0        0        0        0        0        0        0
  1.000000000000E-11                 100  3.264000000000E-01  3.264000000000E-01
  1.958400000000E-02  1.958400000000E-02                   0                   0
                   0                   0                   2                   0
                   2  1.000000000000E-11                 100  3.240000000000E+00
  3.240000000000E+00                  18                  22                 102
                 180                   1                   5                  19
                   1                   0                   1                   5
                   9                   1                   2  8.160000000000E-02
  8.160000000000E-02                   1                   2  2.252160000000E-01
  2.252160000000E-01                   1                   2  1.958400000000E-02
  1.958400000000E-02                   0                   0                   0
                   1                  19                   0                   1
                  10                   0                   2  1.000000000000E-11
                 100                   1                   1                   0
                   2  1.000000000000E-11                 100                   2
  1.000000000000E-11                 100  1.000000000000E-11                 100
                   0                   1                  28                   0
                   2  1.000000000000E-11                 100                   1
                   1                   0                   2  1.000000000000E-11
                 100                   2  1.000000000000E-11                 100
  1.000000000000E-11                 100
 90240.60c 2.40000E+02 0.00000E+00 11/02/97
u235 a, table 9, unperturbed



      82    90240        2        3        2        0        0        0
       0        0        0        0        0        0        0        0
       1       11       18       21       24       27       30       42
      45       45       47        0        0        0        0        0
       0        0        0        0        0       82        0        0
       0        0        0        0        0        0        0        0
  1.000000000000E-11                 100  3.264000000000E-01  3.264000000000E-01
  1.305600000000E-02  1.305600000000E-02                   0                   0
                   0                   0                   2                   0
                   2  1.000000000000E-11                 100  2.700000000000E+00
  2.700000000000E+00                  18                  22                 102
                 180                   1                   5                  19
                   1                   0                   1                   5
                   9                   1                   2  6.528000000000E-02
  6.528000000000E-02                   1                   2  2.480640000000E-01
  2.480640000000E-01                   1                   2  1.305600000000E-02
  1.305600000000E-02                   0                   0                   0
                   1                  19                   0                   1
                  10                   0                   2  1.000000000000E-11
                 100                   1                   1                   0
                   2  1.000000000000E-11                 100                   2
  1.000000000000E-11                 100  1.000000000000E-11                 100
                   0                   1                  28                   0
                   2  1.000000000000E-11                 100                   1
                   1                   0                   2  1.000000000000E-11
                 100                   2  1.000000000000E-11                 100
  1.000000000000E-11                 100
```