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Title:	Using the MCNP Perturbation Feature to Estimate the Taylor Series Coefficients in a keff-Eigenvalue Problem (U)
Author(s):	Jeffrey A. Favorite, XCP-7
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research note

X-Computational Physics Division
Transport Applications Group

Group XCP-7, MS F644
Los Alamos, New Mexico 87545
505/665-7336
Fax: 505/665-7345

To/MS: Distribution
From/MS: Jeffrey A. Favorite / XCP-7, MS F663
Phone/Email: 7-7941 / fave@lanl.gov
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SUBJECT: Using the MCNP Perturbation Feature to Estimate the Taylor Series Coefficients in a k_{eff}-Eigenvalue Problem (U)

Abstract

The MCNP perturbation capability was tested in a two-region spherical fuel-reflector 30-group k_{eff}-eigenvalue problem in which the density of the reflector was perturbed. The MCNP perturbation estimates of the coefficients of two-term Taylor series expansions for Δk_{eff} and for the changes in the groupwise fluxes in the fuel were compared with direct estimates obtained from central-difference formulas. Generally, the second-order coefficients (for the quadratic terms) were more accurately estimated than the first-order coefficients (for the linear terms), but none of the coefficients were estimated accurately. The first-order terms estimated for the change in the groupwise fluxes had the wrong sign for 29 out of 30 groups, indicating a possible bug. If the MCNP perturbation capability could accurately estimate the coefficients of the Taylor series for Δk_{eff}, the resulting approximation would be more accurate than an adjoint-based first-order perturbation theory approximation for this problem. Thus, more work should go into improving the estimates of the coefficients, and retaining the differential operator method as a user option for Δk_{eff} is suggested.

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.[6–11] Although some analytic results have been well matched for k_∞ problems,[6,11] in general it has been found that the perturbation capability is ill-suited for k_{eff}-eigenvalue problems.[6,7,10,12]

In this paper, a new test problem is introduced, a two-region spherical fuel-reflector 30-group k_{eff}-eigenvalue problem in which the density of the reflector is perturbed. The goal is to determine the accuracy of the MCNP perturbation estimates of the coefficients of a two-term Taylor series expansion, rather than of the first-order term alone (as for sensitivities) or the combination of terms for a specific perturbation amount. The reference values are obtained using central-difference formulas applied to the results of direct calculations of perturbed systems.

The next section of this paper discusses the Taylor series expansion of a perturbation and the MCNP perturbation capability. In Sec. III, the test problem is presented. MCNP perturbation results for the Taylor series coefficients are

compared with direct results in Sec. IV, and the accuracy of the Taylor series expansion for Δk_{eff} is discussed in Sec. V. The paper is summarized in Sec. VI. The input files are given in an attachment.

II. Taylor Series and MCNP Perturbations

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

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

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

$$\Delta c_1 \equiv \left.\frac{dc}{d\sigma_x}\right|_{\sigma_{x,0}} \Delta\sigma_x \tag{3}$$

and

$$\Delta c_2 \equiv \frac{1}{2}\left.\frac{d^2c}{d\sigma_x^2}\right|_{\sigma_{x,0}} (\Delta\sigma_x)^2, \tag{4}$$

respectively. Define p_x as the relative cross-section change,

$$p_x \equiv \frac{\Delta\sigma_x}{\sigma_{x,0}}. \tag{5}$$

Then, using the chain rule, the Taylor series terms can be written conveniently as

$$\Delta c_1 = \left.\frac{dc}{dp_x}\right|_{p_x=0} p_x \tag{6}$$

and

$$\Delta c_2 = \frac{1}{2}\left.\frac{d^2c}{dp_x^2}\right|_{p_x=0} p_x^2. \tag{7}$$

At present, the MCNP perturbation capability, invoked with the PERT card, uses a two-term Taylor expansion with no cross terms.[3,13] The perturbation estimate of $\Delta c(p_x) \equiv c(\sigma_x) - c(\sigma_{x,0})$ is

$$\Delta c_{\text{PERT}}(p_x) = \Delta c_1(p_x) + \Delta c_2(p_x). \tag{8}$$

Define coefficients

$$c_1 \equiv \left.\frac{dc}{dp_x}\right|_{p_x=0} \tag{9}$$

and

$$c_2 \equiv \frac{1}{2}\left.\frac{d^2c}{dp_x^2}\right|_{p_x=0}. \tag{10}$$

These coefficients can be computed from any single arbitrary reference perturbation amount $p_{x,r}$ using

$$c_1 = \Delta c_1(p_{x,r}) \big/ p_{x,r} \tag{11}$$

and

$$c_2 = \Delta c_2(p_{x,r}) \big/ p_{x,r}^2. \tag{12}$$

The standard deviations of the Monte Carlo estimates of c_1 and c_2, s_{c_1} and s_{c_2}, are

$$s_{c_1} = s_{\Delta c_1} \big/ |p_{x,r}| \tag{13}$$

and

$$s_{c_2} = s_{\Delta c_2} \big/ p_{x,r}^2, \tag{14}$$

where $s_{\Delta c_1}$ and $s_{\Delta c_2}$ are the standard deviations of the Monte Carlo estimates of Δc_1 and Δc_2.

Now the perturbed response due to any perturbation p_x can be computed using

$$\Delta c_{\mathrm{PERT}}(p_x) = c_1 p_x + c_2 p_x^2, \tag{15}$$

and its standard deviation is

$$s_{\Delta c_{\mathrm{PERT}}} = \left|\frac{p_x}{p_{x,r}}\right| \sqrt{s_{\Delta c_1}^2 + \left(\frac{p_x}{p_{x,r}}\right)^2 s_{\Delta c_2}^2}\,. \tag{16}$$

Equation (16) is exact if Δc_1 and Δc_2 are uncorrelated. If these terms are computed in a single Monte Carlo calculation, as they ordinarily would be, then they are correlated, and Eq. (16) is only approximate.

We emphasize that c_1 is computed using only the first-order Taylor series term [Eq. (11)] and c_2 is computed using only the second-order Taylor series term [Eq. (12)]. In MCNP parlance, this means the PERT card for computing c_1 must have METHOD=2 and the PERT card for computing c_2 must have METHOD=3. We also emphasize that the estimate of these coefficients is independent of the size of the perturbation p_x; it is the accuracy of the perturbation estimates computed with the coefficients that may depend on the size of the perturbation, the absence of third- and higher order terms, and the absence of cross terms, as well as the accuracy of the coefficients.

III. UOFl Test Problem

An enriched uranium oxyfluoride solution[14] (with a density of 1.0262 g/cm^3) fills a spherical aluminum tank with an inner radius of 27.9244 cm and a thickness of 0.2 cm. The system is reflected with a 15-cm thick spherical shell of water (with a nominal density of 0.99705 g/cm^3), which is neutronically infinite. Material compositions are given in the input files in the attachment.

The problem is to estimate the effect of a perturbation in the reflector density on the system k_{eff} and the total (volume-integrated) energy-dependent neutron flux in the UOFl. The problem was done in MCNP5 using multigroup calculations with MENDF5 cross sections in 30 energy groups with no self-shielding correction and no $S(\alpha,\beta)$ scattering. The unperturbed track-length k_{eff} using 500 000 neutrons per cycle, 30 settle cycles, 500 active cycles, and an initial guess of 1. was 0.981993 ± 0.000052. The problem was also done using the PARTISN multigroup discrete-ordinates code[15] with S_{64} quadrature, P_4 scattering, and a convergence criterion of 10^{-8}, and the unperturbed k_{eff} was 0.97520837. The deterministic MENDF5 library includes only prompt fission data, but the Monte-Carlo MENDF5 library includes both prompt and total.[16]

The object is to compare c_1 and c_2 estimated using MCNP PERT cards and Eqs. (11) and (12) with direct values computed using Eqs. (9) and (10). The direct values $c_{1,d}$ and $c_{2,d}$ were estimated using central difference formulas. Let $p_{x,c}$ be an arbitrary positive value of a relative perturbation amount, and let $c_+ = c(+p_{x,c})$, $c_- = c(-p_{x,c})$, and $c_0 = c(p_x = 0)$. The central difference formulas are then

$$c_{1,d} \approx \frac{c_+ - c_-}{2p_{x,c}} \tag{17}$$

and

$$c_{2,d} \approx \frac{1}{2}\frac{c_+ - 2c_0 + c_-}{p_{x,c}^2}. \tag{18}$$

The parameter $p_{x,c}$ must be large enough to make the numerators of Eqs. (17) and (18) statistically meaningful but small enough that the approximations are accurate. A value of $p_{x,c} = 0.10$ was used. When the responses c are computed from independent Monte Carlo runs, the standard deviations $s_{c_{1,d}}$ and $s_{c_{2,d}}$ of the direct values are

$$s_{c_{1,d}} = \frac{1}{2p_{x,c}}\sqrt{s_{c_+}^2 + s_{c_-}^2} \tag{19}$$

and

$$s_{c_{2,d}} = \frac{1}{2p_{x,c}^2}\sqrt{s_{c_+}^2 + 4s_{c_0}^2 + s_{c_-}^2}\,. \tag{20}$$

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 and to write more significant figures for k_{eff} and the "predicted changes in keff". The three calculations used to obtain the direct estimates of Eqs. (17) and (18) used 2 000 000 neutrons per cycle, 30 settle cycles, 1000 active cycles, and an initial guess of 1. None of the bugs that have been previously reported[6,8,11] appear to affect the results of this paper.

IV. Results for Coefficients

IV.A. k_{eff}

The coefficients of a second-order Taylor series expansion of the change in k_{eff} due to a change in the reflector density are given in Table I. (In this section, the accuracy of the second-order expansion itself is not considered.) The first-order coefficient c_1 is very badly estimated by the perturbation capability. The second-order coefficient c_2 is apparently well estimated, just outside one standard deviation from the direct result, but the direct result is quite uncertain.

Table I. Coefficients for k_{eff} (Direct Results from MCNP).

			Difference	
Coefficient	Direct[a]	PERT Estimate[a]	Rel. to Direct	Num. Std. Devs.
c_1	1.545E-02 ± 0.89%	2.567E-02 ± 0.51%	66.14%	38.162
c_2	–1.660E-02 ± 13.99%	–1.337E-02 ± 6.59%	–19.47%	1.009

[a] Relative errors of one standard deviation are given.

To gain more insight, PARTISN was also used for the direct estimates of the coefficients. Results are shown in Table II. Although the PARTISN calculations use prompt fission data and the MCNP calculations use total, the changes in k_{eff} that are caused by reflector density changes are nearly identical when computed with the two codes (compare the "Direct" columns of Table I and Table II). Table II confirms that c_1 is very badly estimated by the MCNP perturbation capability, but the table also indicates that c_2 is also poorly estimated, though not as poorly as c_1.

Table II. Coefficients for k_{eff} (Direct Results from PARTISN).

			Difference	
Coefficient	Direct	PERT Estimate[a]	Rel. to Direct	Num. Std. Devs.
c_1	1.544E-02	2.567E-02 ± 0.51%	66.21%	78.700
c_2	–1.629E-02	–1.337E-02 ± 6.59%	–17.95%	3.321

[a] Relative errors of one standard deviation are given.

IV.B. Flux in Fuel

The total (volume-integrated) group-dependent flux in the UOFl fuel was also a quantity of interest. The usual multigroup indexing is used; group 30 is the most thermal.

Results are shown in Table III for c_1 and Table IV for c_2 with direct results computed with MCNP. The direct results were difficult to achieve with precision. For c_1 (Table III), only two values (group 30 and the energy-integrated total) have relative statistical errors less than 1%. For group 30, the MCNP perturbation estimate of c_1 is in error by ~63%. For the total, the MCNP perturbation estimate of c_1 is in error by ~200%. For groups other than 30, the MCNP estimate of c_1 has the wrong sign, which is why c_1 for the energy-integrated total is much less accurate than that for group 30.

For c_2 (Table IV), again, only two direct values (group 30 and the energy-integrated total) have relative statistical errors less than 1%. For group 30, the MCNP perturbation estimate of c_2 is in error by ~20%. For the total, the MCNP perturbation estimate of c_1 is in error by only ~6% and the direct and estimated values are within one standard deviation. However, the large uncertainty in the direct values makes these comparisons ambiguous.

Table III. c_1 for Flux in Fuel (Direct Results from MCNP).

Energy Group	Direct[a]	PERT Estimate[a]	Difference Rel. to Direct	Difference Num. Std. Devs.
30	2.340E-01 ± 0.06%	3.825E-01 ± 0.54%	63.48%	67.740
29	–8.650E-04 ± 31.53%	5.003E-03 ± 0.83%	–678.37%	18.671
28	–8.600E-04 ± 31.57%	5.216E-03 ± 0.80%	–706.56%	19.390
27	–1.060E-03 ± 25.62%	5.021E-03 ± 0.81%	–573.71%	19.478
26	–9.900E-04 ± 27.30%	4.913E-03 ± 0.79%	–596.26%	19.092
25	–1.380E-03 ± 19.50%	4.784E-03 ± 0.77%	–446.65%	20.156
24	–1.660E-03 ± 16.14%	4.568E-03 ± 0.76%	–375.17%	20.569
23	–1.690E-03 ± 15.79%	4.399E-03 ± 0.74%	–360.31%	20.323
22	–1.965E-03 ± 13.54%	4.178E-03 ± 0.73%	–312.62%	20.698
21	–2.185E-03 ± 12.14%	3.987E-03 ± 0.71%	–282.49%	21.010
20	–2.395E-03 ± 11.06%	3.766E-03 ± 0.70%	–257.23%	21.163
19	–2.600E-03 ± 10.13%	3.648E-03 ± 0.67%	–240.31%	21.692
18	–2.705E-03 ± 9.70%	3.579E-03 ± 0.65%	–232.30%	21.996
17	–3.525E-03 ± 7.37%	3.744E-03 ± 0.64%	–206.22%	25.616
16	–4.525E-03 ± 5.65%	4.424E-03 ± 0.62%	–197.77%	31.612
15	–3.350E-03 ± 9.99%	2.840E-03 ± 0.75%	–184.78%	17.395
14	–4.085E-03 ± 8.10%	3.285E-03 ± 0.76%	–180.41%	20.718
13	–6.200E-03 ± 5.08%	4.044E-03 ± 0.71%	–165.23%	29.836
12	–7.250E-03 ± 4.41%	3.548E-03 ± 0.76%	–148.94%	31.145
11	–4.860E-03 ± 9.19%	1.734E-03 ± 1.01%	–135.69%	14.212
10	–5.970E-03 ± 8.01%	1.528E-03 ± 1.03%	–125.59%	15.172
9	–5.745E-03 ± 8.70%	1.858E-03 ± 1.07%	–132.34%	14.635
8	–5.050E-03 ± 11.29%	1.409E-03 ± 1.10%	–127.90%	11.027
7	–6.115E-03 ± 9.75%	1.183E-03 ± 1.06%	–119.35%	11.985
6	–1.155E-03 ± 128.47%	2.181E-04 ± 2.44%	–118.89%	0.922
5	–2.965E-04 ± 908.41%	5.319E-05 ± 4.31%	–117.94%	0.130
4	–1.130E-04 ± 5661%	7.923E-06 ± 10.70%	–107.01%	0.019
3	–2.280E-05 ± 65540%	8.840E-07 ± 27.35%	–103.88%	0.002
2	–5.785E-06 ± 473167%	7.334E-08 ± 85.56%	–101.27%	0.000
1	3.550E-07 ± 12350125%	0.000E+00 ± 0.00%	–100.00%	0.000
Total	1.555E-01 ± 0.05%	4.655E-01 ± 0.46%	199.35%	140.758

[a] Relative errors of one standard deviation are given.

Table IV. c_2 for Flux in Fuel (Direct Results from MCNP).

Energy Group	Direct[a]	PERT Estimate[a]	Difference Rel. to Direct	Difference Num. Std. Devs.
30	–2.500E-01 ± 0.96%	–2.031E-01 ± 6.30%	–18.76%	3.086
29	2.350E-03 ± 201.01%	1.390E-03 ± 7.03%	–40.85%	0.199
28	1.000E-03 ± 470.23%	1.564E-03 ± 6.16%	56.42%	0.118
27	3.900E-03 ± 120.62%	1.721E-03 ± 5.33%	–55.86%	0.454
26	5.000E-04 ± 936.23%	1.888E-03 ± 4.55%	277.63%	0.291
25	–5.000E-04 ± 931.98%	1.812E-03 ± 4.35%	–462.39%	0.488
24	1.500E-03 ± 309.36%	1.965E-03 ± 3.71%	31.00%	0.099
23	8.000E-04 ± 577.89%	2.025E-03 ± 3.27%	153.12%	0.261
22	1.650E-03 ± 279.40%	2.207E-03 ± 2.74%	33.79%	0.119
21	3.150E-03 ± 145.89%	2.314E-03 ± 2.36%	–26.53%	0.180
20	4.750E-03 ± 96.55%	2.428E-03 ± 1.99%	–48.89%	0.501
19	3.500E-03 ± 130.38%	2.570E-03 ± 1.71%	–26.58%	0.202
18	9.500E-04 ± 478.15%	2.719E-03 ± 1.49%	186.20%	0.386
17	7.750E-03 ± 58.09%	3.217E-03 ± 1.24%	–58.49%	0.998
16	5.500E-04 ± 805.75%	4.166E-03 ± 1.04%	657.38%	0.808
15	6.600E-03 ± 87.81%	2.885E-03 ± 1.12%	–56.29%	0.638
14	1.155E-02 ± 49.62%	3.473E-03 ± 1.05%	–69.93%	1.400
13	6.000E-03 ± 90.88%	5.100E-03 ± 0.83%	–15.00%	0.164
12	7.500E-03 ± 73.84%	3.943E-03 ± 0.92%	–47.43%	0.638
11	–4.000E-04 ± 1934%	2.266E-03 ± 1.05%	–666.46%	0.344
10	–4.200E-03 ± 197.28%	1.819E-03 ± 1.18%	–143.31%	0.725
9	4.950E-03 ± 174.80%	3.229E-03 ± 0.87%	–34.77%	0.198
8	1.090E-02 ± 90.61%	1.529E-03 ± 1.19%	–85.97%	0.947
7	7.450E-03 ± 138.68%	7.074E-04 ± 1.86%	–90.51%	0.652
6	9.250E-03 ± 277.89%	1.035E-04 ± 4.02%	–98.88%	0.356
5	–6.050E-04 ± 7711%	6.665E-06 ± 18.71%	–101.10%	0.013
4	1.417E-03 ± 7819%	–1.360E-07 ± 100%	–100.01%	0.013
3	2.100E-04 ± 123164%	–9.979E-08 ± 66.59%	–100.05%	0.001
2	2.201E-04 ± 215190%	5.111E-08 ± 100%	–99.98%	0.000
1	–2.411E-04 ± 314011%	0.000E+00 ± 0.00%	–100.00%	0.000
Total	–1.550E-01 ± 0.92%	–1.461E-01 ± 8.79%	–5.76%	0.626

[a] Relative errors of one standard deviation are given.

Direct results were also calculated using PARTISN. The direct results from PARTISN are compared with the direct results from MCNP in Table V for c_1 and Table VI for c_2. The point of this comparison is to be assured that the PARTISN results, which are more precise than the MCNP results, are also accurate. For c_1 (Table V), the PARTISN results are generally within one standard deviation of the MCNP results and they are all within two standard deviations, except for group 30, where the relative difference is less than 1%. For c_2 (Table VI), most of the uncertainties in the MCNP results are greater than 100%, so the comparison for most of the groups isn't meaningful. However, for group 30, the MCNP and PARTISN results agree well (they are 2% and just greater than two standard deviations apart). For the energy-integrated total, the PARTISN result differs from the MCNP result by –19% and 21 standard deviations, which is surprisingly large given the excellent agreement of the largest component, the group-30 value.

It should be noted that the MCNP and PARTISN fluxes agreed extremely well, within 0.01% for 15 energy groups (and the energy-integrated total), within 0.10% for 26 groups, and within 0.20% for 29 groups. The largest difference, 0.58%, was for the fastest group. Although the k_{eff}-eigenvalues differed, the fluxes were not renormalized for this comparison. Both codes normalize the fluxes so that the volume- and energy-integrated fission neutron production equals k_{eff}. The different eigenvalues were due to the lack of total fission data in the deterministic cross sections, not to different eigenfunctions (fission distributions or neutron fluxes).

Table V. Direct Results for c_1 from MCNP and PARTISN.

Energy Group	PARTISN	MCNP[a]	Difference	
			Rel. to MCNP	Num. Std. Devs.
30	2.355E-01	2.340E-01 ± 0.06%	0.641%	10.872
29	–7.400E-04	–8.650E-04 ± 31.53%	–14.451%	0.458
28	–9.300E-04	–8.600E-04 ± 31.57%	8.140%	0.258
27	–1.100E-03	–1.060E-03 ± 25.62%	3.774%	0.147
26	–1.275E-03	–9.900E-04 ± 27.30%	28.788%	1.055
25	–1.440E-03	–1.380E-03 ± 19.50%	4.348%	0.223
24	–1.620E-03	–1.660E-03 ± 16.14%	–2.410%	0.149
23	–1.790E-03	–1.690E-03 ± 15.79%	5.917%	0.375
22	–1.960E-03	–1.965E-03 ± 13.54%	–0.254%	0.019
21	–2.130E-03	–2.185E-03 ± 12.14%	–2.517%	0.207
20	–2.305E-03	–2.395E-03 ± 11.06%	–3.758%	0.340
19	–2.525E-03	–2.600E-03 ± 10.13%	–2.885%	0.285
18	–2.830E-03	–2.705E-03 ± 9.70%	4.621%	0.477
17	–3.425E-03	–3.525E-03 ± 7.37%	–2.837%	0.385
16	–4.690E-03	–4.525E-03 ± 5.65%	3.646%	0.645
15	–3.445E-03	–3.350E-03 ± 9.99%	2.836%	0.284
14	–4.540E-03	–4.085E-03 ± 8.10%	11.138%	1.375
13	–6.650E-03	–6.200E-03 ± 5.08%	7.258%	1.429
12	–7.800E-03	–7.250E-03 ± 4.41%	7.586%	1.720
11	–5.015E-03	–4.860E-03 ± 9.19%	3.189%	0.347
10	–5.350E-03	–5.970E-03 ± 8.01%	–10.385%	1.296
9	–6.095E-03	–5.745E-03 ± 8.70%	6.092%	0.701
8	–4.970E-03	–5.050E-03 ± 11.29%	–1.584%	0.140
7	–6.135E-03	–6.115E-03 ± 9.75%	0.327%	0.034
6	–1.240E-03	–1.155E-03 ± 128.47%	7.359%	0.057
5	–4.180E-04	–2.965E-04 ± 908.41%	40.978%	0.045
4	–8.005E-05	–1.130E-04 ± 5661%	–29.159%	0.005
3	–1.580E-05	–2.280E-05 ± 65540%	–30.702%	0.000
2	–4.810E-06	–5.785E-06 ± 473167%	–16.854%	0.000
1	–1.995E-06	3.550E-07 ± 12350125%	–661.972%	0.000
Total	1.555E-01	1.555E-01 ± 0.05%	0.000%	0.000

[a] Relative errors of one standard deviation are given.

Table VI. Direct Results for c_2 from MCNP and PARTISN.

Energy Group	PARTISN	MCNP[a]	Difference	
			Rel. to MCNP	Num. Std. Devs.
30	–2.450E-01	–2.500E-01 ± 0.96%	–2.000%	2.093
29	2.400E-03	2.350E-03 ± 201.01%	2.128%	0.011
28	2.600E-03	1.000E-03 ± 470.23%	160.000%	0.340
27	2.800E-03	3.900E-03 ± 120.62%	–28.205%	0.234
26	2.950E-03	5.000E-04 ± 936.23%	490.000%	0.523
25	3.100E-03	–5.000E-04 ± 931.98%	–720.000%	0.773
24	3.300E-03	1.500E-03 ± 309.36%	120.000%	0.388
23	3.500E-03	8.000E-04 ± 577.89%	337.500%	0.584
22	3.500E-03	1.650E-03 ± 279.40%	112.121%	0.401
21	3.700E-03	3.150E-03 ± 145.89%	17.460%	0.120
20	3.850E-03	4.750E-03 ± 96.55%	–18.947%	0.196
19	4.050E-03	3.500E-03 ± 130.38%	15.714%	0.121
18	4.400E-03	9.500E-04 ± 478.15%	363.158%	0.760
17	5.250E-03	7.750E-03 ± 58.09%	–32.258%	0.555
16	6.900E-03	5.500E-04 ± 805.75%	1155%	1.433
15	4.950E-03	6.600E-03 ± 87.81%	–25.000%	0.285
14	6.400E-03	1.155E-02 ± 49.62%	–44.589%	0.899
13	9.500E-03	6.000E-03 ± 90.88%	58.333%	0.642
12	1.000E-02	7.500E-03 ± 73.84%	33.333%	0.451
11	6.450E-03	–4.000E-04 ± 1934%	–1713%	0.886
10	6.700E-03	–4.200E-03 ± 197.28%	–259.524%	1.315
9	7.650E-03	4.950E-03 ± 174.80%	54.545%	0.312
8	6.200E-03	1.090E-02 ± 90.61%	–43.119%	0.476
7	7.450E-03	7.450E-03 ± 138.68%	0.000%	0.000
6	1.500E-03	9.250E-03 ± 277.89%	–83.784%	0.301
5	5.000E-04	–6.050E-04 ± 7711%	–182.645%	0.024
4	9.650E-05	1.417E-03 ± 7819%	–93.190%	0.012
3	1.900E-05	2.100E-04 ± 123164%	–90.952%	0.001
2	5.600E-06	2.201E-04 ± 215190%	–97.456%	0.000
1	2.250E-06	–2.411E-04 ± 314011%	–100.933%	0.000
Total	–1.250E-01	–1.550E-01 ± 0.92%	–19.355%	20.949

[a] Relative errors of one standard deviation are given.

The direct values from PARTISN are compared with the MCNP perturbation estimates in Table VII for c_1 and Table VIII for c_2. For c_1 (Table VII), the results are essentially the same as those of Table III, where the direct results were computed with MCNP. The MCNP perturbation estimate gives values with the wrong sign for 29 of 30 energy groups. For group 30 and the energy-integrated total, differences between the direct results and the MCNP perturbation results are 62% and 200%, respectively.

Table VII. c_1 for Flux in Fuel (Direct Results from PARTISN).

Energy Group	Direct	PERT Estimate[a]	Difference Rel. to Direct	Difference Num. Std. Devs.
30	2.355E-01	3.825E-01 ± 0.54%	62.441%	71.558
29	–7.400E-04	5.003E-03 ± 0.83%	–776.069%	138.170
28	–9.300E-04	5.216E-03 ± 0.80%	–660.906%	146.701
27	–1.100E-03	5.021E-03 ± 0.81%	–556.486%	150.718
26	–1.275E-03	4.913E-03 ± 0.79%	–485.332%	158.954
25	–1.440E-03	4.784E-03 ± 0.77%	–432.208%	169.295
24	–1.620E-03	4.568E-03 ± 0.76%	–381.961%	177.551
23	–1.790E-03	4.399E-03 ± 0.74%	–345.772%	189.274
22	–1.960E-03	4.178E-03 ± 0.73%	–313.159%	200.379
21	–2.130E-03	3.987E-03 ± 0.71%	–287.200%	214.938
20	–2.305E-03	3.766E-03 ± 0.70%	–263.366%	230.753
19	–2.525E-03	3.648E-03 ± 0.67%	–244.474%	251.346
18	–2.830E-03	3.579E-03 ± 0.65%	–226.457%	273.558
17	–3.425E-03	3.744E-03 ± 0.64%	–209.318%	300.667
16	–4.690E-03	4.424E-03 ± 0.62%	–194.333%	334.546
15	–3.445E-03	2.840E-03 ± 0.75%	–182.440%	295.845
14	–4.540E-03	3.285E-03 ± 0.76%	–172.353%	315.467
13	–6.650E-03	4.044E-03 ± 0.71%	–160.818%	374.786
12	–7.800E-03	3.548E-03 ± 0.76%	–145.491%	420.702
11	–5.015E-03	1.734E-03 ± 1.01%	–134.583%	386.585
10	–5.350E-03	1.528E-03 ± 1.03%	–128.556%	435.000
9	–6.095E-03	1.858E-03 ± 1.07%	–130.482%	398.791
8	–4.970E-03	1.409E-03 ± 1.10%	–128.345%	409.797
7	–6.135E-03	1.183E-03 ± 1.06%	–119.288%	584.410
6	–1.240E-03	2.181E-04 ± 2.44%	–117.591%	273.478
5	–4.180E-04	5.319E-05 ± 4.31%	–112.724%	205.736
4	–8.005E-05	7.923E-06 ± 10.70%	–109.897%	103.782
3	–1.580E-05	8.840E-07 ± 27.35%	–105.595%	69.014
2	–4.810E-06	7.334E-08 ± 85.56%	–101.525%	77.828
1	–1.995E-06	0.000E+00 ± 0.00%	–-100.000%	N/A[b]
Total	1.555E-01	4.655E-01 ± 0.46%	199.349%	146.250

[a] Relative errors of one standard deviation are given.
[b] Not applicable due to division by zero.

For c_2 (Table VIII), the MCNP perturbation estimates are generally within ~35-60% of the direct results from PARTISN, with larger relative differences where the c_2 values are smaller (in magnitude). The differences for group 30 and the energy-integrated total are ~17%.

Table VIII. c_2 for Flux in Fuel (Direct Results from PARTISN).

Energy Group	Direct	PERT Estimate[a]	Difference	
			Rel. to Direct	Num. Std. Devs.
30	–2.450E-01	–2.031E-01 ± 6.30%	–17.097%	3.272
29	2.400E-03	1.390E-03 ± 7.03%	–42.082%	10.336
28	2.600E-03	1.564E-03 ± 6.16%	–39.837%	10.754
27	2.800E-03	1.721E-03 ± 5.33%	–38.525%	11.752
26	2.950E-03	1.888E-03 ± 4.55%	–35.996%	12.360
25	3.100E-03	1.812E-03 ± 4.35%	–41.550%	16.358
24	3.300E-03	1.965E-03 ± 3.71%	–40.456%	18.311
23	3.500E-03	2.025E-03 ± 3.27%	–42.144%	22.272
22	3.500E-03	2.207E-03 ± 2.74%	–36.929%	21.376
21	3.700E-03	2.314E-03 ± 2.36%	–37.454%	25.410
20	3.850E-03	2.428E-03 ± 1.99%	–36.945%	29.394
19	4.050E-03	2.570E-03 ± 1.71%	–36.554%	33.697
18	4.400E-03	2.719E-03 ± 1.49%	–38.206%	41.387
17	5.250E-03	3.217E-03 ± 1.24%	–38.724%	51.163
16	6.900E-03	4.166E-03 ± 1.04%	–39.629%	63.188
15	4.950E-03	2.885E-03 ± 1.12%	–41.724%	64.001
14	6.400E-03	3.473E-03 ± 1.05%	–45.742%	80.015
13	9.500E-03	5.100E-03 ± 0.83%	–46.315%	103.527
12	1.000E-02	3.943E-03 ± 0.92%	–60.574%	166.973
11	6.450E-03	2.266E-03 ± 1.05%	–64.871%	175.812
10	6.700E-03	1.819E-03 ± 1.18%	–72.848%	227.960
9	7.650E-03	3.229E-03 ± 0.87%	–57.793%	157.649
8	6.200E-03	1.529E-03 ± 1.19%	–75.337%	257.117
7	7.450E-03	7.074E-04 ± 1.86%	–90.505%	513.109
6	1.500E-03	1.035E-04 ± 4.02%	–93.098%	335.677
5	5.000E-04	6.665E-06 ± 18.71%	–98.667%	395.597
4	9.650E-05	–1.360E-07 ± 100%	–100.141%	710.418
3	1.900E-05	–9.979E-08 ± 66.59%	–100.525%	287.434
2	5.600E-06	5.111E-08 ± 100%	–99.087%	108.566
1	2.250E-06	0.000E+00 ± 0.00%	–100.000%	N/A[b]
Total	–1.250E-01	–1.461E-01 ± 8.79%	16.853%	1.640

[a] Relative errors of one standard deviation are given.
[b] Not applicable due to division by zero.

IV.C. Summary

In summary, the results of this section indicate that the first-order Taylor series terms for the change in k_{eff} and the group-dependent fluxes in the fuel are very poorly estimated by the MCNP perturbation capability. For the fluxes, the perturbation capability gave the wrong sign for 29 of 30 groups, indicating a possible bug. The second-order Taylor series terms are more accurately estimated, but they are still in error by ~20% for the major values.

V. Accuracy of the Taylor Series Expansion for Δk_{eff}

The accuracy of the MCNP perturbation estimates of the Taylor series coefficients is but one component of the total accuracy of the capability. The other component is the accuracy of the two-term Taylor series estimate itself.

Figure 1 shows the reactivity worth of the reflector density change as a function of p. The reactivity worth ρ is related to Δk_{eff} through

$$\rho = \frac{\Delta k_{eff}}{k_{eff,0} k'_{eff}} = \frac{\Delta k_{eff}}{k_{eff,0}(k_{eff,0} + \Delta k_{eff})}. \tag{21}$$

Dropping the subscript "eff" for convenience, the standard deviation in ρ due to statistical variations in k_0 and Δk is

$$s_\rho = \frac{1}{(k_0 + \Delta k)^2} \sqrt{s_{\Delta k}^2 + \frac{\Delta k^2 (2k_0 + \Delta k)^2}{k_0^4} s_{k_0}^2} \tag{22}$$

if k_0 and Δk are computed independently, which is not the case if Δk is estimated using coefficients calculated during the same run from which k_0 is obtained, but even then we still use Eq. (22) as an estimate. Errors of one standard deviation are shown in Figure 1 (except for the "Deterministic" curves).

The "MCNP exact" and "deterministic exact" curves are virtually indistinguishable.

Figure 1 includes a deterministic first-order adjoint-based perturbation theory[17] curve. The adjoint calculation was done with PARTISN using the same discretization and convergence criterion as the forward. This curve is perfectly linear with p with a slope of 0.016053. This is the curve that the continuous-energy adjoint feature,[18] currently under development, should compute (for this multigroup problem).

The "MCNP PERT" curve uses the coefficients c_1 and c_2 as calculated using the perturbation capability and given in Table I. The "Two-term Taylor series exact" uses the direct values of c_1 and c_2 given in Table I. This curve represents the best that a two-term Taylor series can do on this problem. It shows the results that the MCNP perturbation capability would produce if it could accurately estimate c_1 and c_2.

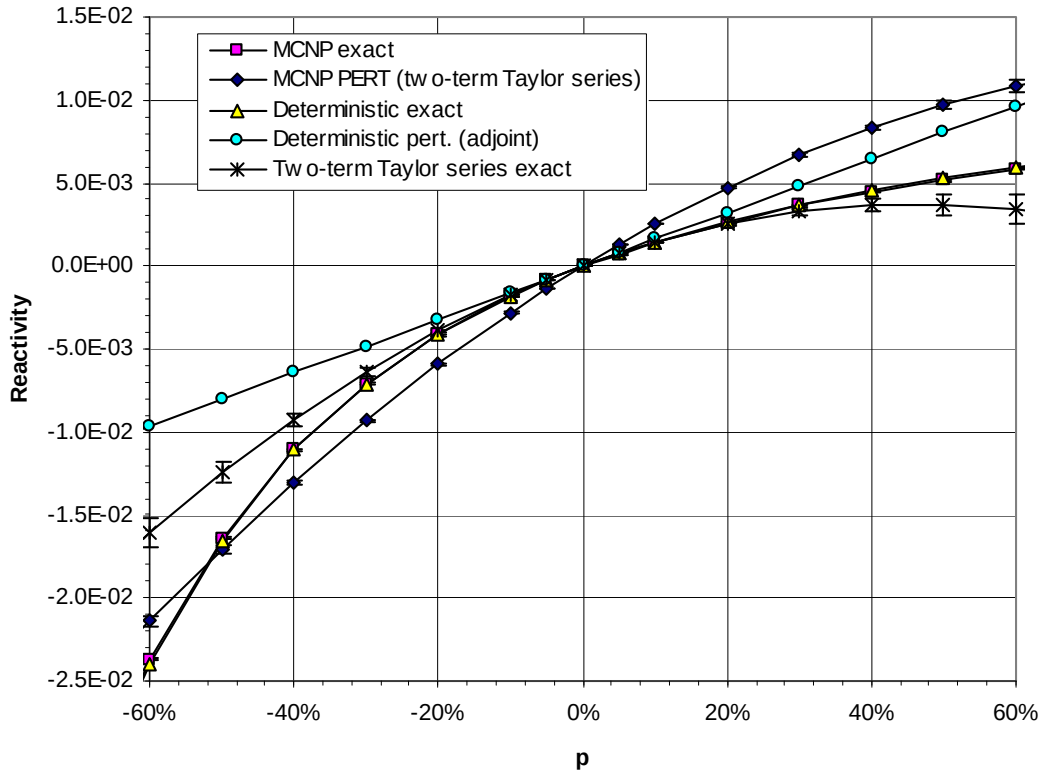

Figure 1. The reactivity worth of the reflector density change as a function of p, the relative change in the reflector density.

The first conclusion to be drawn from Figure 1 is that the MCNP perturbation capability is quite inaccurate for this problem. This conclusion is not surprising given the results for the coefficients in Sec. IV.A. However, if the perturbation capability could accurately estimate the coefficients, it would be fairly accurate out to $p \approx \pm 30\%$.

The second conclusion is that, in fact, if the perturbation capability could accurately estimate the coefficients of the two-term Taylor expansion, the perturbation capability would be more accurate over a wider range of p than the adjoint-based first-order perturbation theory.

This insight suggests that it may be worth putting some work into improving the differential operator method in MCNP and allowing users to choose it instead of (or in addition to) the continuous-energy capability to estimate Δk_{eff}.

VI. Summary and Conclusions

In this paper, the MCNP perturbation capability was tested in a multigroup spherical two-region k_{eff} problem consisting of fuel and reflector. The reflector mass density was perturbed.

Coefficients of a two-term Taylor series expansion for Δk_{eff} were computed using the MCNP perturbation capability and compared with those calculated directly using central-difference formulas. The first-order coefficient (for the linear term) was in error by 66% and the second-order coefficient (for the quadratic term) was in error by –20%.

Coefficients of a two-term Taylor series expansion for the change in the groupwise fluxes in the fuel were computed using the MCNP perturbation capability and compared with those calculated directly using central-difference formulas. For the first-order coefficients, the MCNP perturbation estimate gave values with the wrong sign for 29 of 30 energy groups (indicating a possible bug), and for group 30 and the energy-integrated total, differences between the direct results and the MCNP perturbation results were 62% and 200%, respectively. For the second-order coefficients, the MCNP perturbation estimate was more accurate, being in error by only ~35-60% for most of the groups and ~17% for group 30 and the energy-integrated total.

The differential operator method could be more accurate than standard adjoint-based first-order perturbation theory for Δk_{eff} and the reactivity in this problem if the coefficients could be more accurately estimated. Thus, more work should go into improving the estimates of the coefficients. Keeping the differential operator method as a user option for Δk_{eff} is suggested.

The standard adjoint-based first-order perturbation theory cannot be used for changes in reaction rates, so users are forced to use the differential operator method if reaction rates are of interest to them. Unfortunately, the MCNP perturbation capability failed utterly when asked to estimate the coefficients of a two-term Taylor expansion for the change in groupwise fluxes in the fuel.

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JAF:jaf

Distribution:
A. Sood, XCP-7, MS F663, sooda@lanl.gov
J. S. Hendricks, D-5, MS A143, jxh@lanl.gov
G. W. McKinney, D-5, MS K575, gwm@lanl.gov
R. C. Little, T-DO, MS B259, rcl@lanl.gov
F. B. Brown, XCP-3, MS A143, fbrown@lanl.gov
J. T. Goorley, XCP-3, MS A143, jgoorley@lanl.gov
B. C. Kiedrowski, XCP-3, MS A143, bckiedro@lanl.gov
D. K. Parsons, XCP-5, MS F663, dkp@lanl.gov
J. A. Favorite, XCP-7, MS F663, fave@lanl.gov
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ATTACHMENT 1

All files used in this paper are available electronically from the author.

MCNP INPUT FILE

```
uofl test problem
10    1     -1.0262      -10         imp:n=1
20    2     -2.7         -11 10      imp:n=1
30    3     -0.99705     -12 11      imp:n=1
99    0                      12      imp:n=0

10     so     27.9244
11     so     28.1244
12     so     43.1244

mode n
mgopt f 30
idum 1
rand gen=2 seed=30000000001
kcode 500000   1.    30    530
prdmp j 100
sdef pos=0. 0. 0.  rad=d1  erg=d2
si1  0.  27.9244
sp1  -21 2
sp2  -3
m1   92234 -2.09775E-04 92235 -1.99458E-02 92236 -1.07029E-04
     92238 -1.14305E-03  9019 -3.45810E-03  8016 -8.66328E-01
      1001 -1.08808E-01
m2   13027 -1.0
m3    1001 -1.11916E-01  8016 -8.88084E-01
c
e0    1.390E-10 1.520E-07 4.140E-07 1.130E-06 3.060E-06
      8.320E-06 2.260E-05 6.140E-05 1.670E-04 4.540E-04
      1.235E-03 3.350E-03 9.120E-03 2.480E-02 6.760E-02
      1.840E-01 3.030E-01 5.000E-01 8.230E-01 1.353E+00
      1.738E+00 2.232E+00 2.865E+00 3.680E+00 6.070E+00
      7.790E+00 1.000E+01 1.200E+01 1.350E+01 1.500E+01
      1.700E+01
fc004 flux in the fuel
 f004:n  10
sd004   1.
c
c p=1.
pert202:n cell=30   rho=-1.9941       method=2
pert203:n cell=30   rho=-1.9941       method=3
c
print -30
```

PARTISN INPUT FILE

```
     1     0     0
 uranium oxyfluoride, reflector density
/ * * * * block i * * * *
 igeom=sphere isn= 64 ngroup=  30
 niso=  0 mt= 3 nzone= 3
 im=  3 it= 10831
 t
/ * * * * block ii * * * *
 xmesh= 0.
        2.79244000E+01
        2.81244000E+01
        4.31244000E+01
 xints=   6981  100  3750
 zones=  1
         2
         3
 t
/ * * * * block iii * * * *
 lib=ndilib /fissneut=1
 libname=mendf5 glibname=mendf5g
 lng= 30
 t
/ * * * * block iv * * * *
 matspec=wtfrac;
 matls= m01 "92234.501nm"   0.0002098
            "92235.501nm"   0.0199458
            "92236.501nm"   0.0001070
            "92238.501nm"   0.0011431
            " 9019.501nm"   0.0034581
            " 8016.501nm"   0.8663282
            " 1001.501nm"   0.1088080 ;
        m02 "13027.501nm"   1.0000000 ;
        m03 " 1001.501nm"   0.1119160
            " 8016.501nm"   0.8880840 ;
 assign= zone01   m01    1.02620000 ;
         zone02   m02    2.70000000 ;
         zone03   m03    0.99705000 ;
 t
/ * * * * block v * * * *
 ievt=1  ith=0  isct=4
 epsi= 1.00E-06 norm=1.0
 balp=1
 iitm=999 iitl=0 oitm=9999
/srcacc=no  xsectp=2
 t
/ * * * * block vi * * * *
 zned=1 igrped=3
 ajed=0
 rsfe=  30r 1.
 t
]eof
     1     0     0
uranium oxyfluoride, reflector density, neutron production
/ * * * * block i * * * *
 igeom=sphere isn= 64 ngroup=  30
 niso=  0 mt= 3 nzone= 3
 im=  3 it= 10831
 nosolv=1
 t
/ * * * * block vi * * * *
 zned=1 igrped=3
 ajed=0
 edxs=  nusigf
 resdnt=1
 t
```