Using the MCNP Taylor series perturbation feature (efficiently) for shielding problems

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Abstract. The Taylor series or differential operator perturbation method, implemented in MCNP and invoked using the PERT card, can be used for efficient parameter studies in shielding problems. This paper shows how only two PERT cards are needed to generate an entire parameter study, including statistical uncertainty estimates (an additional three PERT cards can be used to give exact statistical uncertainties). One realistic example problem involves a detailed helium-3 neutron detector model and its efficiency as a function of the density of its high-density polyethylene moderator. The MCNP differential operator perturbation capability is extremely accurate for this problem. A second problem involves the density of the polyethylene reflector of the BeRP ball and is an example of first-order sensitivity analysis using the PERT capability. A third problem is an analytic verification of the PERT capability.

1 Introduction

The Taylor series or differential operator perturbation feature [1, 2] was introduced into MCNP [3] in version 4B in the mid-1990s. The perturbation feature has been shown to be unreliable for estimating perturbations in eigenvalue (k_{eff}) problems [4, 5]. However, for fixed-source (shielding) problems, the perturbation feature can be extremely accurate and deserves to be more widely used. The Taylor series perturbation feature is invoked with the PERT card.

In publications until now [e.g., 2], a separate MCNP PERT card was used for each perturbed point in a parameter study. In fact, the MCNP manual [3] recommends two PERT cards for each perturbation so that the first- and second-order Taylor terms can be examined independently. The manual says that "each perturbation increases running time by 10%-20%" [3]. Limiting the number of PERT cards is therefore desirable.

This paper shows how to compute the two coefficients of a two-term Taylor expansion using only two PERT cards. These coefficients can then be used to estimate the perturbed response for *any* point in a parameter study. The statistical uncertainty can be well estimated from these two PERT cards; it can be computed exactly using three more PERT cards.

In addition, this paper shows how to use the PERT card to perform first-order sensitivity analysis such as may be used in uncertainty quantification.

We emphasize that the results of this paper apply only to fixed-source problems, *not* eigenvalue problems.

2 Taylor series coefficients

A Taylor series expansion of a response c that is a function of some reaction cross section σ_x is

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

where $\sigma_{x,0}$ is the reference value of the cross section and

$$\Delta\sigma_x \equiv \sigma_x - \sigma_{x,0}. \quad (2)$$

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

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

and

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

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

$$p_x \equiv \frac{\Delta\sigma_x}{\sigma_{x,0}}. \quad (5)$$

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

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

and

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

For notational convenience, define $c_0 \equiv c(\sigma_{x,0})$.

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3 Taylor series coefficients and the MCNP PERT card

3.1 Computing the coefficients

At present, the MCNP perturbation capability, invoked with the PERT card, uses a two-term Taylor expansion with no cross terms [6, 3]. The perturbation feature estimates the derivatives in Eqs. (6) and (7) and multiplies them by the relative perturbation p_x (or p_x^2) computed from the user input.

Define coefficients

$$c_1 \equiv \left.\frac{dc}{dp_x}\right|_{p_x=0} \tag{8}$$

and

$$c_2 \equiv \left.\frac{1}{2}\frac{d^2c}{dp_x^2}\right|_{p_x=0}. \tag{9}$$

These coefficients can be computed from any single arbitrary reference perturbation amount $p_{x,r}$ using, from Eqs. (6) and (7),

$$c_1 = \frac{\Delta c_1(p_{x,r})}{p_{x,r}} \tag{10}$$

and

$$c_2 = \frac{\Delta c_2(p_{x,r})}{p_{x,r}^2}. \tag{11}$$

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

$$c_{\text{PERT}}(p_x) = c_0 + c_1 p_x + c_2 p_x^2. \tag{12}$$

Equation (12) [with Eqs. (10) and (11)] is the main conclusion of this paper. With this equation, a parameter study can be done for any number of perturbed values of the parameter with only two MCNP PERT cards, rather than the two PERT cards per perturbation that are recommended in the manual. A detailed prescription is given in Sec. 4.

3.2 Approximate uncertainty

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

$$s_{c_1} = \frac{s_{\Delta c_1}}{\left|p_{x,r}\right|} \tag{13}$$

and

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

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 [meaning $\Delta c_1(p_{x,r})$ and $\Delta c_2(p_{x,r})$ here and in the rest of this paper]. The standard deviation of the unperturbed tally c_0 is s_{c_0}. With these quantities, the variance of the estimated perturbed tally of Eq. (12), estimated by assuming that c_0, Δc_1, and Δc_2 are uncorrelated (subscript "*unc.*"), is

$$s^2_{c_{\text{PERT},unc.}} = s^2_{c_0} + s^2_{c_1} p_x^2 + s^2_{c_2} p_x^4. \tag{15}$$

3.3 Exact uncertainty

Typically, and in the prescription given in Sec. 4, c_0, Δc_1, and Δc_2 are all computed from the same set of histories in the same cells. They are likely to be highly correlated. The effect of the correlations among c_0, Δc_1, and Δc_2 on the variance $s^2_{c_{\text{PERT}}}$ can be computed exactly.

The covariance matrix for c_{PERT} is

$$\underline{\underline{C}} = \begin{bmatrix} s^2_{c_0} & \rho_{c_0\Delta c_1} & \rho_{c_0\Delta c_2} \\ \rho_{c_0\Delta c_1} & s^2_{\Delta c_1} & \rho_{\Delta c_1\Delta c_2} \\ \rho_{c_0\Delta c_2} & \rho_{\Delta c_1\Delta c_2} & s^2_{\Delta c_1} \end{bmatrix}, \tag{16}$$

where the covariances are

$$\rho_{xy} \equiv r_{xy} s_x s_y, \tag{17}$$

where the correlation coefficients are

$$r_{xy} \equiv \frac{N\sum(x_i y_i) - \left(\sum x_i\right)\left(\sum y_i\right)}{\sqrt{\left[N\sum x_i^2 - \left(\sum x_i\right)^2\right]\left[N\sum y_i^2 - \left(\sum y_i\right)^2\right]}}, \tag{18}$$

where N is the number of histories sampled and x_i and y_i are the x and y scores for the ith history.

We now find the correlation coefficient r_{xy} in terms of x, y, and z, where $z = x + y$. The variance in a Monte Carlo estimate of z, implicitly accounting for correlations in x and y, is

$$\begin{aligned} s_z^2 &= \frac{1}{N^2}\sum z_i^2 - \frac{1}{N^3}\left(\sum z_i\right)^2 \\ &= \frac{1}{N^2}\sum(x_i + y_i)^2 - \frac{1}{N^3}\left(\sum(x_i + y_i)\right)^2 \\ &= \frac{1}{N^2}\left(\sum x_i^2 + \sum y_i^2 + 2\sum(x_i y_i)\right) \\ &\quad - \frac{1}{N^3}\left[\left(\sum x_i\right)^2 + \left(\sum y_i\right)^2 + 2\left(\sum x_i\right)\left(\sum y_i\right)\right]. \end{aligned} \tag{19}$$

The variance in a Monte Carlo estimate of the sum $x + y$, *not* accounting for correlations in x and y, is

$$\begin{aligned} s^2_{x+y} &= s_x^2 + s_y^2 \\ &= \frac{1}{N^2}\left(\sum x_i^2 + \sum y_i^2\right) - \frac{1}{N^3}\left[\left(\sum x_i\right)^2 + \left(\sum y_i\right)^2\right]. \end{aligned} \tag{20}$$

Using Eq. (20) in Eq. (19) yields

$$s_z^2 = s^2_{x+y} + \frac{2}{N^3}\left[N\sum(x_i y_i) - \left(\sum x_i\right)\left(\sum y_i\right)\right]. \tag{21}$$

Rearranging Eq. (21) and using the result in Eq. (18) [with the first line of Eq. (19), replacing z with x and y] yields

$$\begin{aligned} r_{xy} &= \frac{\frac{N^3}{2}\left(s_z^2 - s^2_{x+y}\right)}{\sqrt{\left(N^3 s_x^2\right)\left(N^3 s_y^2\right)}} \\ &= \frac{s_z^2 - s^2_{x+y}}{2 s_x s_y}, \end{aligned} \tag{22}$$

and using the first line of Eq. (20) yields

$$r_{xy} = \frac{s_z^2 - s_x^2 - s_y^2}{2 s_x s_y}. \tag{23}$$

Equation (23) will be applied for $(x, y) \in (c_0, \Delta c_1, \Delta c_2)$ and $z \in (c_0 + \Delta c_1, c_0 + \Delta c_2, \Delta c_1 + \Delta c_2)$. Using Eq. (23) in Eq. (17) yields

$$\rho_{xy} = \tfrac{1}{2}(s_z^2 - s_x^2 - s_y^2). \tag{24}$$

The sensitivity vector for c_{PERT} [from Eq. (12) with Eqs. (10) and (11)] is

$$\underline{S} = \left[\frac{\partial c_{\text{PERT}}}{\partial c_0}, \frac{\partial c_{\text{PERT}}}{\partial \Delta c_1}, \frac{\partial c_{\text{PERT}}}{\partial \Delta c_2} \right]^T$$

$$= \left[1, \frac{p_x}{p_{x,r}}, \left(\frac{p_x}{p_{x,r}} \right)^2 \right]^T. \tag{25}$$

where superscript T indicates the transpose.

Using the "sandwich rule," the total variance in c_{PERT} is

$$s_{c_{\text{PERT}}}^2 = (\underline{S})^T \underline{\underline{C}}(\underline{S}). \tag{26}$$

Using Eqs. (15), (16), (24), and (25), Eq. (26) becomes

$$s_{c_{\text{PERT}}}^2 = s_{c_{\text{PERT},unc.}}^2 + \left(s_{c_0+\Delta c_1}^2 - s_{c_0}^2 - s_{\Delta c_1}^2 \right) \left(\frac{p_x}{p_{x,r}} \right)$$

$$+ \left(s_{c_0+\Delta c_2}^2 - s_{c_0}^2 - s_{\Delta c_2}^2 \right) \left(\frac{p_x}{p_{x,r}} \right)^2 \tag{27}$$

$$+ \left(s_{\Delta c_1+\Delta c_2}^2 - s_{\Delta c_1}^2 - s_{\Delta c_2}^2 \right) \left(\frac{p_x}{p_{x,r}} \right)^3.$$

4 Prescription for perturbations

4.1 Basic

The prescription to estimate a response c for any number of perturbations of a parameter p_x is as follows:

Choose a reference perturbation $p_{x,r}$; a convenient choice is $p_{x,r} = 1$.

Set up two PERT cards with the density equal to [from Eqs. (2) and (5)] $\sigma_{x,r} = \sigma_{x,0}(1 + p_{x,r})$. Obviously, if $p_{x,r} = 1$, then $\sigma_{x,r} = 2\sigma_{x,0}$. One PERT card uses METHOD = 2 and the other uses METHOD = 3.

Run the problem using MCNP.

The METHOD = 2 perturbation result is $\Delta c_1(p_{x,r}) \pm s_{\Delta c_1}$; use Eq. (10) to compute c_1. The METHOD = 3 perturbation result is $\Delta c_2(p_{x,r}) \pm s_{\Delta c_2}$; use Eq. (11) to compute c_2. Compute the standard deviations using Eqs. (13) and (14).

A practically continuous curve of $c_{\text{PERT}}(p_x)$ can now be created using Eq. (12) with uncertainties estimated using Eq. (15).

4.2 Checking accuracy

As stated in the manual, it is a good idea to test whether a second-order Taylor expansion is accurate for the largest perturbation that is expected. One way to do this is to compare the first- and second-order terms $c_1 p_x$ and $c_2 p_x^2$ with the total $c_{\text{PERT}}(p_x)$, as suggested in the manual. This can be done for all values of p_x used in the analysis without additional PERT cards. From Eq. (12), the ratio of the second-order term to the first-order term is

$$\frac{\text{2nd}}{\text{1st}} = \frac{c_2 p_x^2}{c_1 p_x} = \frac{c_2}{c_1} p_x, \tag{28}$$

which is linear with the relative perturbation.

However, contrary to statements in the manual, it is not always true that the second-order term should contribute much less to the total than the first-order term. For example, consider the notional curve shown in Fig. 1. The base case of $\sigma_0 = 2$ is at or near the optimum for response R. The first-order Taylor term is zero or close to zero, and the second-order term dominates. Higher-order terms may be zero. Caution is advised.

Where possible, it is wise to use a direct calculation of the perturbed tally to test $c_{\text{PERT}}(p_x)$ for the maximum values of $\pm|p_x|$ that are of interest.

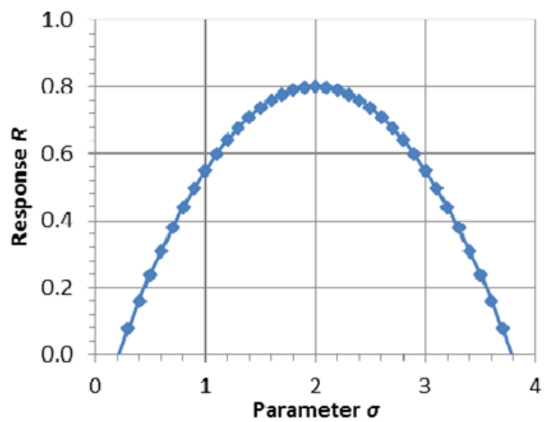

Fig. 1. Notional graph of a response R as a function of a parameter σ; $\sigma_0 = 2$.

4.3 Exact uncertainty

Exact uncertainties that account for the correlations among c_0, Δc_1, and Δc_2 can be computed as follows:

Set up three more PERT cards in addition to those set up in Sec. 4.1 (with the same density as in Sec. 4.1). One of the new PERT cards uses METHOD = –2, one uses METHOD = –3, and one uses METHOD = 1.

Run the problem using MCNP.

The METHOD = –2 perturbation result is $c_0 + \Delta c_1(p_{x,r}) \pm s_{c_0+\Delta c_1}$. The METHOD = –3 perturbation result is $c_0 + \Delta c_2(p_{x,r}) \pm s_{c_0+\Delta c_2}$. The METHOD = 1 perturbation result is $\Delta c_1(p_{x,r}) + \Delta c_2(p_{x,r}) \pm s_{\Delta c_1+\Delta c_2}$.

Exact uncertainties may now be computed using Eqs. (15) and (27). Note that the perturbation results for METHOD = –2, –3, and 1 are not used; only the corresponding uncertainties are used.

5 Prescription for first-order sensitivity analysis

5.1 Basic

The first-order relative sensitivity coefficient of a response c to some reaction cross section σ_x is defined as

$$S_{c,\sigma_x} \equiv \frac{\sigma_{x,0}}{c_0} \frac{dc}{d\sigma_x}\bigg|_{\sigma_{x,0}} . \tag{29}$$

Using $\sigma_x = \sigma_{x,0}(1+p_x)$ in Eq. (29) with the chain rule yields

$$S_{c,\sigma_x} = \frac{1}{c_0} \frac{dc}{dp_x}\bigg|_{p_x=0} , \tag{30}$$

or, from Eq. (8),

$$S_{c,\sigma_x} = \frac{c_1}{c_0} . \tag{31}$$

The prescription to estimate the first-order sensitivity coefficient is now clear: Follow the prescription of Sec. 4.1 to compute c_1, and divide the result by the unperturbed response c_0. The estimated variance of the sensitivity coefficient, assuming c_0 and c_1 are uncorrelated (subscript "*unc.*"), is

$$s^2_{S_{unc.}} = S^2_{c,\sigma_x} \left[\left(\frac{s_{c_0}}{c_0} \right)^2 + \left(\frac{s_{c_1}}{c_1} \right)^2 \right] . \tag{32}$$

Equation (13) gives s_{c_1}. In this approximation, only METHOD = 2 is required.

5.2 Exact uncertainty

The sensitivity vector for S_{c,σ_x} [from Eq. (31) with Eq. (10)] is

$$\underline{S} = \left[\frac{\partial S_{c,\sigma_x}}{\partial c_0}, \frac{\partial S_{c,\sigma_x}}{\partial \Delta c_1} \right]^T = \left[\frac{-\Delta c_1}{p_{x,r} c_0^2}, \frac{1}{p_{x,r} c_0} \right]^T . \tag{33}$$

The covariance matrix for S_{c,σ_x} is

$$\underline{\underline{C}} = \begin{bmatrix} s^2_{c_0} & \rho_{c_0 \Delta c_1} \\ \rho_{c_0 \Delta c_1} & s^2_{\Delta c_1} \end{bmatrix} , \tag{34}$$

with

$$\rho_{c_0 \Delta c_1} = \tfrac{1}{2} (s^2_{c_0+\Delta c_1} - s^2_{c_0} - s^2_{\Delta c_1}) , \tag{35}$$

as in Sec. 3.3. Using Eq. (26) (the sandwich rule) and Eqs. (31) and (32), the total variance of the sensitivity coefficient is

$$s^2_S = s^2_{S_{unc.}} - \left(s^2_{c_0+\Delta c_1} - s^2_{c_0} - s^2_{\Delta c_1} \right) \left(\frac{S^2_{c,\sigma_x}}{c_0 \Delta c_1} \right) . \tag{36}$$

In this case, as in Sec. 4.3, the METHOD = 2 result gives $s_{\Delta c_1}$, and a PERT card with METHOD = –2 is needed to give $s_{c_0+\Delta c_1}$.

6 Numerical examples

6.1 Neutron detector polyethylene density

As an example, consider a detailed model of a neutron detector consisting of 15 helium-3 tubes with an active height of 15 in. (Fig. 2) and pressure of 10 atm. arranged in three rows in a high-density polyethylene (HDPE) moderator (Fig. 3). The nominal density of the HDPE is

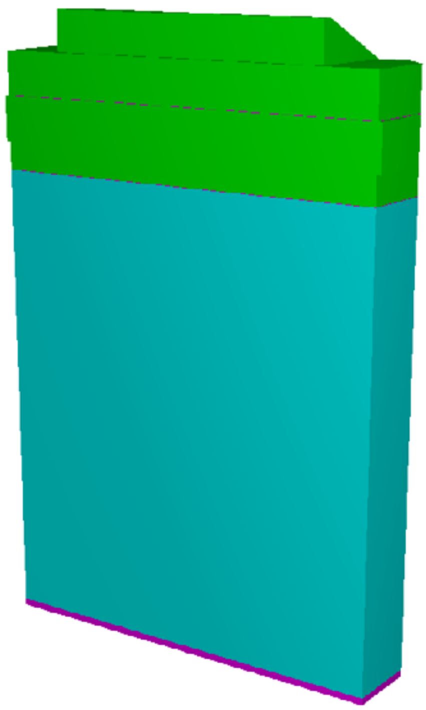

Fig. 2. Three-dimensional rendering of the neutron detector. The light blue material is HDPE, within which are arranged the helium-3 tubes. The height of the HDPE is 16.59 in.

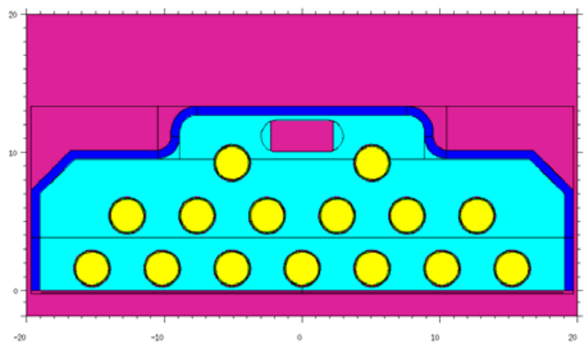

Fig. 3. Cross section of the neutron detector. The light blue material is HDPE, yellow is helium-3, and pink is air. Scales in centimeters.

taken to be 0.962 g/cm^3. How does the response of the detector change as the HDPE density changes?

An Am-Be source was modeled 30 cm from the front face of the detector and centered vertically with respect to the active height of the tubes. Detector counts were modeled as captures in helium-3 in the active part of the tubes.

The total efficiency as a function of HDPE density is plotted in Fig. 4. (The total efficiency is the number of counts per source particle emitted, and for this calculation it is not necessary to specify the source strength.) Seven direct calculations (using perturbed densities) as well as the unperturbed (reference) direct result are compared with a second-order Taylor series estimate computed using coefficients calculated during the run of the unperturbed reference case. Uncertainties for the Taylor series estimates are the uncorrelated estimates of Eq. (15). Figure 4 shows that the Taylor series estimate of the MCNP PERT card provides an extremely accurate and fast method for performing this sensitivity study.

Adding the two PERT cards increased the run time by 6%.

Including all correlations among the Taylor series coefficients changes the standard deviation from 4.67 × 10^{-6} to 4.43 × 10^{-6} for the largest negative perturbation and from 4.42 × 10^{-6} to 4.49 × 10^{-6} for the largest positive perturbation. Adding three more PERT cards increased the run time (from the case with two PERT cards) by only 5%.

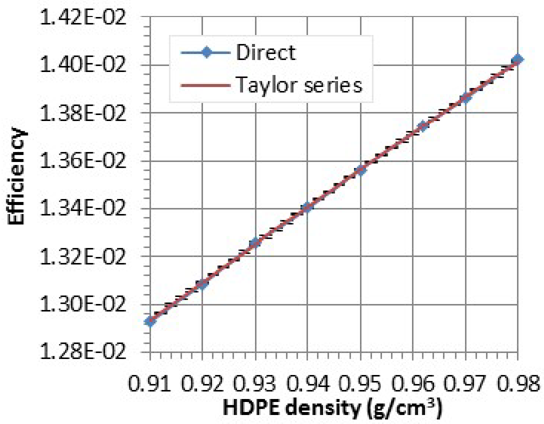

Fig. 4. Efficiency for the neutron detector.

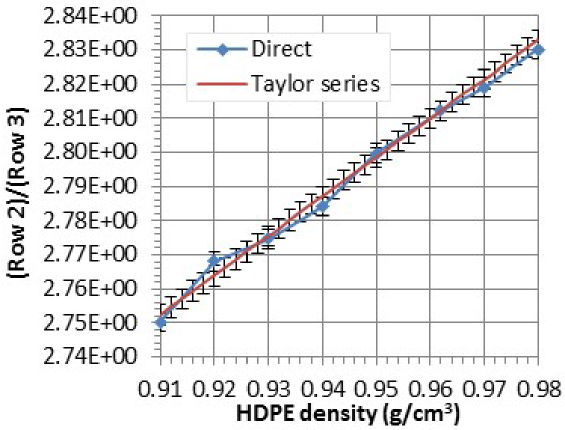

Fig. 5. Row ratio for the neutron detector.

The advantage of a continuous parameter study is not apparent in Fig. 4 since the direct results are relatively easy to acquire. However, another quantity of interest for the neutron detector is the "row ratio," or the ratio of the sum of the counts in the second, third, fourth, and fifth tubes in the middle row (called row 2) to the sum of the counts in the two tubes in the back row (called row 3, the top row in Fig. 3).

Figure 5 shows the row ratio for the seven perturbed configurations and the unperturbed reference case. Statistical uncertainty causes "wiggle" in the curve through the points.

The Taylor series estimate, also shown on Fig. 5, was obtained as the ratio of the individual Taylor series estimates for the count rates for rows 2 and 3. Uncertainties for the Taylor series estimates use the uncorrelated estimate of Eq. (15) for each row.

Including all correlations among the Taylor series coefficients changes the standard deviation from 3.10 × 10^{-3} to 2.99 × 10^{-3} for the largest negative perturbation and from 2.85 × 10^{-3} to 2.88 × 10^{-3} for the largest positive perturbation.

Comparing the contributions of the first- and second-order terms, as suggested in the MCNP manual [3], can easily be done for each perturbed point using Eq. (12).

6.2 Neutron reflector polyethylene density

This problem illustrates the use of the PERT card for the sensitivity of a response to the mass density of a neutron reflector. The response is the total neutron leakage from a spherical system. The system is the polyethylene-reflected BeRP ball [7, 8] described in Table 1. The density of the polyethylene is perturbed.

Table 1. BeRP ball geometry and materials.

Material	Outer Radius (cm)	Density (g/cm^3)
α-Pu	3.794	19.6
NO Gas Fill	3.82829	0.00129
Steel	3.85879	7.62
Polyethylene	11.47879	0.95

The exact leakage for each perturbation is compared with the first- and second-order Taylor series perturbation estimates in Fig. 6. Error bars of one standard deviation are present but not visible. The second-order estimate of Eq. (12) produces the correct curvature near the unperturbed density (0.95 g/cm^3), but it is too large for negative density perturbations and too small for positive density perturbations. A higher-order

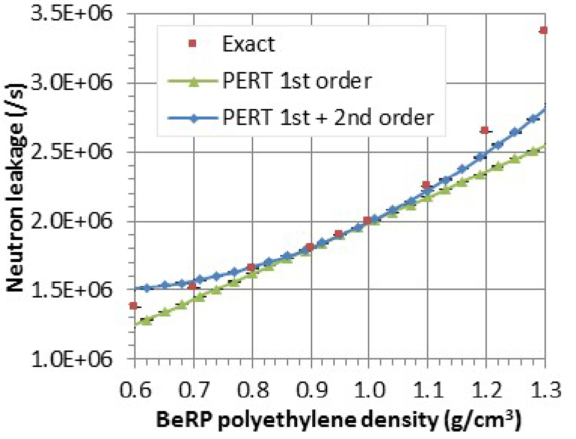

Fig. 6. Neutron leakage as a function of BeRP polyethylene density.

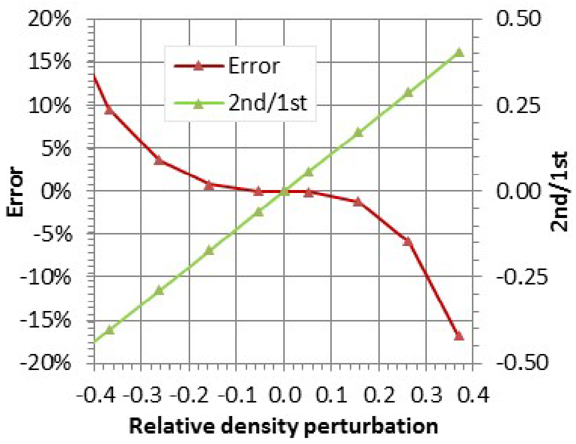

Fig. 7. Error in the second-order perturbation estimate and ratio of second-order term to first-order term for the BeRP ball problem.

Taylor expansion is needed for more accuracy in the range of perturbations shown.

The error is quantified in Fig. 7 and presented with the ratio of the second-order term to the first-order term, as given by Eq. (28). For this problem, the error is within ±10% when the ratio is –0.40 to 0.33.

We turn now to the first-order sensitivity of the leakage to the polyethylene density, computed using Eq. (31). The first-order PERT method is compared with central-difference estimates computed using

$$S_{c,\rho}^{CD} \approx \frac{\rho_0}{c_0}\left(\frac{c(\rho_0+h)-c(\rho_0-h)}{2h}\right), \tag{37}$$

where h is the change made in the density to compute the central difference. It is important to choose the perturbation h small enough that the points $c(\rho_0-h)$, c_0, and $c(\rho_0+h)$ are on a line but large enough that the difference $c(\rho_0+h)-c(\rho_0-h)$ can be calculated accurately [9], and, if a Monte Carlo code is used, with a small uncertainty. Central-difference estimates using Eq. (37) with different values of h and MCNP results for c are shown in Table 2 with Monte Carlo relative uncertainties (1s). The difference between the PERT

Table 2. Sensitivity of neutron leakage to polyethylene density.

Method	h (g/cm^3)	Sensitivity (%/%)	Diff. w.r.t. PERT (Ns)(a)
PERT	N/A	0.9270 ± 0.23%	N/A
Central Diff.	0.05	0.9370 ± 0.32%	1.94
Central Diff.	0.15	0.9949 ± 0.11%	20.7
Central Diff.	0.25	1.136 ± 0.07%	69.4

(a) Number of standard deviations of difference.

estimate and the central-difference estimate is shown in terms of the number of standard deviations of difference.

The central-difference estimate using the smallest value of h (0.05 g/cm^3) is just within 2s of the first-order PERT value of the sensitivity. Which is the more accurate value? The three points of the sensitivity are not exactly on a line: The Pearson correlation coefficient for the points is 0.9994. In our judgment, the PERT value is the most accurate.

6.3 Analytic monodirectional one-group slab

This problem applies the PERT card to the reaction rate inside a slab when there is a monodirectional source and no scattering. The solution is analytic, so this is a good verification problem for the PERT capability.

A boundary source of strength q impinges on the left, at x = 0 cm, and the width of the slab is X. The macroscopic cross section is Σ. The flux $\phi(x)$ at any point x within the slab is

$$\phi(x) = qe^{-\Sigma x} \tag{38}$$

and the total reaction rate R within the slab is

$$\begin{aligned} R &= \int_0^X dx\Sigma\phi(x) \\ &= \int_0^X dx\Sigma q e^{-\Sigma x} \\ &= q\left(1-e^{-\Sigma X}\right). \end{aligned} \tag{39}$$

The cross section Σ is perturbed a relative amount p; in accordance with Eq. (5), we write the cross section as

$$\Sigma = \Sigma_0(1+p). \tag{40}$$

Using Eq. (40) in Eq. (39), the reaction rate is

$$R = q\left(1-e^{-\Sigma_0(1+p)X}\right). \tag{41}$$

From Eq. (41), the first derivative of R with respect to p is

$$\frac{\partial R}{\partial p} = q\Sigma_0 X e^{-\Sigma_0(1+p)X}. \tag{42}$$

The second derivative is

$$\frac{\partial^2 R}{\partial p^2} = -q(\Sigma_0 X)^2 e^{-\Sigma_0(1+p)X}. \tag{43}$$

The derivatives evaluated at p = 0 are

$$\left.\frac{\partial R}{\partial p}\right|_{p=0} = q\Sigma_0 X e^{-\Sigma_0 X} \tag{44}$$

and

$$\left.\frac{\partial^2 R}{\partial p^2}\right|_{p=0} = -q(\Sigma_0 X)^2 e^{-\Sigma_0 X}. \quad (45)$$

The two-term Taylor series expansion is

$$R_{TS}(p) = R_0 + \left.\frac{\partial R}{\partial p}\right|_{p=0} p + \frac{1}{2}\left.\frac{\partial^2 R}{\partial p^2}\right|_{p=0} p^2$$
$$= R_0 + R_1 p + R_2 p^2, \quad (46)$$

where R_1 and R_2 are c_1 and c_2 of Eqs. (8) and (9).

We now apply the parameters of Table 3 to this problem. Analytic values of R_0, R_1, and R_2 [from Eqs. (41), (44), and (45), respectively] are shown in Table 4 and compared with values computed using MCNP. R_0 is, of course, a regular reaction-rate cell tally. R_1 and R_2 were computed using the PERT card as discussed in Sec. 4.1. The differences between the MCNP results and the analytic values are well within one standard deviation.

A parameter study is shown in Fig. 8. The exact reaction rate, from Eq. (41), is compared with the two-term Taylor series of Eq. (46) when the coefficients are computed analytically and when the coefficients are from the MCNP PERT capability. The two curves for the Taylor series are indistinguishable. Figure 8 shows that a two-term Taylor expansion is extremely accurate for cross-section perturbations of ±10% for this problem; beyond that, higher-order terms may be needed.

Figure 9 quantifies these observations, showing the error in the second-order PERT estimate as well as the ratio of the second- to the first-order Taylor term. For this problem, even when the second-order term is about the same size as the first-order term, the error in the Taylor series estimate is less than 0.6%.

Table 3. Parameters of the analytic slab problem.

Parameter	Value
q	1.0 cm^{-2}s^{-1}
X	1.0 cm
Σ_0	5.2 cm^{-1}

Table 4. Coefficients of the Taylor expansion.

Coefficient[(a)]	Analytic	MCNP PERT	N_S[(b)]
R_0 (s^{-1})	0.994483	0.994428 ± 0.01%	0.57
R_1 (s^{-1})	0.0286861	0.0287011 ± 0.83%	0.06
R_2 (s^{-1})	–0.0745840	–0.0746330 ± 0.48%	0.14

(a) The right side of Eq. (39) is multiplied by a unit area, making the units work out to s^{-1}.
(b) Number of standard deviations of difference.

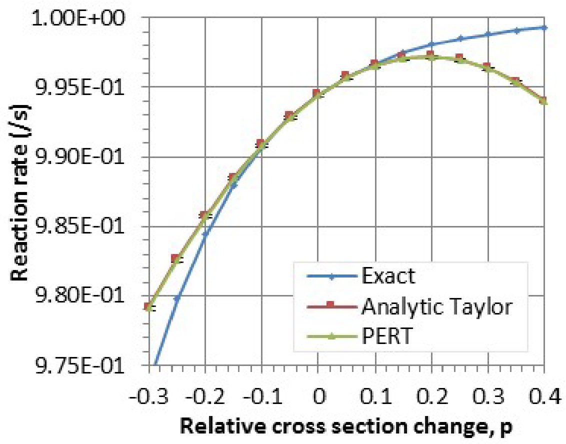

Fig. 8. Exact reaction rate and Taylor series estimates for the analytic problem.

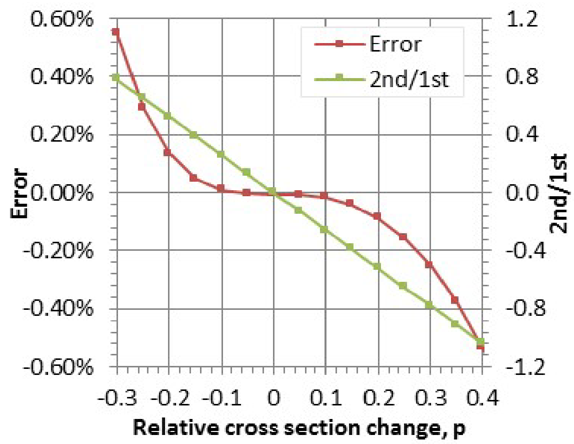

Fig. 9. Error in the second-order perturbation estimate and ratio of second-order term to first-order term for the analytic problem.

7 Summary and conclusions

The MCNP perturbation capability can be extremely accurate for shielding problems. This paper has demonstrated that it is not necessary to use a PERT card (or two PERT cards) for every perturbed point in a parameter study. Just two PERT cards suffice to obtain the Taylor series coefficients, generate a near-continuous curve of the resulting perturbed response, and estimate the statistical uncertainty in the perturbed response.

This paper has focused on cross-section and density perturbations. Material-substitution perturbations require special treatment [6], but it might be possible to apply the methods of this paper. On the other hand, the first-order sensitivity of a response to material composition changes can be computed using the first-order sensitivity to each of the individual nuclide densities, computed as described in Sec. 5. This topic is receiving new attention [10, 11].

The run times for the test problem of Sec. 6.1 increased by only ~20% of the rule of thumb quoted in the manual [3].

The PERT card must not be used to perturb problem parameters that would cause the source spatial, spectral, or angular distribution to be perturbed.

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