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DISTRIBUTION IN MCNP

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ESTIMATION OF CHANGE IN k_{eff} DUE TO PERTURBED FISSION SOURCE DISTRIBUTION IN MCNP

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ABSTRACT

The Monte Carlo perturbation method based on the differential operator sampling method has been widely used to obtain a small change in neutronic parameters or sensitivity. The method is very effective for fixed-source problems but a difficulty arises for eigenvalue problems because the fission source distribution (eigenfunction) is perturbed. Most Monte Carlo codes assume that the source distribution is unchanged after a perturbation is introduced. However, this assumption can lead to a significant error in the perturbation estimate. Recently, a method to estimate the perturbed fission source effect has been proposed. In this method, the additional weights for the differential coefficient of the fission source at fission sites are normalized in each cycle, and the effect is estimated by propagating the normalized additional weight between cycles. The method has been implemented into MCNP5 and verified with simple benchmark problems including homogeneous and localized perturbation cases. The conventional MCNP perturbation estimates are significantly improved by taking into account the effect estimated with the method in all the cases. The method is, thus, effective not only for a homogeneous perturbation case but also a localized perturbation case, though the statistical uncertainties tend to be large. In addition, it has been verified that the method is applicable to Monte Carlo codes with the normalization scheme used in MCNP.

Key Words: Monte Carlo, perturbation, eigenvalue, differential operator sampling method, MCNP

1. INTRODUCTION

MCNP[1] has the perturbation capability based on the differential operator sampling method and calculates the differential coefficients up to the second order. This capability is becoming more useful for reactor physicists because they can obtain not only sensitivities to neutronic parameters with the first-order differential coefficients but also the change in the parameters such as reactivity worth, etc. with the Taylor series expansion of the change in regard to a perturbation. However, attention must be paid to the limitations that originate from approximations in the perturbation formulation.

The method implemented in MCNP involves only two approximations for fixed-source problems. The third-order and higher terms of the differential coefficients are neglected as the first approximation. Furthermore, the second-order cross terms are neglected as the second approximation. Since these

approximations are not very important in practical applications, the method is actually very efficient for most fixed-source problems and the effectiveness has been well verified[2, 3]. There are some cases where the cross terms become important[4, 5] but Favorite showed that the second-order cross terms can be estimated with the midpoint strategy[5].

On the other hand, an additional approximation is present for eigenvalue problems. MCNP assumes that the fission source distribution does not change, even if a perturbation is introduced into the system. (In other words, it is assumed that the fundamental eigenfunction in the system is constant, regardless of the perturbation.) Therefore the perturbation effect due to the fission source change has not been taken into account in MCNP. This effect can become significant if a locally large perturbation is introduced. Even for a uniform perturbation, the effect accounts for a few percent of the total change in some cases[6].

Recently, one of the authors proposed a method to evaluate the effect due to the perturbed fission source distribution. He also showed that the change in k_{eff} was significantly improved by taking the effect into account, and that the method was applicable not only for uniform but also localized perturbations[6].

In this work, we have implemented the method into a beta version of MCNP Version 5 (MCNP5)[7] and have verified the effectiveness of the method with simple benchmark problems described in Reference [6].

2. DIFFERENTIAL OPERATOR SAMPLING METHOD

2.1. Review of Explicit Formulation for k_{eff}

The effective multiplication factor k_{eff} in the i -th generation can be expressed with the Neumann series as follows[6];

$$k_i = \frac{\int dP \int dP' K_F(P; P') S_{f,i}(P')}{\int dP S_{f,i}(P)}, \quad (1)$$

where $S_{f,i}$ is the fission source in the i -th generation and $K_F(P; P')$ is defined as

$$K_F(P; P') = \int dP'' K_f(P; P'') \sum_{m=0}^{\infty} K_{s,m}(P''; P') \quad (2)$$

$$K_{s,m}(P; P') = \int dP_1 \cdots \int dP_{m-1} K_s(P; P_{m-1}) K_s(P_{m-1}; P_{m-2}) \cdots K_s(P_1; P'). \quad (3)$$

Furthermore, $K_x(x = s \text{ or } f)$ in Eq. (3) is defined as the product of the collision and transport kernels;

$$K_x(P; P') = C_x(P; P'') T(P''; P'). \quad (4)$$

The change in k_i for a perturbed parameter a can be then expressed with the Taylor series expansion as follows;

$$\Delta k_i = \frac{\partial k_i}{\partial a} \Delta a + \frac{1}{2} \frac{\partial^2 k_i}{\partial a^2} (\Delta a)^2 + \cdots + \frac{1}{n!} \frac{\partial^n k_i}{\partial a^n} (\Delta a)^n + \cdots \quad (5)$$

The differential operator sampling method estimates each differential coefficients in Eq.(1). We can obtain the first-order differential coefficient by differentiating Eq.(1);

$$\frac{\partial k_i}{\partial a} = \frac{1}{\int S_{f,i} dP_0} \sum_m \int dP_m \cdots \int dP_0 \left[\frac{1}{C_{f,m}} \frac{\partial C_{f,m}}{\partial a} + \frac{1}{T_m} \frac{\partial T_m}{\partial a} \right]$$

$$\begin{aligned}
 & + \frac{1}{C_{s,m-1}} \frac{\partial C_{s,m-1}}{\partial a} + \frac{1}{T_{m-1}} \frac{\partial T_{m-1}}{\partial a} \cdots + \frac{1}{T_1} \frac{\partial T_1}{\partial a} + \frac{1}{S_{f,i}} \frac{\partial S_{f,i}}{\partial a} \Big] \\
 & \times C_{f,m} T_m C_{s,m-1} T_{m-1} \cdots C_{s,1} T_1 S_{f,i},
 \end{aligned} \tag{6}$$

where T_m is the transport kernel of the m -th flight, $C_{x,m}$ the collision kernel of the m -th collision. The last term in the bracket represents the first-order perturbation effect due to the fission source change.

Since MCNP calculates the differential coefficients without the perturbed fission source effect, it is convenient to separate the term for it explicitly;

$$\frac{\partial k_i}{\partial a} = \frac{\partial k_i}{\partial a} (\text{no perturbed FS effect}) + \frac{\partial k_i}{\partial a} (\text{perturbed FS effect}), \tag{7}$$

where

$$\begin{aligned}
 \frac{\partial k_i}{\partial a} (\text{no perturbed FS effect}) = & \\
 & \frac{1}{\int S_{f,i} dP_0} \sum_m \int dP_m \cdots \int dP_0 \left[\frac{1}{C_{f,m}} \frac{\partial C_{f,m}}{\partial a} + \frac{1}{T_m} \frac{\partial T_m}{\partial a} + \frac{1}{C_{s,m-1}} \frac{\partial C_{s,m-1}}{\partial a} \right. \\
 & \left. + \frac{1}{T_{m-1}} \frac{\partial T_{m-1}}{\partial a} \cdots + \frac{1}{T_1} \frac{\partial T_1}{\partial a} \right] C_{f,m} T_m C_{s,m-1} T_{m-1} \cdots C_{s,1} T_1 S_{f,i},
 \end{aligned} \tag{8}$$

$$\begin{aligned}
 \frac{\partial k_i}{\partial a} (\text{perturbed FS effect}) = & \\
 & \frac{1}{\int S_{f,i} dP_0} \sum_m \int dP_m \cdots \int dP_0 \left[\frac{1}{S_{f,i}} \frac{\partial S_{f,i}}{\partial a} \right] C_{f,m} T_m C_{s,m-1} T_{m-1} \cdots C_{s,1} T_1 S_{f,i}.
 \end{aligned} \tag{9}$$

Eq.(8) and (9) represent the first-order differential coefficient without the perturbed fission source effect and the first-order effect due to the perturbed fission source distribution, respectively. The perturbation capability in most Monte Carlo codes is based on Eq.(8) and perturbations in the fission source are not accounted for.

To evaluate Eq.(9), we apply a method developed by one of the authors[6]. In this method, the differential coefficient of the fission source in the bracket of Eq.(9) ($\partial S_{f,i}/\partial a$) is obtained from the following equation;

$$\begin{aligned}
 \frac{\partial}{\partial a} S_{f,i}(P) = & \frac{\int S_{f,i-1} dP'}{\int dP \int dP' K_F S_{f,i-1}} \left(\int dP' \frac{\partial}{\partial a} [K_F S_{f,i-1}] \right. \\
 & \left. - \int dP \int dP' \frac{\partial}{\partial a} [K_F S_{f,i-1}] \frac{\int dP' K_F S_{f,i-1}}{\int dP \int dP' K_F S_{f,i-1}} \right).
 \end{aligned} \tag{10}$$

This equation represents the normalization of the additional weights for the differential coefficient of the fission source at fission sites selected in the $(i-1)$ -st generation as shown later.

Similarly, we can derive the second-order differential coefficient for k_i by differentiating Eq.(8) with regard to a as presented in Reference [6]. The coefficient includes the first- and second-order differential coefficients of the fission source ($\partial S_{f,i}/\partial a$, $\partial^2 S_{f,i}/\partial a^2$) but we neglect these terms in the evaluation of the second-order differential coefficient in this work.

2.2. Implementation of the Method to Evaluate the Perturbed Fission Source Effect into MCNP5

In this section, we describe how to implement the above method into MCNP. The following procedure can be applied to other Monte Carlo codes that have the same normalization scheme for fission neutrons between cycles.

In MCNP, an integral number of fission sites is generated at collisions based on $\nu\sigma_f/(\sigma_t * k_{eff})$. These sites are assumed to have equal weight and are stored for use as the source in the next cycle. The number of banked fission sites varies in each cycle. At the conclusion of a cycle, the banked particle weights are normalized so that the total weight in each cycle is constant, equal to the total starting weight for the cycle. That is, the number of starting sites may vary from cycle to cycle, but the total starting weight is constant for each cycle. Letting the number of particles generated in the $(i - 1)$ -st cycle and the total weight be M_{i-1} and N_c , respectively, the weight of each source particle in the i -th cycle $\bar{w}_{f,i}$ can be simply expressed as follows;

$$\bar{w}_{f,i} = \frac{N_c}{M_{i-1}}. \quad (11)$$

Now we consider each term that appears in Eq.(10). The term $\int dP' K_F S_{f,i-1}$ represents the score of the fission rate at each fission site. Of course, the score varies depending on the site but, for estimating the effects of changing source distribution, we can consider that the weight defined by Eq.(11) is assigned to each fission neutron (particle) in the normalization process. Therefore, the term is estimated by the following expression;

$$\int dP' K_F S_{f,i-1} \Rightarrow \bar{w}_{f,i}. \quad (12)$$

The term $\int dP \int dP' K_F S_{f,i-1}$ can be estimated as the sum of $\int dP' K_F S_{f,i-1}$ over all fission sites.

$$\int dP \int dP' K_F S_{f,i-1} \Rightarrow \bar{w}_{f,i} M_{i-1}. \quad (13)$$

Likewise, the differential terms $\int dP' \partial [K_F S_{f,i-1}] / \partial a$ and $\int dP \int dP' \partial [K_F S_{f,i-1}] / \partial a$ are estimated by the following expressions;

$$\int dP' \frac{\partial}{\partial a} [K_F S_{f,i-1}] \Rightarrow w'_{f,\hat{m}} \bar{w}_{f,i} \quad (14)$$

$$\int dP \int dP' \frac{\partial}{\partial a} [K_F S_{f,i-1}] \Rightarrow \sum_{\hat{m}=1}^{M_{i-1}} w'_{f,\hat{m}} \bar{w}_{f,i}, \quad (15)$$

where $w'_{f,\hat{m}}$ is the additional weight for the score of the fission rate and defined as

$$w'_{f,\hat{m}} = \frac{1}{C_{f,m}} \frac{\partial C_{f,m}}{\partial a} + \frac{1}{T_m} \frac{\partial T_m}{\partial a} + \frac{1}{C_{s,m-1}} \frac{\partial C_{s,m-1}}{\partial a} + \frac{1}{T_{m-1}} \frac{\partial T_{m-1}}{\partial a} \dots + \frac{1}{T_1} \frac{\partial T_1}{\partial a}. \quad (16)$$

Using the expressions above, the additional weight for the differential coefficient of the fission source (the term in the bracket of Eq.(9)) can be estimated as follows;

$$\frac{1}{S_{f,i}} \frac{\partial S_{f,i}}{\partial a} \Rightarrow w'_{f,\hat{m}} - \frac{1}{M_{i-1}} \sum_{\hat{m}=1}^{M_{i-1}} w'_{f,\hat{m}}. \quad (17)$$

Here we used the following expressions;

$$\int S_{f,i-1} dP' \Rightarrow N_c \quad (18)$$

$$S_{f,i} \Rightarrow \bar{w}_{f,i}. \quad (19)$$

Expression (17) represents the normalization for the additional weight for the score of the fission rate. Since the fission source is normalized in each cycle, the additional weight must be also normalized according to Expression (17).

It is straightforward to estimate the perturbed fission source effect (Eq.(9)) when the additional weight for the differential coefficient of the fission source is obtained. Since the additional weight does not change during the history of each particle, Eq.(9) can be estimated by multiplying the score of the fission rate by the additional weight.

3. CALCULATED RESULTS

3.1. Godiva Assembly

The Godiva density perturbation problems[6] were solved with the modified MCNP5 code. There are two problems; one is the homogeneous density perturbation problem and the other is the localized one. The former problem addresses the case where the fission source distribution does not change significantly and the latter problem addresses the case where the perturbation of the distribution is enhanced.

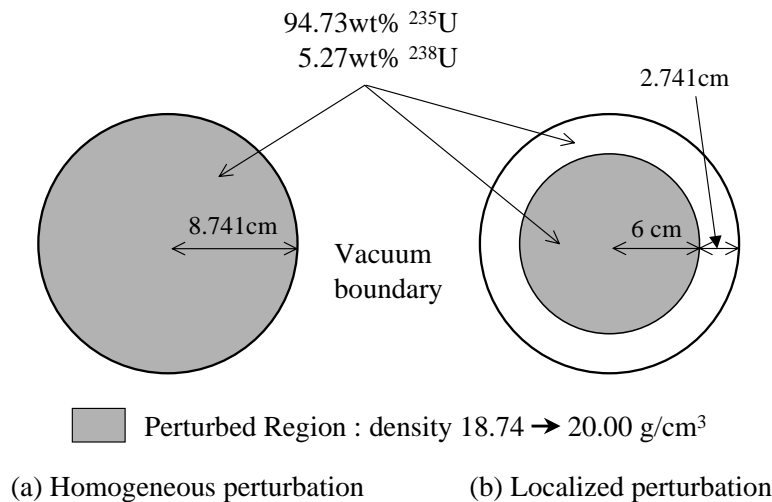


Figure 1. Godiva Geometry and Perturbed Regions

Figure 1 shows the geometry of the Godiva assembly and the perturbed regions. The geometry is a bare uranium sphere of a radius of 8.741 cm. The original density is 18.74 g/cm³ and the composition is 94.73 wt% ^{235}U and 5.27 wt% ^{238}U . The perturbed regions are the whole region and the central region of a radius of 6 cm in the homogeneous and localized cases, respectively. The density is perturbed from 18.74 g/cm³ to 20.00 g/cm³ in both the cases.

All MCNP eigenvalue calculations including perturbation calculations were performed for 60 inactive and 90 active cycles with 10000 histories per cycle. The JENDL-3.2 MCNP library[8] was used. The k_{eff} value for the unperturbed case was 1.00205 ($1\sigma = 0.062\%$).

Table I. Results for the Godiva Homogeneous Perturbation Problem

Method	Δk	1σ	$\Delta k/k$	1σ
ONEDANT (70 groups, S8P0)	5.400E-2	—	5.430E-2	—
2 Independent MCNP Runs	5.454E-2	0.086E-2	5.443E-2	0.085E-2
MCNP 1st-Order Differential Operator	5.370E-2	0.012E-2	5.359E-2	0.012E-2
MCNP 2nd-Order Differential Operator	5.252E-2	0.012E-2	5.241E-2	0.012E-2
Only Perturbed Fission Source Effect	0.177E-2	0.037E-2	0.176E-2	0.037E-2
Sum of 2nd-Order & Perturbed Effect	5.428E-2	0.039E-2	5.417E-2	0.039E-2

Table I shows the results for the Godiva homogeneous perturbation problem. The second and fourth columns list the change in k_{eff} and its fractional change, respectively. The reference solution was obtained from the difference of two k_{eff} values with the ONEDANT code[9]. The reference calculations were performed for S_8 angular quadrature and P_0 scattering cross section with a 70-group cross section library JFS-3-J3.2[10, 11] based on JENDL-3.2[12]. The Δk (or $\Delta k/k$) value obtained from two independent MCNP runs agrees with the reference one within a standard deviation but the statistical uncertainty is slightly large.

On the other hand, the result of the conventional MCNP estimate up to the second-order underestimates the reference one by $\sim 3\%$. There are two possible causes for the underestimation; one is the higher-order effect and the other is the perturbed fission source effect. Since the second-order perturbation estimate is $\sim 2\%$ of the reference change in k_{eff} , the higher-order effect can be assumed to be less. Thus, there exists somewhat the perturbed fission source effect even in the homogeneous perturbation case. The effect was estimated to be $\sim 3\%$ of the reference Δk with the modified MCNP. The original MCNP estimate can be improved by taking this effect into account as shown in Table I.

Table II shows the results for the Godiva localized perturbation problem. As in the homogeneous case, we obtained the reference Δk ($\Delta k/k$) with the ONEDANT code, the direct estimate from two independent MCNP runs and the conventional MCNP perturbation estimates. The direct estimate is in very good agreement with the reference one but the statistical uncertainty is rather large. The conventional MCNP estimate up to the second-order underestimates the reference result significantly and the discrepancy is $\sim 36\%$. Obviously, the higher-order effect is very small and the perturbed fission source effect is dominant in this case.

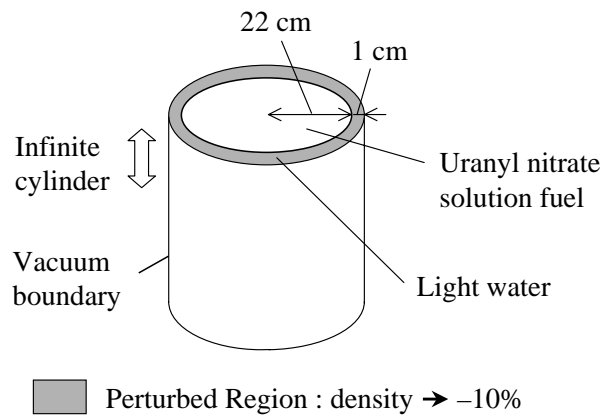
On the other hand, the result with the perturbed fission source effect is in good agreement with the reference one and the conventional MCNP estimate is improved significantly as shown in Table II. Therefore, the effect is estimated correctly and it is found that our method to estimate the effect is also effective for relatively large fission source distortion.

Table II. Results for the Godiva Localized Perturbation Problem

Method	Δk	1σ	$\Delta k/k$	1σ
ONEDANT (70 groups, S8P0)	2.968E-2	—	2.984E-2	—
2 Independent MCNP Runs	2.968E-2	0.090E-2	2.962E-2	0.090E-2
MCNP 1st-Order Differential Operator	1.936E-2	0.009E-2	1.932E-2	0.009E-2
MCNP 2nd-Order Differential Operator	1.899E-2	0.009E-2	1.896E-2	0.009E-2
Only Perturbed Fission Source Effect	1.109E-2	0.041E-2	1.107E-2	0.041E-2
Sum of 2nd-Order & Perturbed Effect	3.009E-2	0.042E-2	3.002E-2	0.042E-2

3.2. Simplified STACY Model

We also performed perturbation calculations for the simplified STACY model[6] to ensure our method implemented in MCNP. The geometry of the model is shown in Fig. 2 and the details such as composition etc. are described in Reference [6]. A perturbation is introduced by decreasing the density in the reflector region by 10%.

**Figure 2. Geometry for the Simplified STACY Model**

All MCNP calculations were performed for 70 inactive and 430 active cycles with 10000 histories per cycle and the JENDL-3.2 library was used. The k_{eff} value for the unperturbed case was 1.00284 ($1\sigma = 0.033\%$).

Table III shows the results for the simplified STACY model. The reference Δk value is the ANISN result obtained from two eigenvalue calculations with S_8 angular quadrature and the 107-group JENDL-3.2 library including P_1 scattering cross sections[6]. The result of two independent MCNP runs agrees with the reference one within a standard deviation but the statistical uncertainty is more than 30%. The conventional MCNP perturbation estimate is not trustworthy at all and the discrepancy is more than 100%. Thus the perturbed fission source effect is considered to be significant and we cannot obtain the correct Δk value

without the effect. Even in this case, our method is effective and the estimated perturbed fission source effect improves the conventional MCNP estimate.

Table III. Results for the Simplified STACY Problem

Method	Δk	1σ	$\Delta k/k$	1σ
ANISN (107 groups, S8P1)	-1.70E-3	—	-1.69E-3	—
2 Independent MCNP Runs	-1.40E-3	0.47E-3	-1.40E-3	0.47E-3
MCNP 1st-Order Differential Operator	-3.67E-3	0.03E-3	-3.66E-3	0.03E-3
MCNP 2nd-Order Differential Operator	-3.71E-3	0.03E-3	-3.70E-3	0.03E-3
Only Perturbed Fission Source Effect	1.80E-3	0.28E-3	1.80E-3	0.28E-3
Sum of 2nd-Order & Perturbed Effect	-1.90E-3	0.28E-3	-1.90E-3	0.28E-3

4. CONCLUSIONS

In this work, we have implemented a method to estimate the perturbed fission source effect into MCNP5 and have verified it with simple benchmark problems. We have shown that the method is very effective not only for the homogeneous perturbation case but also the localized perturbation cases. It has, thus, verified that the method can be applicable for Monte Carlo codes that have the same normalization scheme between cycles.

One area for future work concerns the relatively large statistical uncertainty for the perturbed fission source effect. Currently, the additional weight for the differential coefficient of the fission source is propagated between cycles. This may result in relatively large uncertainty, possibly diverging in pathological cases. Further investigation is required for the uncertainty analysis.

Another area for future work is the estimation of accurate statistical uncertainties. In the current scheme, we estimate the statistical uncertainties of differential coefficients and the perturbed fission source effect in the same way as the usual k_{eff} estimation. Namely, the correlations between the coefficients and between cycles are ignored. The accurate statistical uncertainties must be presented for the Monte Carlo perturbation technique with our method to provide a reference result in eigenvalue problems.

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