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**On the Accuracy of the Differential Operator Monte Carlo Perturbation Method for Eigenvalue Problems**

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**INTRODUCTION**

The differential operator Monte Carlo perturbation method [1, 2] can be used to estimate $k_{eff}$ eigenvalue perturbations and sensitivities in MCNP5 [3]. However, the method was originally developed for fixed-source problems in which the perturbation does not affect the source, and its application to eigenvalue problems must be made cautiously [4–6]. Recently [6, 7], it was observed that the differential operator method in MCNP5 had some trouble with scattering cross section perturbations compared with other cross section perturbations. This paper attempts to explain the differences using an approach that was previously presented [5].

**THE $k_{eff}$-EIGENVALUE AND THE DIFFERENTIAL OPERATOR METHOD**

Consider the one-group homogeneous transport equation with isotropic scattering,

$$\hat{\mathbf{\Omega}} \cdot \vec{\nabla} \psi(r,\hat{\mathbf{\Omega}}) + \Sigma_t(r)\psi(r,\hat{\mathbf{\Omega}}) - \Sigma_s(r)\phi(r)$$
$$= \frac{1}{k_{eff}} \nu\Sigma_f(r)\phi(r). \tag{1}$$

The notation is standard and vacuum boundary conditions are assumed. The scalar flux is $\phi(r) \equiv \int_{4\pi} d\hat{\mathbf{\Omega}} \psi(r,\hat{\mathbf{\Omega}})$. The total cross section is

$$\Sigma_t(r) = \Sigma_c(r) + \Sigma_f(r) + \Sigma_s(r). \tag{2}$$

Whether Eq. (1) is solved with Monte Carlo or deterministic methods, the following discussion is valid. Let the flux be normalized to

$$\int dV\, \nu\Sigma_f(r)\phi(r) = k_{eff}. \tag{3}$$

Define the fission source as $S(r) \equiv \nu\Sigma_f(r)\phi(r)$. When the fission source distribution is converged and the flux is normalized as in Eq. (3), then the inhomogeneous equation

$$L\psi(r,\hat{\mathbf{\Omega}}) = \hat{\mathbf{\Omega}} \cdot \vec{\nabla}\psi(r,\hat{\mathbf{\Omega}}) + \Sigma_t(r)\psi(r,\hat{\mathbf{\Omega}}) - \Sigma_s(r)\phi(r)$$
$$= S(r) \tag{4}$$

has the same solution as the homogeneous equation [Eq. (1)], and this solution satisfies the normalization of Eq. (3). Note that the transport operator $L$ of Eq. (4) does not include the fission source, but the total cross section does include fission; thus, in Eq. (4), fission is treated as capture.

One way of thinking about Monte Carlo estimates of $k_{eff}$ is that "inactive cycles" are used to converge the fission source, then "active cycles" are run as fixed-source problems to estimate tallies (the quoted terminology is MCNP's). The $k_{eff}$ eigenvalue can be estimated as a track-length flux tally, as in Eq. (3).

In the differential operator Monte Carlo perturbation method, the tally (in this case, $k_{eff}$) is expanded in a Taylor series about the initial, unperturbed parameter. For example, for a cross-section perturbation, $\Delta k_{eff}$ is estimated using

$$\Delta k_{eff,DO}(\Delta\Sigma_x) = \frac{\partial k_{eff}}{\partial\Sigma_x}\bigg|_{\Sigma_{x,0}} (\Delta\Sigma_x) +$$
$$\frac{1}{2}\frac{\partial^2 k_{eff}}{\partial\Sigma_x^2}\bigg|_{\Sigma_{x,0}} (\Delta\Sigma_x)^2 + \cdots, \tag{5}$$

where subscript $DO$ indicates the differential operator estimate, subscript 0 indicates initial, unperturbed quantities, and $\Delta X = X' - X_0$, with a prime indicating perturbed quantities.

The derivatives in Eq. (5) are calculated during active cycles using the normal neutron histories. Contributions are scored based on what the neutrons might have done if the cross section were $\Sigma_x'$ rather than $\Sigma_{x,0}$. Thus, the unperturbed fission source is used, but the goal is to estimate the effect of the perturbed transport operator.

To summarize, the initial, unperturbed system satisfies

$$L_0\psi_0(r,\hat{\mathbf{\Omega}}) = S_0(r), \tag{6}$$

where the source is the converged, properly normalized fission source. The perturbed system satisfies

$$L'\psi'(r,\hat{\mathbf{\Omega}}) = S'(r). \tag{7}$$

The exact value of the eigenvalue perturbation is

$$\Delta k_{eff} = \int dV\, \nu\Sigma'_f(r)\phi'(r) - \int dV\, \nu\Sigma_{f,0}(r)\phi_0(r). \qquad (8)$$

The differential operator estimate of the eigenvalue perturbation is

$$\Delta k_{eff,DO} = \int dV\, \nu\Sigma'_f(r)\widetilde{\phi}(r) - \int dV\, \nu\Sigma_{f,0}(r)\phi_0(r), \qquad (9)$$

where

$$L'\widetilde{\psi}(r,\hat{\mathbf{\Omega}}) = S_0(r). \qquad (10)$$

For later convenience, define $\widetilde{k}$ to be the first term on the right side of Eq. (9): $\widetilde{k} \equiv \int dV\, \nu\Sigma'_f(r)\widetilde{\phi}(r)$.

Assuming that the Taylor expansion order is sufficient and that necessary cross terms are included, the accuracy of the differential operator method is limited only by the assumption that the fission source is unperturbed. However, the issue is not only whether $S_0(r)$ is a good approximation of $S'(r)$ [Eq. (10)], but, more importantly, whether $\widetilde{\psi}(r,\hat{\mathbf{\Omega}})$ is a good approximation of $\psi'(r,\hat{\mathbf{\Omega}})$ [Eq. (9)].

This analysis of the differential operator method as applied to $k_{eff}$-eigenvalue problems has been presented previously [5]. In this paper, the first numerical demonstration is given. This demonstration was developed to understand why the differential operator method was less accurate for computing the sensitivity of $k_{eff}$ with respect to scattering cross sections than to capture cross sections [6, 7].

**TEST PROBLEM AND RESULTS**

The one-group $k_{eff}$ test problem is a homogeneous spherical fuel region (radius 6.12745 cm) surrounded by a spherical reflector shell (thickness 3.063725 cm). It is problem 16 from [8]. The macroscopic cross sections are listed in Table I. Scattering is isotropic. This problem was also used in [6]. Using 30 000 neutrons per cycle, 20 inactive cycles, and 300 active cycles, the MCNP5 track-length value of $k_{eff}$ was $0.999916 \pm 0.0000675$. Using a mesh spacing of 0.004 cm and $S_{128}$ quadrature, the PARTISN [9] value of $k_{eff}$ was 1.0000128.

Fuel capture and fuel scattering cross section perturbations were considered (independently). For perturbations to the capture cross section, Eq. (10) is

TABLE I. Test Problem Cross Sections.

| Material | $\nu$ | $\Sigma_f$ (cm$^{-1}$) | $\Sigma_c$ (cm$^{-1}$) | $\Sigma_s$ (cm$^{-1}$) | $\Sigma_t$ (cm$^{-1}$) |
|---|---|---|---|---|---|
| Fuel[a] | 2.797101 | 0.065280 | 0.013056 | 0.248064 | 0.32640 |
| Reflector[b] | 0.0 | 0.0 | 0.032640 | 0.293760 | 0.32640 |

[a] U-235 (b), Table 9 [8].
[b] H$_2$O (refl), Table 9 [8].

$$L_0\widetilde{\psi}(r,\hat{\mathbf{\Omega}}) + \Delta\Sigma_c(r)\widetilde{\psi}(r,\hat{\mathbf{\Omega}}) = S_0(r), \qquad (11)$$

and for perturbations to the scattering cross section, Eq. (10) is

$$L_0\widetilde{\psi}(r,\hat{\mathbf{\Omega}}) + \Delta\Sigma_s(r)\left[\widetilde{\psi}(r,\hat{\mathbf{\Omega}}) - \widetilde{\phi}(r)\right] = S_0(r). \qquad (12)$$

Results for a –20% perturbation in the fuel capture cross section and a +5% perturbation in the fuel scattering cross section (independently) are shown in Table II. The first four rows were computed using PARTISN. The sixth row ($\Delta k_{eff,DO}$) was computed using the differential operator method with a second-order Taylor expansion (via the PERT card in MCNP5). The error in $\Delta k_{eff,DO}$ was computed by comparing with the PARTISN value of $\Delta k_{eff}$, which introduces a slight inconsistency.

TABLE II. Perturbation Results.

|  | $\Sigma_c$ Pert. | $\Sigma_s$ Pert. |
|---|---|---|
| $k'_{eff}$ | 1.0130141 | 1.0069433 |
| $\widetilde{k}$ | 1.0132118 | 1.0060818 |
| $k'_{eff} - k_{eff,0}$ | 0.0130013 | 0.0069305 |
| $\widetilde{k} - k_{eff,0}$ | 0.0131990 | 0.0060690 |
| Error | 1.52% | –12.43% |
| $\Delta k_{eff,DO}$ | $0.0131810 \pm 0.01\%$ | $0.0060493 \pm 0.12\%$ |
| Error | 1.38% | –12.71% |

Note that $k_{eff}$ is much more sensitive to the fuel scattering cross section than to the fuel capture cross section, since a 5% change in the former has about half the effect of a –20% change in the latter.

Although the $\Sigma_s$ perturbation is smaller than the $\Sigma_c$ perturbation and has a smaller effect on $k_{eff}$, the differential operator method is much less accurate at predicting the effect.

However, in both cases, the differential operator method very accurately estimates $\widetilde{k} - k_{eff,0}$. This result *suggests* the correctness of both the analysis of the preceding section and the differential operator implementation in MCNP5, but it does not *prove* either.

Perturbed fluxes $\phi'(r)$ and $\widetilde{\phi}(r)$ are plotted in Figs. 1 and 2 for each problem. For readability, the fluxes are plotted as differences from the unperturbed flux $\phi_0(r)$.

For comparision, the maximum unperturbed flux (at $r = 0$ cm) is $9.745 \times 10^{-3}$ cm$^{-2}$s$^{-1}$. The flux shift $[\phi'(r) - \phi_0(r)]/\phi_0(r)$ at r = 0 cm is 1.12% for the capture cross section perturbation and 1.52% for the scattering cross section perturbation.
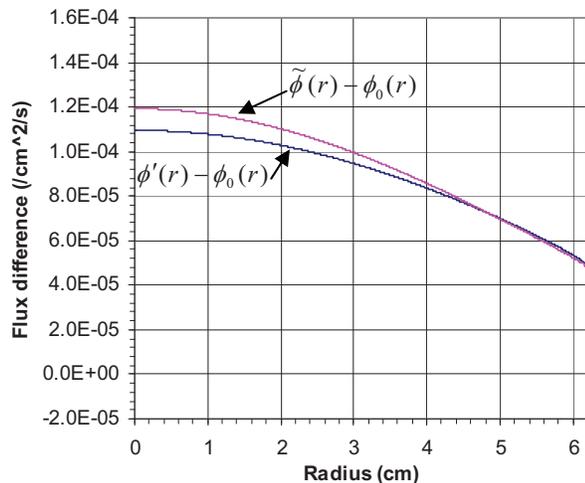
Fig. 1. Fluxes for the capture cross section perturbation.



Fig. 2. Fluxes for the scattering cross section perturbation.

The exact perturbed flux distribution $\phi'(r)$ more closely approximates the unperturbed flux distribution $\phi_0(r)$ for the capture cross section perturbation than for the scattering cross section perturbation (the difference is flatter). In addition, $\tilde{\phi}(r)$ more closely matches $\phi'(r)$ for the capture cross section perturbation than for the scattering cross section perturbation.

**CONCLUSIONS**

The notion that the differential operator method works by essentially solving the inhomogeneous transport equation with a perturbed transport operator and an unperturbed fission source [Eq. (10)] and using the resulting flux $\tilde{\phi}(r)$ to estimate $\Delta k_{eff}$ [Eq. (9)] has been demonstrated in a numerical test problem solved deterministically and with Monte Carlo. MCNP5 has more trouble estimating $\Delta k_{eff}$ due to scattering cross section perturbations than capture cross section perturbations because $\tilde{\phi}(r)$ differs more significantly from $\phi'(r)$ when the scattering cross section is perturbed, even when the effect on $\Delta k_{eff}$ is smaller.

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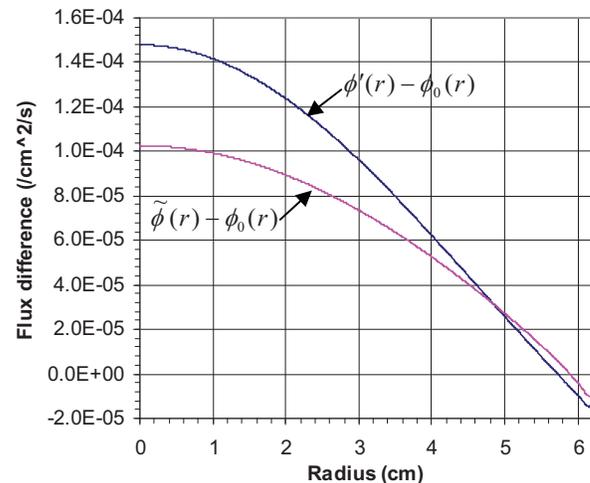3. X-5 MONTE CARLO TEAM, "MCNP–A General Monte Carlo N-Particle Transport Code, Version 5," Chap. 2, Vol. I, LA–UR–03–1987, Los Alamos National Laboratory (April 24, 2003).
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