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Submitted to:

http://lib-www.lanl.gov/la-pubs/00367167.pdf

M&C 2001 Salt Lake City, Utah, USA, September 2001.

SECOND-ORDER CROSS TERMS IN MONTE CARLO DIFFERENTIAL OPERATOR PERTURBATION ESTIMATES

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Keywords: Perturbations, Monte Carlo, differential operator, Taylor series

ABSTRACT

Given some initial, unperturbed problem and a desired perturbation, a second-order accurate Taylor series perturbation estimate for a Monte Carlo tally that is a function of two or more perturbed variables can be obtained using an implementation of the differential operator method that ignores cross terms, such as in MCNP4C™. This requires running a base case defined to be halfway between the perturbed and unperturbed states of all of the perturbed variables and doubling the first-order estimate of the effect of perturbing from the "midpoint" base case to the desired perturbed case. The difference between such a midpoint perturbation estimate and the standard perturbation estimate (using the endpoints) is a second-order estimate of the sum of the second-order cross terms of the Taylor series expansion. This technique is demonstrated on an analytic fixed-source problem, a Godiva k_{eff} eigenvalue problem, and a concrete shielding problem. The effect of ignoring the cross terms in all three problems is significant.

1. INTRODUCTION

The effect of small perturbations in criticality or fixed-source problems may be difficult to calculate directly using the Monte Carlo method because the inherent statistical uncertainty in the calculation may be larger than the effect of the perturbation for reasonable sample sizes. One Monte Carlo perturbation method is the differential operator (or Taylor series) method (Olhoeft, 1962; Takahashi, 1970; Hall, 1982; Rief, 1984), in which the tally of interest is expressed as a Taylor series expansion about the initial, unperturbed parameters that are to be perturbed. The coefficients and derivatives of the expansion are determined using Monte Carlo methods as the initial, unperturbed tally is computed.

The second- and higher-order terms of a Taylor series expansion of a function of two or more variables include "cross terms" that involve mixed partial derivatives of the function with respect to each of the variables. These cross terms represent the interaction between the perturbations. If none of the variables interact in their influence on the function, then the function can be represented as the sum of Taylor series expansions of the function with respect to each of the variables independently because the cross terms are all zero. This assumption of independently-acting perturbations is a standard feature of common Monte Carlo codes.

However, the importance of the cross terms is difficult to predict. Peplow (2000) found that the cross term for seemingly independent perturbations (the average number of neutrons per fission and the mass density in a one-group k_{eff} eigenvalue problem) was not only non-zero, but important.

Thus, it is important for users of an implementation of the differential operator perturbation method that ignores cross terms to have a way of estimating the importance of this effect. This paper provides such an estimate and demonstrates its use on three sample problems.

2. TAYLOR SERIES EXPANSIONS FOR PERTURBATIONS

Consider a function of two variables, $c(f_1, f_2)$. A Taylor series expansion of $c(f_1, f_2)$ about some initial, unperturbed values $f_{1,0}$ and $f_{2,0}$ is

$$\begin{aligned} c(f_1, f_2) = c(f_{1,0}, f_{2,0}) &+ \left.\frac{\partial c(f_1, f_2)}{\partial f_1}\right|_{\substack{f_1=f_{1,0},\\ f_2=f_{2,0}}} \left(f_1 - f_{1,0}\right) + \left.\frac{\partial c(f_1, f_2)}{\partial f_2}\right|_{\substack{f_1=f_{1,0},\\ f_2=f_{2,0}}} \left(f_2 - f_{2,0}\right) \\ &+ \frac{1}{2}\left[\left.\frac{\partial^2 c(f_1, f_2)}{\partial f_1^{\,2}}\right|_{\substack{f_1=f_{1,0},\\ f_2=f_{2,0}}} \left(f_1 - f_{1,0}\right)^2 + 2\left.\frac{\partial^2 c(f_1, f_2)}{\partial f_1 \partial f_2}\right|_{\substack{f_1=f_{1,0},\\ f_2=f_{2,0}}} \left(f_1 - f_{1,0}\right)\left(f_2 - f_{2,0}\right) \right. \\ &\left. + \left.\frac{\partial^2 c(f_1, f_2)}{\partial f_2^{\,2}}\right|_{\substack{f_1=f_{1,0},\\ f_2=f_{2,0}}} \left(f_2 - f_{2,0}\right)^2 \right] + \cdots \quad , \end{aligned} \tag{1}$$

where the ellipses represent an infinite series of third- and higher-order terms.

Let f_1' and f_2' be specific perturbed values of f_1 and f_2 for which it is desired to estimate the quantity

$$\Delta c(\Delta f_1', \Delta f_2') \equiv c(f_1', f_2') - c(f_{1,0}, f_{2,0}) \quad , \tag{2}$$

where $\Delta f_1' \equiv f_1' - f_{1,0}$ and $\Delta f_2' \equiv f_2' - f_{2,0}$. Using Eq. (1), a second-order Taylor series estimate of $\Delta c(\Delta f_1', \Delta f_2')$ is

$$\Delta c(\Delta f_1', \Delta f_2') = \left.\frac{\partial c(f_1, f_2)}{\partial f_1}\right|_{\substack{f_1 = f_{1,0},\\ f_2 = f_{2,0}}} \Delta f_1' + \left.\frac{\partial c(f_1, f_2)}{\partial f_2}\right|_{\substack{f_1 = f_{1,0},\\ f_2 = f_{2,0}}} \Delta f_2'$$
$$+ \frac{1}{2}\left[\left.\frac{\partial^2 c(f_1, f_2)}{\partial f_1^{\,2}}\right|_{\substack{f_1 = f_{1,0},\\ f_2 = f_{2,0}}} \Delta f_1'^2 + 2\left.\frac{\partial^2 c(f_1, f_2)}{\partial f_1 \partial f_2}\right|_{\substack{f_1 = f_{1,0},\\ f_2 = f_{2,0}}} \Delta f_1' \Delta f_2' \right. \tag{3}$$
$$\left. + \left.\frac{\partial^2 c(f_1, f_2)}{\partial f_2^{\,2}}\right|_{\substack{f_1 = f_{1,0},\\ f_2 = f_{2,0}}} \Delta f_2'^2 \right] .$$

The second-order cross (mixed derivative) term, the middle term in the brackets in Eq. (3), is the subject of this paper.

Let $f_{1,\frac{1}{2}}$ and $f_{2,\frac{1}{2}}$ represent points halfway between the initial, unperturbed points $f_{1,0}$ and $f_{2,0}$ and the desired perturbed points f_1' and f_2':

$$f_{1,\frac{1}{2}} \equiv \frac{1}{2}\left(f_{1,0} + f_1'\right) \tag{4a}$$

and

$$f_{2,\frac{1}{2}} \equiv \frac{1}{2}\left(f_{2,0} + f_2'\right) \quad . \tag{4b}$$

Manipulating Eqs. (4a) and (4b) gives

$$\left(f_{1,0} - f_{1,\frac{1}{2}}\right) = -\left(f_1' - f_{1,\frac{1}{2}}\right) \tag{5a}$$

and

$$\left(f_{2,0} - f_{2,\frac{1}{2}}\right) = -\left(f_2' - f_{2,\frac{1}{2}}\right) \quad . \tag{5b}$$

Define

$$\Delta c(f_1' - f_{1,\frac{1}{2}}, f_2' - f_{2,\frac{1}{2}}) \equiv c(f_1', f_2') - c(f_{1,\frac{1}{2}}, f_{2,\frac{1}{2}}) \quad . \tag{6}$$

A second-order Taylor series estimate of $\Delta c(f_1' - f_{1,\frac{1}{2}}, f_2' - f_{2,\frac{1}{2}})$ is

$$\Delta c(f_1' - f_{1,1/2}, f_2' - f_{2,1/2}) = \left.\frac{\partial c(f_1,f_2)}{\partial f_1}\right|_{\substack{f_1=f_{1,1/2},\\ f_2=f_{2,1/2}}} \left(f_1' - f_{1,1/2}\right) + \left.\frac{\partial c(f_1,f_2)}{\partial f_2}\right|_{\substack{f_1=f_{1,1/2},\\ f_2=f_{2,1/2}}} \left(f_2' - f_{2,1/2}\right)$$

$$+\frac{1}{2}\left[\left.\frac{\partial^2 c(f_1,f_2)}{\partial f_1^{\,2}}\right|_{\substack{f_1=f_{1,1/2},\\ f_2=f_{2,1/2}}} \left(f_1' - f_{1,1/2}\right)^2 + 2\left.\frac{\partial^2 c(f_1,f_2)}{\partial f_1 \partial f_2}\right|_{\substack{f_1=f_{1,1/2},\\ f_2=f_{2,1/2}}} \left(f_1' - f_{1,1/2}\right)\left(f_2' - f_{2,1/2}\right) \right.$$

$$\left. + \left.\frac{\partial^2 c(f_1,f_2)}{\partial f_2^{\,2}}\right|_{\substack{f_1=f_{1,1/2},\\ f_2=f_{2,1/2}}} \left(f_2' - f_{2,1/2}\right)^2 \right] . \qquad (7)$$

Similarly, define

$$\Delta c(f_{1,0} - f_{1,1/2}, f_{2,0} - f_{2,1/2}) \equiv c(f_{1,0}, f_{2,0}) - c(f_{1,1/2}, f_{2,1/2}) \quad . \qquad (8)$$

A second-order Taylor series estimate of $\Delta c(f_{1,0} - f_{1,1/2}, f_{2,0} - f_{2,1/2})$ is

$$\Delta c(f_{1,0} - f_{1,1/2}, f_{2,0} - f_{2,1/2}) = \left.\frac{\partial c(f_1,f_2)}{\partial f_1}\right|_{\substack{f_1=f_{1,1/2},\\ f_2=f_{2,1/2}}} \left(f_{1,0} - f_{1,1/2}\right) + \left.\frac{\partial c(f_1,f_2)}{\partial f_2}\right|_{\substack{f_1=f_{1,1/2},\\ f_2=f_{2,1/2}}} \left(f_{2,0} - f_{2,1/2}\right)$$

$$+\frac{1}{2}\left[\left.\frac{\partial^2 c(f_1,f_2)}{\partial f_1^{\,2}}\right|_{\substack{f_1=f_{1,1/2},\\ f_2=f_{2,1/2}}} \left(f_{1,0} - f_{1,1/2}\right)^2 + 2\left.\frac{\partial^2 c(f_1,f_2)}{\partial f_1 \partial f_2}\right|_{\substack{f_1=f_{1,1/2},\\ f_2=f_{2,1/2}}} \left(f_{1,0} - f_{1,1/2}\right)\left(f_{2,0} - f_{2,1/2}\right) \right.$$

$$\left. + \left.\frac{\partial^2 c(f_1,f_2)}{\partial f_2^{\,2}}\right|_{\substack{f_1=f_{1,1/2},\\ f_2=f_{2,1/2}}} \left(f_{2,0} - f_{2,1/2}\right)^2 \right] . \qquad (9)$$

Subtracting Eq. (9) from Eq. (7) and using Eqs. (2) and (5) yields

$$\Delta c(\Delta f_1', \Delta f_2') = 2\left[\left.\frac{\partial c(f_1,f_2)}{\partial f_1}\right|_{\substack{f_1=f_{1,1/2},\\ f_2=f_{2,1/2}}} \left(f_1' - f_{1,1/2}\right) + \left.\frac{\partial c(f_1,f_2)}{\partial f_2}\right|_{\substack{f_1=f_{1,1/2},\\ f_2=f_{2,1/2}}} \left(f_2' - f_{2,1/2}\right) \right] . \qquad (10)$$

Equation (10) represents an estimate of $\Delta c(\Delta f_1', \Delta f_2')$ of Eq. (2) that is always second-order accurate because the second-order Taylor series term vanishes. Note that the right hand side of Eq. (10) is double the first-order term for the Taylor series estimate of $\Delta c(f_1' - f_{1,½}, f_2' - f_{2,½})$ [the sum of the first two terms on the right hand side of Eq. (7)].

It is easily seen that generalizing Eqs. (1)–(9) for a function of N variables $c(f_1, f_2, \ldots, f_N)$ would yield a second-order accurate estimate of $\Delta c(\Delta f_1', \Delta f_2', \ldots, \Delta f_N')$:

$$\Delta c(\Delta f_1', \Delta f_2', \ldots, \Delta f_N') = 2\Bigg[\frac{\partial c(f_1, f_2, \ldots, f_N)}{\partial f_1}\Bigg|_{\substack{f_1 = f_{1,½},\\ \ldots, f_N = f_{N,½}}} \left(f_1' - f_{1,½}\right) + \frac{\partial c(f_1, f_2, \ldots, f_N)}{\partial f_2}\Bigg|_{\substack{f_1 = f_{1,½},\\ \ldots, f_N = f_{N,½}}} \left(f_2' - f_{2,½}\right) + \cdots + \frac{\partial c(f_1, f_2, \ldots, f_N)}{\partial f_N}\Bigg|_{\substack{f_1 = f_{1,½},\\ \ldots, f_N = f_{N,½}}} \left(f_N' - f_{N,½}\right) \Bigg] \quad . \tag{11}$$

3. SECOND-ORDER ACCURATE PERTURBATION ESTIMATES

Suppose that it is desired to estimate the change in the neutron flux in a homogeneous fixed-source problem due to a change in the material composition. For simplicity, let the material consist of only two isotopes whose relative fractions change realistically in the perturbation (i.e., their fractions must sum to unity). Using the differential operator perturbation technique to estimate the change while computing the initial, unperturbed case, but ignoring the second-order cross (mixed derivative) term [the middle term in the brackets in Eq. (3)], leads to errors.

On the other hand, define a new material having isotopic fractions exactly halfway between their fractions in the original, unperturbed problem and the desired perturbed problem. Let the new material be used in the base case and run a perturbation from that base case to the desired perturbed case. Now, the first-order term in the Taylor series expansion is the term in brackets in Eq. (10). Doubling this term yields a second-order accurate estimate of the change in the neutron flux due to the change to the desired perturbed material composition from the original, unperturbed material composition.

This "midpoint" strategy can be generalized to a tally with more than two simultaneous perturbations, as suggested by Eq. (11).

This strategy has two drawbacks over the standard "endpoint" strategy. First, it can not generally be used to compute a series of perturbations in a single run. Second, and more serious, it requires an additional Monte Carlo calculation (since it is assumed that the initial, unperturbed case will be computed anyway) for the perturbation from the new (midpoint) base case to the desired perturbed case. If two runs are required, why not run the initial, unperturbed case and the desired perturbed case and compute the perturbation directly as the difference, and be done with any perturbation estimates at all?

First, a small difference between direct calculations will be swamped by the statistics of each calculation, so a reliable perturbation estimate may, in fact, be desirable or even necessary. Thus, it may be that the perturbation estimate can be obtained with far less computer time than the direct calculation of the perturbed case would require.

Second, a second-order perturbation estimate can be used in a way that a direct calculation of the perturbation can not: to calculate the missing cross terms. This point is addressed in the Sec. 4.

4. ESTIMATING SECOND-ORDER CROSS TERMS

Assume that a second-order perturbation estimate for a tally is more desirable than a direct estimate because the perturbation estimate is much cheaper to obtain (even though it too requires a separate calculation from the initial, unperturbed case).

One widely used Monte Carlo code with the differential operator perturbation technique that ignores the second-order cross term is MCNP[TM,a], version 4C (Briesmeister, 2000). The MCNP estimate of $\Delta c(\Delta f_1', \Delta f_2')$ of Eq. (3) is

$$\begin{aligned}\Delta c_{MCNP}(\Delta f_1', \Delta f_2') &= \left.\frac{\partial c(f_1, f_2)}{\partial f_1}\right|_{\substack{f_1 = f_{1,0},\\ f_2 = f_{2,0}}} \Delta f_1' + \left.\frac{\partial c(f_1, f_2)}{\partial f_2}\right|_{\substack{f_1 = f_{1,0},\\ f_2 = f_{2,0}}} \Delta f_2' \\ &+ \frac{1}{2} \left.\frac{\partial^2 c(f_1, f_2)}{\partial f_1^2}\right|_{\substack{f_1 = f_{1,0},\\ f_2 = f_{2,0}}} \Delta f_1'^2 + \frac{1}{2} \left.\frac{\partial^2 c(f_1, f_2)}{\partial f_2^2}\right|_{\substack{f_1 = f_{1,0},\\ f_2 = f_{2,0}}} \Delta f_2'^2 \quad ,\end{aligned} \tag{12}$$

the right hand side of which is just the right hand side of Eq. (3) without the cross term in the second-order term. It was proven in Sec. 2 that, through second order, the right hand side of Eq. (10) is equal to the right hand side of Eq. (3); let these expressions be equal to a new symbol, $\Delta c_{2nd\,order}(\Delta f_1', \Delta f_2')$. Then the difference

$$\Delta c_{2nd\,order}(\Delta f_1', \Delta f_2') - \Delta c_{MCNP}(\Delta f_1', \Delta f_2') = \left.\frac{\partial^2 c(f_1, f_2)}{\partial f_1 \partial f_2}\right|_{\substack{f_1 = f_{1,0},\\ f_2 = f_{2,0}}} \Delta f_1' \Delta f_2' \quad . \tag{13}$$

Generalizing Eq. (12) to the case of a function of *N* variables and using arguments for Eq. (11) instead of Eq. (10), Eq. (13) becomes

[a] MCNP is a trademark of the Regents of the University of California, Los Alamos National Laboratory.

$$
\begin{aligned}
&\Delta c_{2nd\,order}(\Delta f_1', \Delta f_2', \ldots, \Delta f_N') - \Delta c_{MCNP}(\Delta f_1', \Delta f_2', \ldots, \Delta f_N') = \\
&\left.\frac{\partial^2 c(f_1, f_2, \ldots, f_N)}{\partial f_1 \partial f_2}\right|_{\substack{f_1 = f_{1,0},\\ \ldots, f_N = f_{N,0}}} \Delta f_1' \Delta f_2' + \left.\frac{\partial^2 c(f_1, f_2, \ldots, f_N)}{\partial f_1 \partial f_3}\right|_{\substack{f_1 = f_{1,0},\\ \ldots, f_N = f_{N,0}}} \Delta f_1' \Delta f_3' \\
&+ \cdots + \left.\frac{\partial^2 c(f_1, f_2, \ldots, f_N)}{\partial f_1 \partial f_N}\right|_{\substack{f_1 = f_{1,0},\\ \ldots, f_N = f_{N,0}}} \Delta f_1' \Delta f_N' \\
&+ \left.\frac{\partial^2 c(f_1, f_2, \ldots, f_N)}{\partial f_2 \partial f_3}\right|_{\substack{f_1 = f_{1,0},\\ \ldots, f_N = f_{N,0}}} \Delta f_2' \Delta f_3' \\
&+ \cdots + \left.\frac{\partial^2 c(f_1, f_2, \ldots, f_N)}{\partial f_2 \partial f_N}\right|_{\substack{f_1 = f_{1,0},\\ \ldots, f_N = f_{N,0}}} \Delta f_2' \Delta f_N' \\
&+ \cdots + \left.\frac{\partial^2 c(f_1, f_2, \ldots, f_N)}{\partial f_{N-1} \partial f_N}\right|_{\substack{f_1 = f_{1,0},\\ \ldots, f_N = f_{N,0}}} \Delta f_{N-1}' \Delta f_N' \quad ,
\end{aligned}
\tag{14}
$$

the sum of all the cross terms.

In other words, a true second-order accurate estimate of the perturbation, obtained using the midpoint method as described in Sec. 3, can be used with a conventional endpoint MCNP perturbation estimate to determine with second-order accuracy the value of the cross terms ignored by MCNP. Thus, it is now no longer necessary to merely assume (and hope!) that the cross terms are small.

One practical use of such an estimate is as follows. Compute the second-order cross term for an endpoint f_1' and f_2' using Eq. (13). Then an estimate of the cross term for a change to arbitrary points f_1 and f_2 between $f_{1,0}$ and $f_{2,0}$ and f_1' and f_2', respectively, is

$$
\text{cross term} \approx \frac{\Delta c_{2nd\,order}(\Delta f_1', \Delta f_2') - \Delta c_{MCNP}(\Delta f_1', \Delta f_2')}{\Delta f_1' \Delta f_2'} \left(f_1 - f_{1,0}\right)\left(f_2 - f_{2,0}\right) \quad . \tag{15}
$$

An MCNP estimate of the perturbation due to a change from $f_{1,0}$ and $f_{2,0}$ to f_1 and f_2 should be more accurate if the cross term of Eq. (15) is added to it. A numerical example of the use of this idea is given in Sec. 5.2. Equation (15) can easily be generalized for a function of more than two variables.

Note that a direct calculation of the perturbation, $\Delta c_{exact}(\Delta f_1', \Delta f_2')$, used instead of $\Delta c_{2nd\,order}(\Delta f_1', \Delta f_2')$ in Eq. (13) yields

$$\Delta c_{exact}(\Delta f_1', \Delta f_2') - \Delta c_{MCNP}(\Delta f_1', \Delta f_2') = \left.\frac{\partial^2 c(f_1, f_2)}{\partial f_1 \partial f_2}\right|_{\substack{f_1 = f_{1,0},\\ f_2 = f_{2,0}}} \Delta f_1' \Delta f_2' \;+\; \cdots \quad , \tag{16}$$

where, as in Eq. (1), the ellipses represents an infinite series of higher-order terms. Comparing the right hand sides of Eqs. (13) and (16), it is evident that to determine the cross term by itself (to second-order accuracy) requires $\Delta c_{2nd\,order}(\Delta f_1', \Delta f_2')$, not $\Delta c_{exact}(\Delta f_1', \Delta f_2')$.

Finally, note that Eq. (13) holds regardless of the accuracy of the second-order Taylor series estimate $\Delta c_{2nd\,order}(\Delta f_1', \Delta f_2')$ with respect to the true perturbed result.

5. EXAMPLE PROBLEMS

5.1. Analytic Two-Isotope Fixed-Source Problem

Consider a material composed of two isotopes with fractions f_1 and f_2 such that $f_1 + f_2 = 1$. Let the atom density of the material be 1 cm^{-3}, and let there be no scattering or fission. Then the total one-group cross section is $\Sigma = 1 \times (f_1\sigma_1 + f_2\sigma_2) = f_1\Sigma_1 + f_2\Sigma_2$. The total flux within a 1-cm slab made of this material due to a monoenergetic beam normally incident on a surface is

$$\begin{aligned}\phi(f_1, f_2) &= \frac{1}{\Sigma}\left(1 - e^{-\Sigma}\right)\\ &= \frac{1}{f_1\Sigma_1 + f_2\Sigma_2}\left(1 - e^{-(f_1\Sigma_1 + f_2\Sigma_2)}\right) \quad .\end{aligned} \tag{17}$$

Using Eq. (17) in Eq. (1), then applying Eq. (2), yields

$$\begin{aligned}\Delta\phi(\Delta f_1', \Delta f_2') = &\left[-\frac{\left(1 - e^{-(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)}\right)}{(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)^2} + \frac{e^{-(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)}}{(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)}\right]\Sigma_1\Delta f_1'\\ &+\left[-\frac{\left(1 - e^{-(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)}\right)}{(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)^2} + \frac{e^{-(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)}}{(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)}\right]\Sigma_2\Delta f_2'\\ &+\frac{1}{2}\left[\frac{2\left(1 - e^{-(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)}\right)}{(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)^3} - \frac{2e^{-(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)}}{(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)^2} - \frac{e^{-(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)}}{(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)}\right]\Sigma_1^{\,2}\Delta f_1'^{\,2}\\ &+\left[\frac{2\left(1 - e^{-(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)}\right)}{(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)^3} - \frac{2e^{-(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)}}{(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)^2} - \frac{e^{-(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)}}{(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)}\right]\Sigma_1\Sigma_2\Delta f_1'\Delta f_2'\\ &+\frac{1}{2}\left[\frac{2\left(1 - e^{-(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)}\right)}{(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)^3} - \frac{2e^{-(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)}}{(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)^2} - \frac{e^{-(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)}}{(f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2)}\right]\Sigma_2^{\,2}\Delta f_2'^{\,2} \quad .\end{aligned} \tag{18}$$

Let the microscopic total cross sections for isotopes 1 and 2 be $\sigma_1 = 3/2$ and $\sigma_2 = 1/2$. Then since the atom density of the mixture is unity, the macroscopic cross sections for isotopes 1 and 2 are $\Sigma_1 = 3/2$ and $\Sigma_2 = 1/2$. Furthermore, if the unperturbed material is composed of half of each isotope,

$$\begin{aligned}\Sigma_0 &= f_{1,0}\Sigma_1 + f_{2,0}\Sigma_2 \\ &= \frac{1}{2}\cdot\frac{3}{2} + \frac{1}{2}\cdot\frac{1}{2} \\ &= 1 \quad .\end{aligned} \tag{19}$$

Now let the perturbed material be composed of 40% of isotope 1 and 60% of isotope 2. Then

$$\begin{aligned}\Sigma' &= f_1'\Sigma_1 + f_2'\Sigma_2 \\ &= 0.4\cdot\frac{3}{2} + 0.6\cdot\frac{1}{2} \\ &= 0.9 \quad .\end{aligned} \tag{20}$$

In this case, $\Delta f_1' = 0.4 - 0.5 = -0.1$ and $\Delta f_2' = 0.6 - 0.5 = 0.1$.

The sum of the first-order terms for isotopes 1 and 2 for [the first and second terms on the right hand side of Eq. (18)] is

$$\left(-1 + 2e^{-1}\right)\left(\frac{3}{2}\right)(-0.1) + \left(-1 + 2e^{-1}\right)\left(\frac{1}{2}\right)(0.1) = 0.0264241 \quad . \tag{21}$$

The sum of the pure second-derivative terms for isotopes 1 and 2 [the third term plus the fifth term on the right hand side of Eq. (18)] is

$$\frac{1}{2}\left(2 - 5e^{-1}\right)\left(\frac{3}{2}\right)^2(-0.1)^2 + \frac{1}{2}\left(2 - 5e^{-1}\right)\left(\frac{1}{2}\right)^2(0.1)^2 = 0.00200753 \quad . \tag{22}$$

The second-order cross term for $\Delta\phi(-0.1, 0.1)$ [the fourth term on the right hand side of Eq. (18)] is

$$\left(2 - 5e^{-1}\right)\left(\frac{3}{2}\cdot\frac{1}{2}\right)(-0.1)(0.1) = -0.00120452 \quad . \tag{23}$$

The sum of all three second-order terms is

$$\frac{1}{2}\left[\left(\frac{3}{2}\right)^2 + \left(\frac{1}{2}\right)^2 - \left(\frac{3}{2}\right)\right]\left(2 - 5e^{-1}\right)(0.1)^2 = 0.000803014 \quad . \tag{24}$$

The second-order Taylor series estimate of $\Delta\phi(-0.1,0.1)$ is the sum of all the terms, or 0.0272271. The exact analytic value of $\Delta\phi(-0.1,0.1)$ is, using Eq. (17),

$$\frac{1}{0.9}\left(1-e^{-0.9}\right)-\left(1-e^{-1}\right)=0.0272465 \quad . \tag{25}$$

This problem was run with MCNP4C using a one-group cross section library made for the fictitious materials. The unperturbed total flux within the slab was given by an F4 tally with ~ 198 million histories to be 0.632135 ± 0.00%. (The analytic result is 0.632121.) Perturbed tally results are shown in Table 1. The agreement of the computed first-order term with the analytic value [from Eq. (21)] is excellent, but the agreement of the second-order term with the analytic value [from Eq. (24)] is not good because the cross term is ignored in the MCNP calculation. On the other hand, the agreement of the second-order term with the analytic value for the sum of the second derivatives [from Eq. (22)] is excellent.

Table 1. Standard results for $\Delta\phi(-0.1,0.1)$.

Taylor series term	MCNP4C	Analytic
First-order	0.026426 ± 0.02%	0.026424
Second-order	0.002008 ± 0.03%	0.000803
Sum of first- and second-order	0.028434 ± 0.02%	0.027227
Exact (analytic)	N/A	0.027247

The analytic column of Table 1 shows that the first two terms in the Taylor series expansion make up 99.9% of the exact (infinite Taylor series) value. Thus, the absence of third- and higher-order terms from the MCNP calculation leads to inappreciable errors. The missing cross term is the cause of the entire error of 4.4%.

Use of the midpoint method of Sec. 3 enables MCNP4C to obtain second-order accurate results for this material composition perturbation. Define a base case material to contain 45% of isotope 1 ($\sigma = 1.5$) and 55% of isotope 2 ($\sigma = 0.5$), in addition to the previously defined materials of 50% of each isotope (initial, unperturbed problem) and 40% of isotope 1 and 60% of isotope 2 (perturbed case of interest). Table 2 shows the results for the flux (F4 tally) when ~ 476 million histories are run. In this case, the first-order term is itself second-order accurate because it is essentially a numerical first derivative evaluated at the midpoint of two points.

Using Eq. (17) in Eq.(10) with $f_{1,1/2}=0.45$, $f_{2,1/2}=0.55$, $f_1'=0.5$, and $f_2'=0.6$ yields an analytic midpoint result of 0.02724155. This result is compared with the others in Table 2. Comparing the analytic second-order Taylor series estimates (the sum of the first- and second-order terms) for the endpoint and the midpoint methods, it is clear that some of the greater accuracy seen in the differential operator (MCNP4C) midpoint results over the standard endpoint results of Table 1 is due to the fact that the first derivatives in the midpoint method are estimated at an optimal location, halfway between the unperturbed case and each of the perturbed cases.

Table 2. Midpoint results for $\Delta\phi(-0.1,0.1)$.

Taylor series term	"Midpoint" MCNP4C result	Standard (endpoint) analytic	Midpoint analytic
First-order	0.0272416 ± 0.01%	0.026424	0.027242
Second-order	0.0	0.000803	0.0
Sum of first- and second-order	0.0272416 ± 0.01%	0.027227	0.027242
Exact (analytic)	N/A	0.027246	0.027246

This implies that the higher-order terms are smaller for the midpoint method than for the standard method. Indeed, it can be proven that the leading error term, the third-order term, is about four times greater in the standard method than in the midpoint method. (And in Table 2, the error in the endpoint analytic second-order Taylor series estimate is about four times the error in the midpoint result.) How big is this effect compared with the missing second-order cross term? Obviously very small in this simple problem, as Table 2 shows. In general it is expected to be very small, since it is a third-order rather than a second-order effect, but this is an issue that still needs to be addressed.

These results may also be used to estimate the cross term directly. The second-order accurate MCNP estimate of $\Delta\phi(-0.1,0.1)$ of Table 2 minus the MCNP estimate of $\Delta\phi(-0.1,0.1)$ of Table 1 is –0.001192, an excellent estimate of the analytic value of –0.001205 of Eq. (23).

5.2. Godiva Composition Perturbation

The Godiva composition perturbation problem used in the MCNP4C perturbation verification of Hess (1998) was redone. This is a k_{eff} eigenvalue problem in which the composition of the Godiva spherical assembly was perturbed from its original 94.73% ^{235}U and 5.27% ^{238}U to 50% by weight of each isotope. Three intermediate compositions were also calculated. As in Hess (1998), all MCNP KCODE calculations used an initial k_{eff} guess of unity, 20 settle cycles, 200 active cycles, 3000 particles per cycle, and current default cross sections. The k_{eff} eigenvalue for the initial, unperturbed case was 0.99831 ± 0.08%.

Results are shown in Table 3. The second column of Table 3 shows the standard MCNP4C perturbation estimates, which were computed in a single KCODE run of the initial, unperturbed case. The third column of Table 3 shows the estimates obtained using the "midpoint" method of Eq. (10) and Sec. 3; this column required four runs, one for each perturbation. The fourth column of Table 3 shows the reference result obtained by running a KCODE calculation for each case (including the initial, unperturbed case, for a total of five runs) and subtracting. All of these results are also plotted in Fig. 1.

Table 3. Results for the Godiva composition perturbation.

^{238}U weight fraction	MCNP4C result	"Midpoint" MCNP4C result	Reference calculation
0.13	–0.04279 ± 2.0%	–0.04098 ± 0.86%	–0.04298 ± 2.52%
0.26	–0.12719 ± 2.8%	–0.11690 ± 0.67%	–0.11671 ± 0.93%
0.38	–0.21896 ± 3.6%	–0.19568 ± 0.52%	–0.19505 ± 0.51%
0.50	–0.32403 ± 4.3%	–0.27776 ± 0.44%	–0.28381 ± 0.34%

Most of the error in the standard MCNP4C perturbation results is not due to the second-order estimate (i.e., the absence of third- and higher-order terms), but rather to the absence of the cross term in the second-order term. When the cross term is included, as it is in the "Midpoint" estimate of Fig. 1 and Table 3, the second-order Taylor series is quite accurate to better than 20% Δk_{eff}.

The only approximations left in the "Midpoint" curve of Fig. 1 are the absence of third- and higher-order terms in the Taylor series expansion and the inherent assumption that the perturbation does not alter the fission neutron source.

The missing cross term for the largest perturbed case can be computed to second-order accuracy using Eq. (13) to be 0.04627 ± 30% [the uncertainty is, as usual, the

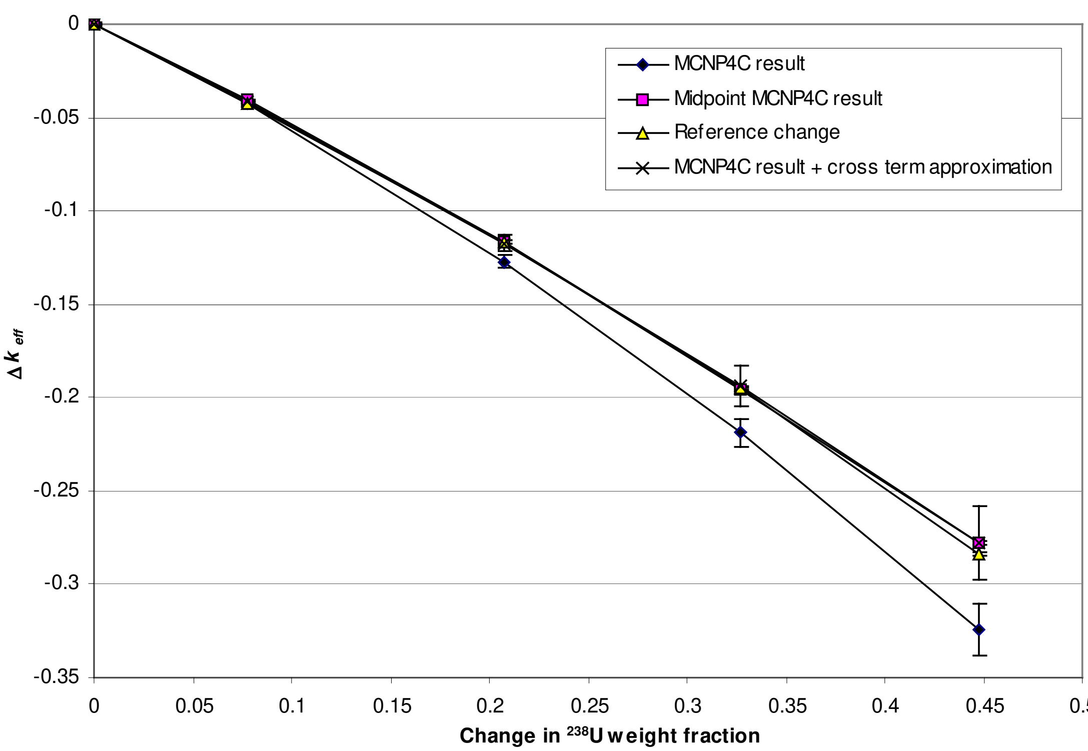

Fig. 1 Δk_{eff} for a Godiva composition change. The cross term approximation of Eq. (15) has been added; it lies on top of the Midpoint MCNP4C PERT curve. Error bars of one standard deviation are shown.

square root of the sum of the squares of the standard deviations of the two terms on the left hand side of Eq. (13)]. Despite the low precision, this value can be used in Eq. (15) to estimate the missing cross term for each of the other perturbed cases. This estimate of the cross term can be added to the standard MCNP4C estimate (the second column of Table 3) for an approximate second-order Taylor series perturbation estimate. The resulting curve is plotted on Fig. 1. The new curve lies almost on top of the midpoint method curve, but the standard deviation is greater.

Thus, second-order accurate perturbation estimates can be obtained with only two Monte Carlo calculations: one for the initial, unperturbed case, where standard second-order (no cross term) perturbations are estimated for all desired cases, and another for the midpoint between the initial, unperturbed case and the endpoint perturbed case, with one standard first-order only perturbation estimated for the perturbation from the midpoint to the endpoint.

A word on the statistical uncertainties of Table 3 is in order. Although it is generally expected that the perturbation methods would yield lower uncertainties than the direct difference method, in this problem the uncertainties in the standard MCNP4C perturbation results are large because the uncertainties of the second-order term are much larger than those of the first-order term. This is a bit unexpected, though it has been seen before (Hess, 1998). The uncertainty of the midpoint method is therefore much smaller than that of the standard method since the midpoint method does not use the second-order terms [c.f. Eq. (10)]. Note that the uncertainty of the midpoint method actually increases as the perturbation decreases, suggesting that it may be unbounded for small perturbations. However, the midpoint method is just a refinement of the standard Taylor series method whose variance is known to be bounded; as the perturbation decreases, the variance of the midpoint method converges to the (bounded) variance of the standard method (within the statistics of the two different Monte Carlo calculations). This has yet to be proven mathematically.

5.3. Shielding Concrete Composition Perturbation

A shielding calculation involving a point source within a spherical concrete shield has also been performed. The source is an isotropic 2.4-MeV neutron source. The sphere has a radius of 30 cm (~ 1 foot). It is desired to determine the leakage for two different concrete compositions (Harmon, 1994), one used by criticality safety engineers at Los Alamos National Laboratory (LANL) and the other used by criticality safety engineers at Oak Ridge National Laboratory (ORNL). The composition of each of the concretes and that of the "midpoint" concrete are given in Table 4. All three concretes had a density of 2.25 g/cm^3 and the current MCNP default cross sections were used for each isotope. The leakage through each concrete is also given in Table 4. Leakage calculations for the LANL, ORNL, and midpoint concretes used an F1 tally with ~ 4.5 million, ~ 2.2 million, and ~ 3.1 million particle histories, respectively (hydrogen slows the calculation!).

From Table 4, a perturbation from the initial, unperturbed case of the LANL concrete to the ORNL concrete causes a change in the leakage of –0.205905 $\pm$ 0.11%.

Table 4. Concrete compositions (mass fractions).

Element/ Isotope	LANL concrete	ORNL concrete	Midpoint concrete
^{1}H	0.00453	0.01000	0.007265
^{16}O	0.51260	0.53200	0.52230
Si	0.36036	0.33700	0.34868
^{27}Al	0.03555	0.03400	0.034775
^{23}Na	0.01527	0.02900	0.022135
Ca	0.05791	0.04400	0.050955
Fe	0.01378	0.01400	0.01389
Leakage	0.912068 ± 0.01%	0.706163 ± 0.03%	0.814627 ± 0.02%

The results of perturbation calculations involving these concretes are shown in Table 5. A standard perturbation estimate of the change from the LANL to the ORNL concrete is in error by 11.6%, while an estimate using the midpoint method is in error by 2.1%.

Table 5. Results for concrete composition perturbation.

Taylor series term	MCNP4C result (LANL → ORNL)	Midpoint result (Midpoint → ORNL – Midpoint → LANL)
First-order	–0.171040 ± 0.67%	–0.210168 ± 0.35%
Second-order	–0.0588281 ± 6.12%	0.0 ± 0.0%
Sum of first- and second-order	–0.229868 ± 1.63%	–0.210168 ± 0.35%
Error in sum	0.023963 ± 15.7%	0.004263 ± 18.1%

Obviously, it is of no benefit to use the midpoint perturbation method in this problem because it is just as expensive to compute the perturbed case (use of the ORNL concrete) directly. However, it is instructive to examine the cross term, which, to second order from Eq. (14), is 0.019700 ± 19%. (Note that the cross term in this case is actually a sum of 21 terms!) This cross term is one-third the magnitude but opposite the sign of the sum of the pure second derivatives computed by MCNP (the second-order term of Table 5), and its absence leads to ~ 9.5% of the error of the PERT estimate. Presumably, the other ~ 2.1% of the error is due to the neglect of third- and higher-order terms.

6. CONCLUSIONS

In this paper, we have demonstrated a method for using MCNP4C to obtain a true second-order Taylor series perturbation estimate of a tally that is a function of two or more perturbed variables. We have shown how such an estimate can be used to obtain a second-order accurate estimate of the second-order cross terms that are ignored by the MCNP4C perturbation feature. Unfortunately, the second-order perturbation estimate requires an additional MCNP calculation that may be quite expensive. However, the estimate of the cross term can be used in an interpolation scheme to improve a series of standard MCNP4C perturbation estimates. In addition, it may be desired to know what effect the absence of the cross term has on a particular problem or class of problems. This note provides a means of assessing the effect by estimating the missing cross term.

It is clear that the method developed in this paper could easily be extended to apply to third- and higher-order Taylor series perturbation methods, but this extension has yet to be developed.

One point of further interest is to examine the third- and higher-order Taylor series terms to understand how accurate the second-order estimate of the cross term is with respect to the second-order estimate of a perturbation using the standard "endpoint" method. Such an effort would lead to insight on how much of the error of the endpoint method is due to the absence of third- and higher-order terms (i.e., the second-order estimate) and how much of the error is due to the absence of the second-order cross terms.

More future work involves studying the variance of the midpoint method, as discussed in Sec. 5.2, and using multi- and one-group fixed-source and k_{eff} eigenvalue problems with analytic solutions. These problems are invaluable aids in evaluating code approximations, and it is generally possible, as in this paper, to generalize them to more realistic problems.

NOMENCLATURE

$c(f_1, f_2)$ a general function of two variables

ϕ total neutron flux in a volume

k_{eff} standard measure of neutron multiplication or criticality; eigenvalue of the Boltzmann transport equation

σ, Σ microscopic and macroscopic total neutron cross section, respectively

Subscripts

1, 2, …, N indices for a set of variables

0 the initial, unperturbed case

½ the "midpoint" case, halfway between the initial, unperturbed case and the desired or endpoint perturbed case

MCNP an estimate of a perturbed tally that uses the differential operator method without including the cross terms, as in the computer code MCNP

2nd order an estimate of a perturbed tally that uses the differential operator method that does include the cross terms

exact a direct calculation of a perturbed tally

Superscripts

′ (prime) the desired perturbed or endpoint case

ACKNOWLEDGMENTS

The authors would like to thank Dr. Avneet Sood for valuable discussions and for bringing to their attention the work of Peplow (2000).

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