

Monte Carlo sensitivity calculation in fixed source problems with the derivative source method

Toshihiro Yamamoto^{a*}, Hiroki Sakamoto^b

^a*Institute for Integrated Radiation and Nuclear Science, Kyoto University, 2 Asashiro Nishi, Kumatori-cho, Sennan-gun, Osaka, 590-0494, Japan*

^b*Radiation Dose Analysis and Evaluation Network, 4-13-14, Kokubunji-shi, Tokyo, 185-0001, Japan*

Abstract

This paper proposes a new Monte Carlo sensitivity analysis method for fixed source radiation transport problems, which is dubbed the derivative source method (DSM). This method is a variation of the formerly proposed perturbation source method. A transport equation of a derivative particle representing a derivative of a flux with respect to a parameter such as a cross section is derived by differentiating the fixed source radiation transport equation. This paper presents a Monte Carlo algorithm to solve this transport equation. The derivative particle is emitted from a region of interest (ROI) when a radiation particle undergoes a collision in the ROI. The derivative particle is tracked in the same manner as the ordinary radiation particles. The derivative particle that undergoes a collision in the ROI can yield another derivative particle whose derivative order is increased by one from the colliding particle. This higher-order derivative particle can be used for calculating the higher-order derivative of a flux. The differential operator sampling method (DOS), which is commonly used for Monte Carlo sensitivity analyses, suffers from poor performance when an ROI is small. For a small ROI, the efficiency of the DSM can be improved by adding a pseudo scattering cross section in the ROI, thereby increasing the pseudo scatterings and the number of derivative particles emitted from the ROI. The efficiency of the new method is evaluated by comparing the DSM to the DOS. Numerical tests are performed for a two-dimensional geometry containing a small inclusion. The results reveal that the DSM definitely outperforms the DOS for these test problems. The efficiency of the DSM depends strongly on the

* Corresponding author. E-mail address: toshihiro.yamamoto223@gmail.com (T. Yamamoto)

pseudo scattering cross section added to the inclusion.

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1. Introduction

The sensitivity and uncertainty analysis of the desired quantity of interest in radiation transport with respect to some input parameters (e.g., cross sections and geometries) has been mainly performed using two different manners: the deterministic method and the stochastic method (i.e., the Monte Carlo method). The former method, the deterministic method, ordinarily uses the adjoint-based method [6]. Applying the adjoint-based method to radiation transport requires storing six-dimensional data for the forward and angular fluxes, which in some cases requires a huge amount of data storage. Some potential solutions to the memory requirement for the transport adjoint formulation have been proposed thus far. The use of a quasi-diffusion method to reduce the overall dimensionality of the transport problem, which is termed as a variable Eddington tensor (VET), is one of them [7].

For the latter method, the Monte Carlo method, several techniques have been developed for sensitivity and uncertainty analyses. The iterated fission probability (IFP) method is one of the techniques, and the IFP method calculates the adjoint flux in the continuous energy Monte Carlo [12, 13, 29, 30]. Another one, which is implemented in the SERPENT code, is the collision-history-based method [1]. Well known production Monte Carlo codes that have the capability of sensitivity analysis are: SCALE [18, 19, 25], MCNP [12, 13], SERPENT [1], MORET [9], McCARD [28], and RMC [22-24]. A quite different approach is the differential operator sampling method (DOS) [5, 9, 16, 26, 31-33]. The unique feature of the DOS lies in that it does not need the calculation of the adjoint flux and the estimates of the derivatives of the variable of interest with respect to nuclear data can be extended to arbitrary orders.

A quite different Monte Carlo approach that has the potential to be adopted in sensitivity and uncertainty analysis is the perturbation source method (PSM) [14, 15, 21]. The method is an exact Monte Carlo perturbation technique that is available in fixed source problems. This method,

1 however, has not been a mainstream Monte Carlo method. Sakamoto and Yamamoto [27, 34, 35]
2 recently revisited the PSM and proposed a new technique to solve the drawback regarding its
3 computation efficiency. Owing to the newly proposed technique, the PSM may have the potential
4 to outperform commonly used Monte Carlo perturbation methods such as the correlated sampling
5 method and the DOS for some fixed source particle transport calculations. In the PSM, each time
6 a particle collides in a perturbed region during the course of a fixed source problem, a perturbation
7 particle representing a flux difference is started from the point of the collision. The perturbation
8 particle is tracked within the whole domain until it is killed or it escapes from the external boundary.
9 The weight of the perturbation particle represents the flux difference caused by the change of the
10 cross section. The PSM can provide the exact flux difference due to the change of the cross sections.
11 While the correlated sampling technique experiences large statistical uncertainties for large cross
12 section changes [26], the PSM method is a robust technique regardless of the magnitude of the
13 perturbation. In particular, for perturbation problems in which the cross sections change in a very
14 small region, the PSM definitely outperforms other Monte Carlo perturbation methods such as the
15 correlated sampling method and the DOS in terms of the computational efficiency.

16 A new Monte Carlo sensitivity and uncertainty analysis method can be derived after a slight
17 modification of the PSM. In this paper, the new method is referred to as the derivative source
18 method (DSM). While a particle that is transported in the PSM represents a perturbed flux, a
19 particle that is transported in the DSM represents the derivative of a flux with respect to a cross
20 section.

21 As a unique feature of the DSM, this method is capable of being expanded to calculate the
22 second- and higher-order derivatives of a flux like the DOS. In most cases, the second-order
23 response sensitivities are much smaller than the corresponding first-order sensitivities. However,
24 in some special cases, the second-order sensitivities are much larger than the corresponding first-
25 order ones [2, 3], which makes the interest in calculating second-order sensitivities increasingly
26 evident. The works on the second-order sensitivities have been performed using deterministic

methods such as the Second-Order Adjoint Sensitivity Analysis Methodology (2nd-ASAM) [4]. The present paper develops a new Monte Carlo method for second- and higher-order sensitivity analysis, which can overcome the deficiency of the DOS.

Section 2 of this paper will present the basic theory of the DSM. Section 3 presents the Monte Carlo algorithm that implements the theory of the DSM. Section 4 presents the expansion of the DSM to higher-order derivatives. Section 5 presents some numerical examples and the evaluation of the performance of the DSM. Section 6 presents the summary and conclusions.

2. Theory of the derivative source method (DSM)

This section presents the theory of the sensitivity analysis method to calculate the derivative of a flux with respect to a parameter that is included in a fixed source radiation transport equation. The theory is simple and very similar to the perturbation source method (PSM) [27, 34, 35]. The fixed source radiation transport equation in a nonmultiplying medium is given by the following:

$$\mathbf{H}\phi(\mathbf{r}, \boldsymbol{\Omega}, E) = S(\mathbf{r}, \boldsymbol{\Omega}, E), \quad (1)$$

where

$$\begin{aligned} \mathbf{H}\phi(\mathbf{r}, \boldsymbol{\Omega}, E) \equiv & \boldsymbol{\Omega} \cdot \nabla \phi(\mathbf{r}, \boldsymbol{\Omega}, E) + \Sigma_t(\mathbf{r}, E)\phi(\mathbf{r}, \boldsymbol{\Omega}, E) \\ & - \int_{4\pi} d\boldsymbol{\Omega}' \int dE' \Sigma_s(\mathbf{r}, \boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega}, E' \rightarrow E)\phi(\mathbf{r}, \boldsymbol{\Omega}', E'), \end{aligned} \quad (2)$$

$\phi(\mathbf{r}, \boldsymbol{\Omega}, E)$ = the flux at position $\mathbf{r}$ with energy E and direction $\boldsymbol{\Omega}$, $S(\mathbf{r}, \boldsymbol{\Omega}, E)$ = the external source term, Σ_t = the total cross section, and Σ_s = the scattering cross section. The transport equation for the first derivative of the flux with respect to parameter α , which can be the total cross section, the scattering cross section, and the angular or energy distribution of the scattered particle, is obtained by differentiating Eq. (1) by parameter α :

$$\mathbf{H}\phi'_\alpha(\mathbf{r}, \boldsymbol{\Omega}, E) = -\mathbf{H}'_\alpha\phi(\mathbf{r}, \boldsymbol{\Omega}, E), \quad (3)$$

where $\phi'_\alpha(\mathbf{r}, \boldsymbol{\Omega}, E)$ = the first derivative of the flux with respect to α , and $\mathbf{H}'_\alpha$ = the first derivative of the transport operator $\mathbf{H}$ with respect to α . Here, it is assumed that the source term $S(\mathbf{r}, \boldsymbol{\Omega}, E)$ is independent of parameter α . In Eq. (3), the right-hand side represents the source term for the transport equation of the first derivative of the flux. It is assumed that the differential scattering cross section is given by the following:

$$\Sigma_s(\mathbf{r}, \boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega}, E' \rightarrow E) = \Sigma_s(\mathbf{r}, E') p(\boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}, E' \rightarrow E), \quad (4)$$

where $p(\boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}, E' \rightarrow E)$ is the probability density function (PDF) of the collision law. Then, the right-hand side is as follows:

$$\begin{aligned} & -H'_\alpha \phi(\mathbf{r}, \boldsymbol{\Omega}, E) \\ & = \begin{cases} -\phi(\mathbf{r}, \boldsymbol{\Omega}, E) & \text{for } \alpha = \Sigma_t(\mathbf{r}, \boldsymbol{\Omega}, E) \text{ or } \Sigma_c(\mathbf{r}, \boldsymbol{\Omega}, E), \\ -\phi(\mathbf{r}, \boldsymbol{\Omega}, E) + \int_{4\pi} d\boldsymbol{\Omega}' \int dE' p(\boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}, E' \rightarrow E) \phi(\mathbf{r}, \boldsymbol{\Omega}', E') & \text{for } \alpha = \Sigma_s(\mathbf{r}, E'), \end{cases} \end{aligned} \quad (5)$$

where Σ_c = the capture cross section. When α is a variable of the PDF of the collision law, the right-hand side of Eq. (3) is as follows:

$$-H'_\alpha \phi(\mathbf{r}, \boldsymbol{\Omega}, E) = \int_{4\pi} d\boldsymbol{\Omega}' \int dE' p'_\alpha(\boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}, E' \rightarrow E) \Sigma_s(\mathbf{r}, E') \phi(\mathbf{r}, \boldsymbol{\Omega}', E'), \quad (7)$$

where $p'_\alpha(\boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}, E' \rightarrow E)$ = the first derivative of the PDF with respect to α .

To solve Eq. (3), the flux $\phi(\mathbf{r}, \boldsymbol{\Omega}, E)$ needs to be calculated by solving the transport equation, Eq. (1), with the fixed source $S(\mathbf{r}, \boldsymbol{\Omega}, E)$. Once we obtain the source term in Eqs. (5), (6), and (7) using the flux $\phi(\mathbf{r}, \boldsymbol{\Omega}, E)$, the first derivative of the flux $\phi'_\alpha(\mathbf{r}, \boldsymbol{\Omega}, E)$ can be obtained by solving the transport equation for the first derivative of the flux, Eq. (3). An equation that is essentially the same as Eq. (3) is already presented in many papers (e.g., Eq. (16) in [3]). However, solving Eq. (3) is computationally inefficient if the number of parameter α s to be evaluated is not small because this equation would need to be solved for every variation of α . In the deterministic method, this computationally inefficient method can be avoided by introducing the adjoint function. On the other hand, in the Monte Carlo method, introducing the technique using the adjoint function is not as straightforwardly simple as the deterministic method. Instead, the differential operator sampling method (DOS) is alternatively available as an easily implemented method for sensitivity analyses. The DOS can be easily expanded to higher-order sensitivity analyses without significantly increasing the computational load. However, the DOS suffers from poor performance when the region where a parameter to be changed exists is tiny compared to the whole calculation domain. In this case, radiation particles rarely enter the tiny region, which makes the scoring of the DOS less efficient. This situation may occur if we are interested in the sensitivity

of the radiation transport due to a small inclusion within a material. Thus, this paper proposes a Monte Carlo method to obtain the derivative of the flux by directly solving Eq. (3). The proposed method uses the same fundamentals as the PSM [27, 34, 35]. The efficiency of the PSM can be improved by adding a pseudo scattering cross section to the region of interest, thereby increasing the additional collisions in the region. With the pseudo scatterings, the PSM outperforms other Monte Carlo methods such as the DOS. Applying the same technique could make the newly proposed method an efficient Monte Carlo technique for the sensitivity analyses of small regions.

3. Monte Carlo algorithm of the derivative source method (DSM)

3.1 Monte Carlo algorithm for calculating the first derivative of a flux

This section presents a Monte Carlo algorithm to solve the transport equation for the first derivative of a flux, Eq. (3). Although the algorithms in this section have much in common with the PSM [27, 34, 35], they are repeatedly presented in this section.

First, an ordinary fixed source Monte Carlo calculation is performed to obtain a flux $\phi(\mathbf{r}, \boldsymbol{\Omega}, E)$ by solving Eq. (1). The flux will be used as the source term in the right-hand side of Eq. (3). This procedure is dubbed the fixed source calculation mode. Each time a particle is stopped by a collision in a region of interest (hereafter ROI) where a parameter whose effect on the radiation transport is to be examined exists, the source term for Eq. (3) is estimated via Eqs. (5), (6), and (7). The source term is defined by the position, energy, direction, and particle weight. Two methods can be considered for estimating the source term. The first one is to perform the fixed source calculation for Eq. (1) until a sufficient number of collisions are stored. However, this would require a huge storage capacity to store a sufficient amount of source information. Hence, as an alternative method, a so-called on-the-fly technique was chosen by the PSM [27, 34, 35]. The on-the-fly technique is also used in this paper for the DSM. Each time a particle is stopped by a collision in the ROI in the fixed source calculation mode, the fixed source calculation is suspended for a while. Next, the source term for Eq. (3) is calculated via Eqs. (5), (6), and (7), and another particle (derivative particle), which stands for the first derivative of the flux ϕ'_α , is started

from the point of the collision. This procedure is dubbed the derivative calculation mode. The derivative particle is transported in the same way as in the fixed source calculation mode. As seen in Eq. (5), the source particle has a negative weight for $\alpha = \Sigma_t$ or Σ_c . After the particle that represents the first derivative is killed, the derivative calculation mode for solving Eq. (3) is over and the fixed source calculation mode is restarted. This procedure is iterated until the sufficient statistics for the derivative of the flux are attained.

Next, a Monte Carlo algorithm for calculating the source term defined by Eqs. (5), (6), and (7) is presented as follows. When a particle undergoes a collision in the ROI in the fixed source calculation mode, the calculation mode is changed to the derivative calculation mode.

[1] Source term for $\alpha = \Sigma_t$ or Σ_c

According to Eq. (5), the source term for $\alpha = \Sigma_t$ or Σ_c is equal to the flux at the point of the collision. The weight of the source term is given by the following:

$$W_t = -\frac{W}{\Sigma_t(\mathbf{r}, E)}, \quad (8)$$

where W = the weight of the colliding particle. A new derivative particle with the weight of W_t is started from the point of the collision. The direction and energy of the derivative particle are the same as the particle that undergoes the collision in the fixed source calculation mode. This derivative particle is tracked until it is killed. If $\alpha = \Sigma_c$, no other source particle has to be emitted from the point of the collision. The weight of the first source term in Eq. (6) is also given by Eq. (8).

[2] Source term for $\alpha = \Sigma_s$

The source term for $\alpha = \Sigma_s$ is obtained by the following steps.

1) According to Eq. (6), the weight of the second source term is given by the following:

$$W_s = \frac{W}{\Sigma_t(\mathbf{r}, E)}. \quad (9)$$

2) The direction $\boldsymbol{\Omega}'$ and the energy E' of the derivative particle are determined by sampling from the collision law $p(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}', E \rightarrow E')$.

This derivative particle is emitted from the point of the collision in addition to the derivative

particle defined by Eq. (8). That is, when $\alpha = \Sigma_s$, two derivative particles need to be started sequentially and tracked until they are killed.

[3] Source term for a collision-related parameter α

When α is a parameter of the collision law $p(\boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}, E' \rightarrow E)$, the source term is obtained by the following steps:

1) According to Eq. (7), the weight of the source term is given by the following:

$$W_p = \frac{p'_\alpha(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}', E \rightarrow E') \Sigma_s(\mathbf{r}, E)}{p(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}', E \rightarrow E') \Sigma_t(\mathbf{r}, E)} W. \quad (10)$$

2) The direction $\boldsymbol{\Omega}'$ and the energy E' of the derivative particle are determined by sampling from the collision law $p(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}', E \rightarrow E')$.

If parameter α does not affect any cross sections other than the collision law, only one particle with the weight of W_p needs to be emitted from the point of the collision.

A schematic flow diagram of the DSM is shown in Figs. 1(a) and 1(b). The total score of the derivative particles divided by the total sum of the weights emitted from the source $S(\mathbf{r}, \boldsymbol{\Omega}, E)$ represents the estimate of the first derivative of the flux $\phi'_\alpha(\mathbf{r}, \boldsymbol{\Omega}, E)$.

[Fig. 1(a)], [Fig. 1(b)]

3.2 Pseudo scattering method for the derivative source method

The derivative calculation mode is not initiated until a particle collides in an ROI. Even when the particle gets into the ROI, the particle that penetrates the ROI without a collision does not initiate the derivative calculation mode. If the ROI occupies only a small fraction of the whole calculation region, collisions in the ROI seldom occur, making the derivative calculation less efficient. As proposed by Sakamoto and Yamamoto [27, 34, 35], a pseudo scattering cross section is added to the cross section of the ROI in order to increase the number of derivative particles. For this purpose, the total cross section Σ_t in the ROI is increased by a factor of $C (>1)$ as follows:

$$\Sigma_t^* = C \cdot \Sigma_t. \quad (11)$$

The fixed source calculation mode uses this pseudo total cross section for the ROI. Each time a particle collides in the ROI where the pseudo total cross section is Σ_t^* , a derivative particle is

started from the point of the collision. The initial weight of the derivative particle is decreased to compensate for the increased pseudo total cross section as follows:

$$W'_t = \frac{W_t}{C}, \quad (12)$$

$$W'_s = \frac{W_s}{C}, \quad (13)$$

$$W'_p = \frac{W_p}{C}, \quad (14)$$

where W_t , W_s , and W_p are given by Eqs. (8), (9), and (10), respectively. After the derivative particle is killed, the suspended fixed source calculation mode is restarted. When restarting the fixed source calculation mode, whether the pseudo collision in the ROI is accepted as the real collision is determined based on the following criteria:

$$\xi < \frac{\Sigma_t}{\Sigma_t^*} = \frac{1}{C}, \quad (15)$$

where ξ is a pseudo random number from 0 to 1. Unless the criterion is met, the particle maintains its direction, energy, and weight before the pseudo collision. As the factor C increases, the number of collisions increases in the ROI, which increases the number of derivative particles that are started from the ROI. As already demonstrated in [27], the pseudo scattering method improves the computation efficiency of the PSM by a factor of more than 10 when a perturbed region is small.

4. Monte Carlo method for calculating the second derivative of a flux

4.1 Theory of the derivative source method for the second derivative of a flux

The transport equation for the second derivative of a flux can be obtained as follows by differentiating Eq. (3) by a parameter α :

$$\mathbf{H}\phi''_{\alpha}(\mathbf{r}, \boldsymbol{\Omega}, E) = -\mathbf{H}''_{\alpha}\phi(\mathbf{r}, \boldsymbol{\Omega}, E) - 2\mathbf{H}'_{\alpha}\phi'_{\alpha}(\mathbf{r}, \boldsymbol{\Omega}, E), \quad (16)$$

where the double prime symbol denotes the second derivative with respect to α . The right-hand side is the source term for the transport equation of the second derivative of the flux. The first term on the right-hand side of Eq. (16) is as follows:

$$-\mathbf{H}''_{\alpha}\phi(\mathbf{r}, \boldsymbol{\Omega}, E) = 0 \quad \text{for } \alpha = \Sigma_t, \Sigma_c, \text{ or } \Sigma_s, \quad (17)$$

because $\mathbf{H}'_{\alpha}$ includes neither Σ_t , Σ_c , or Σ_s . The second term on the right-hand side of Eq. (16) is

1 as follows:

$$2 \quad -2\mathbf{H}'_{\alpha}\phi'_{\alpha}(\mathbf{r}, \boldsymbol{\Omega}, E)$$

$$3 \quad = \begin{cases} -2\phi'_{\alpha}(\mathbf{r}, \boldsymbol{\Omega}, E) & \text{for } \alpha = \Sigma_t \text{ or } \Sigma_c, \quad (18) \\ -2\phi'_{\alpha}(\mathbf{r}, \boldsymbol{\Omega}, E) + 2 \int_{4\pi} d\boldsymbol{\Omega}' \int dE' p(\boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}, E' \rightarrow E) \phi'_{\alpha}(\mathbf{r}, \boldsymbol{\Omega}', E') & \text{for } \alpha = \Sigma_s. \quad (19) \end{cases}$$

4 For a collision-related parameter α , the first and second terms on the right-hand side of Eq. (16)
5 are, respectively,

$$6 \quad -\mathbf{H}''_{\alpha}\phi(\mathbf{r}, \boldsymbol{\Omega}, E) = \int_{4\pi} d\boldsymbol{\Omega}' \int dE' p''_{\alpha}(\boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}, E' \rightarrow E) \Sigma_s(\mathbf{r}, E') \phi(\mathbf{r}, \boldsymbol{\Omega}', E'), \quad (20)$$

$$7 \quad -2\mathbf{H}'_{\alpha}\phi'_{\alpha}(\mathbf{r}, \boldsymbol{\Omega}, E) = 2 \int_{4\pi} d\boldsymbol{\Omega}' \int dE' p'_{\alpha}(\boldsymbol{\Omega}' \cdot \boldsymbol{\Omega}, E' \rightarrow E) \Sigma_s(\mathbf{r}, E') \phi'_{\alpha}(\mathbf{r}, \boldsymbol{\Omega}', E'). \quad (21)$$

8 Eq. (16) says that the source term of the transport equation for the second derivative of the flux
9 requires the calculation for ϕ'_{α} that is obtained by solving Eq. (3) and the calculation for ϕ that
10 is obtained by solving Eq. (1).

11

12 **4.2 Monte Carlo algorithm for calculating the second derivative of a flux**

13 This section presents the Monte Carlo algorithm for calculating the second derivative of a
14 flux. The calculation for the first term on the right-hand side of Eq. (16), which requires ϕ , can
15 be performed during the calculation for the first derivative. When parameter α is a cross section,
16 this calculation can be omitted because the source term is zero, as shown in Eq. (17). When α is
17 a collision-related parameter, the source term defined by Eq. (20) can be calculated in the same
18 manner as [3] in Sec. 3.1. The only difference is that the weight for this source term is given by
19 the following:

$$20 \quad W_{p1} = \frac{\partial}{\partial \alpha} \left(\frac{p'_{\alpha}(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}', E \rightarrow E')}{p(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}', E \rightarrow E')} \right) \frac{\Sigma_s(\mathbf{r}, E)}{\Sigma_t(\mathbf{r}, E)} W. \quad (22)$$

21 To calculate the second term on the right-hand side of Eq. (16), a new calculation mode for
22 the second derivative needs to be initiated. As seen in Fig. 1(b), when a particle representing the
23 first derivative of a flux undergoes a collision in an ROI in the first derivative calculation mode
24 (the left part of Fig. 1(b)), the calculation mode is switched to the second derivative calculation

mode (the right part of Fig. 1(b)). During the second derivative calculation mode, the first derivative calculation mode is suspended. The procedure in the second derivative calculation mode is the same as the first derivative calculation mode except for the weight of the starting particle. When parameter α is the total cross section, the weight of the source term defined by Eq. (18) is as follows:

$$W_t = -\frac{2W'}{\Sigma_t(\mathbf{r}, E)}, \quad (23)$$

where W' is the weight of the particle that undergoes a collision in the ROI in the first derivative calculation mode and it represents the first derivative of the flux. The weight of the first source term defined by Eq. (19) is also given by Eq. (23). Similarly, when parameter α is the scattering cross section, the weight of the second source term defined by Eq. (19) is as follows:

$$W_s = \frac{2W'}{\Sigma_t(\mathbf{r}, E)}. \quad (24)$$

In the same manner as in the calculation for the first derivative, two derivative particles need to be started for $\alpha = \Sigma_s$. When α is the collision-related parameter, the weight of the source term defined by Eq. (21) is as follows:

$$W_{p2} = 2 \frac{p'_\alpha(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}', E \rightarrow E')}{p(\boldsymbol{\Omega} \cdot \boldsymbol{\Omega}', E \rightarrow E')} \frac{\Sigma_s(\mathbf{r}, E)}{\Sigma_t(\mathbf{r}, E)} W'. \quad (25)$$

The technique that uses the pseudo scattering in Sec. 3.2 can also be applied in the second derivative calculation mode in order to improve the calculation efficiency for the second derivative calculation mode. The factor C defined in Eq. (11) can be arbitrarily determined in the second derivative calculation mode regardless of the factor C used in the first derivative calculation.

By repeating the procedure for expanding the first derivative to the second derivative, the DSM can be applied to an arbitrary order of derivatives.

5. Numerical tests for the derivative source method

5.1 Overview of the numerical tests

The proposed DSM is tested for a two-dimensional 4×4 cm rectangular geometry. The energy dependence is neglected and the scattering angular distribution is determined based on the Henyey-Greenstein phase function [8, 20], which is commonly used in optics calculations:

$$p(\theta, g) = \frac{1}{4\pi} \frac{1 - g^2}{(1 + g^2 - 2g \cos \theta)^{3/2}}, \quad (26)$$

where θ is the scattering angle, and g is the anisotropy factor. The factor g is equal to the mean cosine of the scattering angle. The scattering angle distribution is usually approximated by a Legendre polynomial expansion in radiation transport calculations. While the Legendre polynomial expansion requires several expansion coefficients to reproduce the anisotropy of the scattering, the Henyey-Greenstein phase function can yield an approximate angular distribution with the single parameter g . Some studies were performed to compare the angular distributions between the Henyey-Greenstein phase function and the Legendre polynomial expansion [10, 11]. This paper chooses the Henyey-Greenstein phase function as the scattering angular distribution function.

A two-dimensional rectangular is composed of a matrix material and a small inclusion material, as shown in Fig. 2. The region of interest is the inclusion whose section size is 0.02×0.02 cm. In the numerical tests, the first and second derivatives of the surface flux with respect to the cross sections and the anisotropy factor of the inclusion are calculated. The cross sections and the anisotropy factor of the materials used for the calculations are as follows:

Matrix: $\Sigma_s = 4.0 \text{ cm}^{-1}$, $\Sigma_c = 0.1 \text{ cm}^{-1}$, $\Sigma_t = 4.1 \text{ cm}^{-1}$, and $g = 0.9$; and
Inclusion: $\Sigma_s = 10.0 \text{ cm}^{-1}$, $\Sigma_c = 1.0 \text{ cm}^{-1}$, $\Sigma_t = 11.0 \text{ cm}^{-1}$, and $g = 0.9$.

[Fig. 2]

A beam source is perpendicularly injected into the center of Side 3 in Fig. 2. When a particle with a weight of W leaves one of the four sides, the estimate of the surface flux, $W/(\mathbf{n} \cdot \boldsymbol{\Omega})$, is scored, where $\boldsymbol{\Omega}$ = the particle's direction vector and $\mathbf{n}$ = the unit outward vector normal to the surface. The surface flux on the side k ($=1, 2, 3$, and 4) is estimated to be as follows:

$$S_k = \frac{1}{N} \sum_i \frac{W_i}{\mathbf{n} \cdot \boldsymbol{\Omega}_i}, \quad (27)$$

where W_i = the weight of the i th particle leaving side k , i is summed over all particles leaving side k , and N = the total number of particles started from the source. Due to the smallness of the whole geometry, the Russian roulette game is turned off and the particles are tracked until they leave the outer surface.

The differential operator sampling method (DOS) is used to obtain the reference solutions that are compared to the results of the DSM. The first derivatives of S_k with respect to Σ_c , Σ_s , and g in the inclusion are respectively calculated as follows [17, 26, 27]:

$$\frac{\partial S_k}{\partial \Sigma_c} = -\frac{1}{N} \sum_i \frac{W_i}{\mathbf{n} \cdot \boldsymbol{\Omega}_i} T_i, \quad (28)$$

$$\frac{\partial S_k}{\partial \Sigma_s} = \frac{1}{N} \sum_i \frac{W_i}{\mathbf{n} \cdot \boldsymbol{\Omega}_i} \left(\frac{M_i}{\Sigma_s} - T_i \right), \quad (29)$$

$$\frac{\partial S_k}{\partial g} = \frac{1}{N} \sum_i \frac{W_i}{\mathbf{n} \cdot \boldsymbol{\Omega}_i} G_{1i}, \quad (30)$$

where T_i = the sum of the track lengths within the inclusion for the i th detected particle, and M_i = the number of collisions within the inclusion for the i th detected particle. G_{1i} in Eq. (30) is defined by the following:

$$G_{1i} = \sum_j \frac{1}{p(\theta_j, g)} \frac{\partial p(\theta_j, g)}{\partial g}, \quad (31)$$

where the summation symbol for j denotes the sum for all collisions within the inclusion for the i th detected particle.

The second derivative of S_k with respect to Σ_c , Σ_s , and g in the inclusion are respectively calculated as follows [17, 26, 27]:

$$\frac{\partial^2 S_k}{\partial \Sigma_c^2} = -\frac{1}{N} \sum_i \frac{W_i}{\mathbf{n} \cdot \boldsymbol{\Omega}_i} T_i^2, \quad (32)$$

$$\frac{\partial^2 S_k}{\partial \Sigma_s^2} = \frac{1}{N} \sum_i \frac{W_i}{\mathbf{n} \cdot \boldsymbol{\Omega}_i} \left\{ -\frac{M_i}{\Sigma_s^2} + \left(\frac{M_i}{\Sigma_s} - T_i \right)^2 \right\}, \quad (33)$$

$$\frac{\partial^2 S_k}{\partial g^2} = \frac{1}{N} \sum_i \frac{W_i}{\mathbf{n} \cdot \boldsymbol{\Omega}_i} (G_{1i}^2 + G_{2i}), \quad (34)$$

where

$$G_{2i} = \sum_j \frac{\partial}{\partial g} \left(\frac{1}{p(\theta_j, g)} \frac{\partial p(\theta_j, g)}{\partial g} \right). \quad (35)$$

5.2 The first derivative of a surface flux

The reference first derivatives of the surface flux on each surface with respect to Σ_c , Σ_s , and g are compared with the results obtained by the DSM in Tables 1, 2, and 3, respectively. The factor C defined in Eq. (11) is set to 100 for these comparisons. Both results agree well and are

within two standard deviations. Tables 4, 5, and 6 compares the relative figure-of-merit (FOM) defined by the following:

$$FOM = \frac{1}{s^2 T}, \quad (36)$$

where s = one standard deviation of absolute uncertainty and T = the computation time. The FOMs are normalized with respect to the DOS. As seen in Tables 4, 5, and 6, the relative FOMs are less than unity when $C = 1$. That is, the computational efficiency of the DSM is inferior to that of the DOS without introducing the pseudo scatterings. However, the efficiency of the DSM becomes much higher than that of the DOS as C increases. In this numerical test, the particles rarely enter the inclusion due to its smallness, which makes the DOS inefficient. Furthermore, by increasing the number of the pseudo scatterings within the inclusion, many derivative particles are emitted from the collision points, which make the DSM superior to the DOS. Needless to say, the efficiency does not unboundedly increase with C . It decreases after C exceeds a certain value, although it keeps increasing up to $C = 1000$ for Σ_s and g .

[Tables 1, 2, 3, 4, 5, 6]

Fig. 3 shows the geometry of another numerical test where the inclusion is enlarged up to the size of 1×1 cm. The first derivatives of the surface flux are calculated for this numerical test with the DOS and the DSM. The FOMs are compared in Tables 7, 8, and 9. Because too many derivative particles are emitted from the large inclusion, the efficiency of the DSM becomes worse compared to the DOS.

As expected, while the efficiency of the DOS would be improved as the inclusion becomes larger, the DSM becomes less efficient than the DOS because too many derivative particles need to be tracked.

[Tables 7, 8, 9] [Fig. 3]

5.3 The second derivative of a surface flux

The performance of the DSM for the second derivative of a flux is tested in this section. The DOS, which is used for the reference solutions, cannot yield statistically significant results for the second derivatives of the numerical test of Fig. 2 due to the smallness of the inclusion. The

verification work of the DSM for the second derivatives is performed for the numerical test of Fig. 3 that has the large inclusion. The second derivatives of the surface flux with respect to Σ_c, Σ_s , and g are given in Tables 10, 11, and 12, respectively. The results of the DSM agree with those of the DOS within two standard deviations. This agreement suggests that the DSM yields the correct second derivatives. For reference, the comparison between the DSM and DOS for the small inclusion is presented in Appendix.

[Tables 10, 11, 12]

The computational efficiency of the DSM is evaluated for the numerical test of Fig. 2 where the inclusion is small. A different factor C could be respectively assigned to the first and second derivative calculations. However, finding an optimal combination of the factor C is not an easy task. In this paper, the same C value is assigned to both derivative calculations. Tables 13, 14, and 15 compare the relative FOMs of the second derivative with respect to Σ_c, Σ_s , and g , respectively. The efficiency improvement caused by the pseudo scattering is the most notable for the scattering cross section. The efficiency is improved by a factor of several hundred at most compared with the DOS for the scattering cross section. The superiority of the DSM to the DOS could be further enhanced for a smaller ROI or by finding an optimal combination of the factor C .

[Tables 13, 14, 15]

5.4 Effect of the inclusion size

As stated above, the efficiency of the DSM is expected to increase as the inclusion size decreases. Table 16 compares the relative FOM with respect to the DOS for the inclusion sizes of 0.02×0.02 cm and 0.05×0.05 cm. The factor C used for the results in Table 16 is chosen so that it maximizes the FOM; otherwise, $C = 100$. As seen from Table 16, the FOMs are larger for the smaller inclusion.

[Table 16]

6. Conclusions

A new Monte Carlo sensitivity analysis method for fixed source problems is proposed, which is dubbed the derivative source method (DSM). An arbitrary order of sensitivity analyses can be easily performed with the differential operator sampling method (DOS). However, the DOS has a

1 weakness in that it suffers from poor performance when a region of interest (ROI) is small within
2 the whole domain because particles rarely enter the ROI. The DSM can overcome this weakness
3 by adding a pseudo scattering cross section to the ROI. The pseudo scatterings increase the number
4 of derivative particles emitted from the ROI, which improves the performance of the derivative
5 calculations. The efficiency increases with the added pseudo scattering cross section up to a certain
6 maximum point. The DSM is inferior to the DOS for larger ROIs because too many derivative
7 particles have to be tracked. On the other hand, the DSM further outperforms the DOS in the
8 sensitivity analysis of a small inclusion.

9 This paper demonstrates the viability of expanding the DSM to higher-order sensitivity
10 analyses. When an n th-order derivative particle undergoes a collision in an ROI, then the
11 subsequent higher order particle is emitted from the collision point. By performing this process
12 successively, the DSM can be expanded to an arbitrary order of sensitivity analyses. The numerical
13 tests for the small inclusion show that the DSM is superior to the DOS for the calculations of the
14 second derivatives of the surface flux. The DSM can be applied to continuous energy Monte Carlo
15 simulations that can be handled with the DOS. The advantage of the DSM over the DOS in
16 sensitivity analyses for a small region is still valid even for continuous energy simulations. Future
17 work will be focused on developing a method to find an optimal combination of the factors of the
18 pseudo scattering for higher-order sensitivity analyses.

19 Appendix

20
21 The numerical tests for the small inclusion shown in Fig. 2 are not suitable for verification of
22 the second order derivatives due to the large uncertainties in the DOS. However, the second
23 derivatives of the surface flux with respect to Σ_c , Σ_s , and g are compared between the DSM and
24 DOS in Tables A.1, A.2, and A.3, respectively.

25 [Tables A.1, A.2, A.3]

26 Although a precise comparison cannot be made for the small inclusion, the second derivatives
27 with the DSM agree with those with the DOS within the statistical uncertainties.

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Figure legends

- 1
- 2 Fig. 1(a) Flow chart of the fixed source calculation mode. The connector boxes 1 and 2 are
- 3 connected to those in Fig. 1(b).
- 4 Fig. 1(b) Flow chart of the derivative calculation mode.
- 5 Fig. 2 Geometry for the numerical test (small inclusion).
- 6 Fig. 3 Geometry for the numerical test (large inclusion).

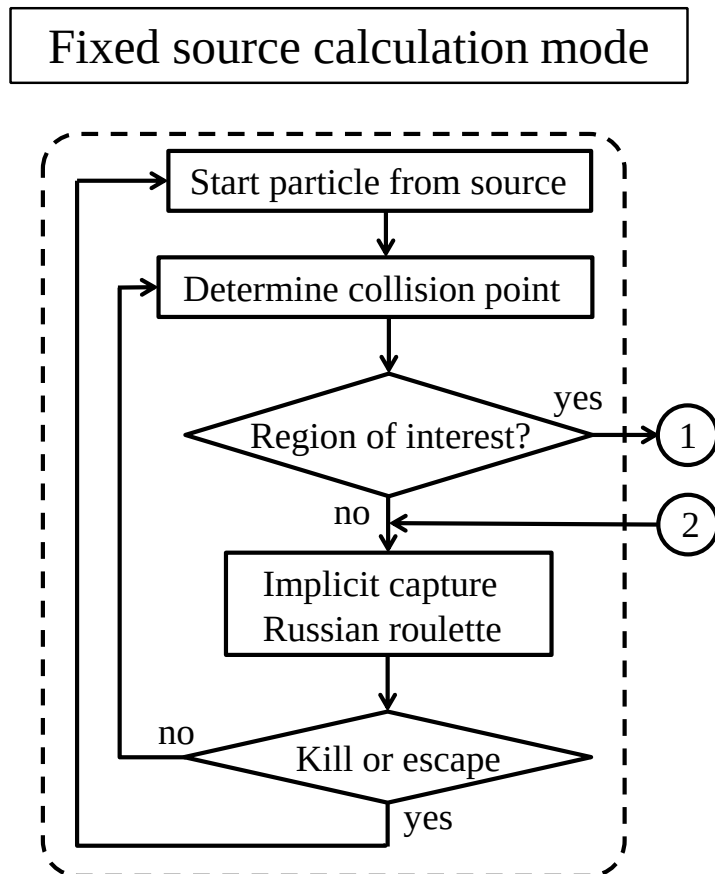


Fig. 1(a) Flow chart of the fixed source calculation mode. The connector boxes 1 and 2 are connected to those in Fig. 1(b).

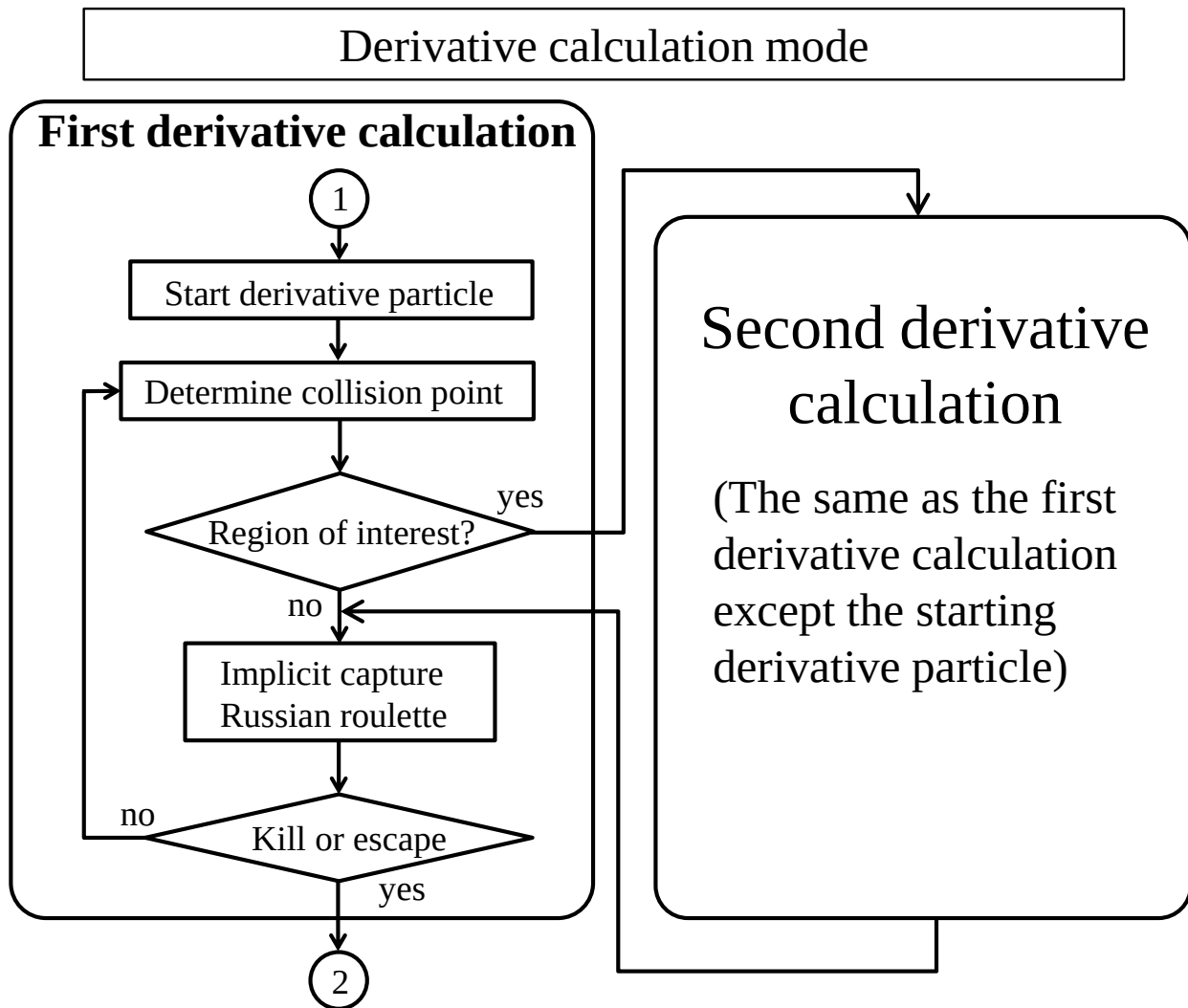


Fig. 1(b) Flow chart of the derivative calculation mode.

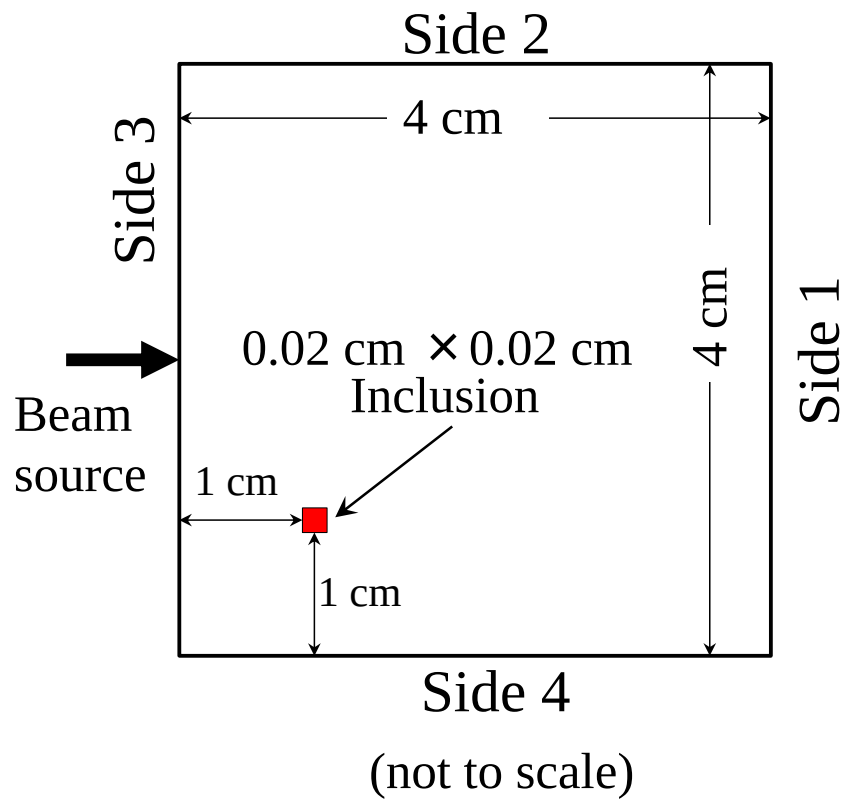


Fig. 2 Geometry for the numerical test (small inclusion).

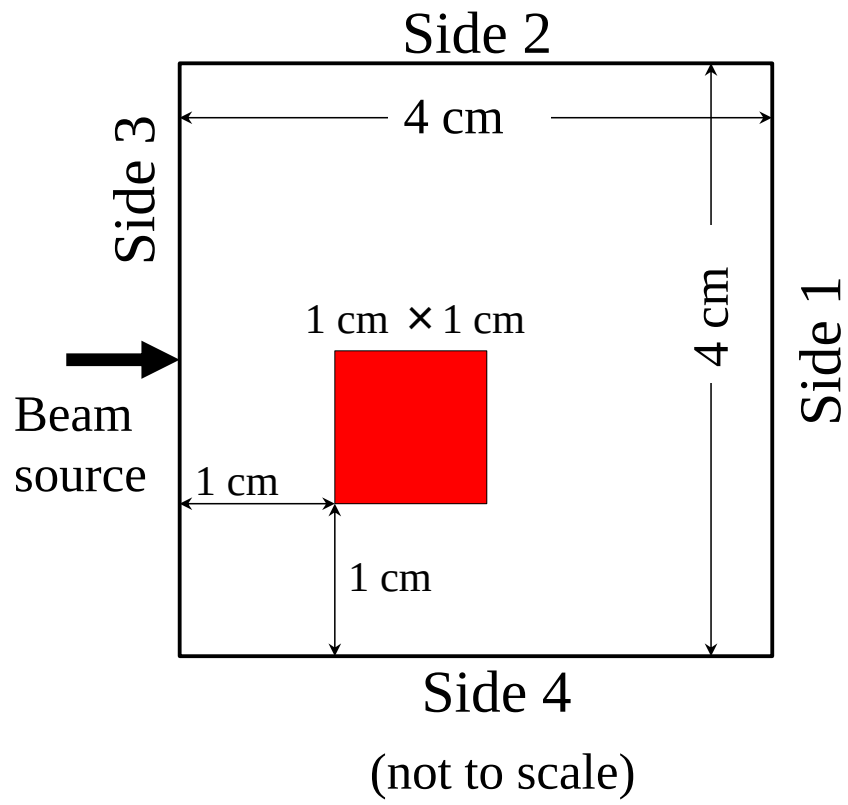


Fig. 3 Geometry for the numerical test (large inclusion).

Table 1 First derivative of the surface flux with respect to Σ_c .

	Side 1	Side 2	Side 3	Side 4
DSM	$-5.19\text{E-}6^a$	$-3.67\text{E-}6$	$-2.18\text{E-}5$	$-5.08\text{E-}5$
$C=100$	$(3.38\text{E-}9)^b$	$(2.63\text{E-}9)$	$(1.25\text{E-}8)$	$(2.33\text{E-}8)$
DOS	$-5.20\text{E-}6$	$-3.67\text{E-}6$	$-2.18\text{E-}5$	$-5.08\text{E-}5$
	$(6.92\text{E-}9)$	$(5.42\text{E-}9)$	$(1.61\text{E-}8)$	$(2.50\text{E-}8)$

^a Read as -5.19×10^{-6}

^b One standard deviation

Table 2 First derivative of the surface flux with respect to Σ_s .

	Side 1	Side 2	Side 3	Side 4
DSM	$4.22\text{E-}7^a$	$3.80\text{E-}7$	$9.52\text{E-}7$	$-2.30\text{E-}6$
$C=100$	$(4.88\text{E-}9)^b$	$(3.92\text{E-}9)$	$(1.09\text{E-}8)$	$(1.76\text{E-}8)$
DOS	$4.31\text{E-}7$	$3.75\text{E-}7$	$9.91\text{E-}7$	$-2.33\text{E-}6$
	$(1.30\text{E-}8)$	$(9.50\text{E-}9)$	$(2.91\text{E-}8)$	$(4.60\text{E-}8)$

^a Read as 4.22×10^{-7}

^b One standard deviation

Table 3 First derivative of the surface flux with respect to the anisotropy factor g .

	Side 1	Side 2	Side 3	Side 4
DSM	$-4.20\text{E-}5^a$	$-3.89\text{E-}5$	$-9.48\text{E-}5$	$2.29\text{E-}4$
$C=100$	$(2.77\text{E-}7)^b$	$(2.27\text{E-}7)$	$(6.53\text{E-}7)$	$(1.06\text{E-}6)$
DOS	$-4.06\text{E-}5$	$-3.85\text{E-}5$	$-9.12\text{E-}5$	$2.34\text{E-}4$
	$(1.30\text{E-}6)$	$(9.20\text{E-}7)$	$(2.89\text{E-}6)$	$(4.62\text{E-}6)$

^a Read as -4.20×10^{-5}

^b One standard deviation

Table 4 Relative FOM of the first derivative with respect to Σ_c .

		Side 1	Side 2	Side 3	Side 4
DOS		1	1	1	1
DSM	$C=1$	0.329	0.338	0.243	0.253
DSM	$C=10$	2.76	2.89	2.51	1.96
DSM	$C=20$	5.47	5.60	3.72	2.81
DSM	$C=30$	7.62	7.06	4.58	3.48
DSM	$C=50$	11.2	11.7	5.83	4.21
DSM	$C=100$	18.4	18.6	7.21	5.06
DSM	$C=200$	25.2	26.0	7.72	5.30
DSM	$C=300$	27.8	28.5	7.52	5.12
DSM	$C=500$	29.5	31.1	7.14	4.81
DSM	$C=1000$	27.9	29.5	6.10	4.09

Table 5 Relative FOM of the first derivative with respect to Σ_s .

		Side 1	Side 2	Side 3	Side 4
DOS		1	1	1	1
DSM	$C=1$	0.498	0.443	0.530	0.505
DSM	$C=10$	5.30	4.70	5.53	5.28
DSM	$C=20$	9.66	8.41	10.3	9.87
DSM	$C=30$	16.1	13.1	16.1	16.0
DSM	$C=50$	24.6	21.1	25.5	24.5
DSM	$C=100$	47.2	38.9	47.0	44.9
DSM	$C=200$	85.6	71.2	82.8	77.2
DSM	$C=300$	112	94.3	106	97.8
DSM	$C=500$	154	131	138	123
DSM	$C=1000$	212	178	164	138

Table 6 Relative FOM of the first derivative with respect to the anisotropy factor g .

		Side 1	Side 2	Side 3	Side 4
DOS		1	1	1	1
DSM	$C=1$	1.04	0.601	0.817	0.959
DSM	$C=10$	9.56	8.08	9.29	9.91
DSM	$C=20$	18.8	15.2	18.6	18.8
DSM	$C=30$	27.2	21.9	26.1	27.3
DSM	$C=50$	48.6	36.0	45.0	44.8
DSM	$C=100$	92.9	70.0	83.2	81.3
DSM	$C=200$	158	124	145	138
DSM	$C=300$	229	176	190	183
DSM	$C=500$	346	264	266	245
DSM	$C=1000$	546	421	348	300

Table 7 Relative FOM of the first derivative with respect to Σ_c (large inclusion).

		Side 1	Side 2	Side 3	Side 4
DOS		1	1	1	1
DSM	$C=1$	1.09	0.992	1.01	1.11
DSM	$C=2$	0.979	0.946	0.898	0.906
DSM	$C=5$	0.700	0.788	0.647	0.573

Table 8 Relative FOM of the first derivative with respect to Σ_s (large inclusion).

		Side 1	Side 2	Side 3	Side 4
DOS		1	1	1	1
DSM	$C=1$	0.0464	0.0381	0.0397	0.0469
DSM	$C=2$	0.0487	0.0397	0.0416	0.0491
DSM	$C=5$	0.0489	0.0401	0.0415	0.0491

Table 9 Relative FOM of the first derivative with respect to the anisotropy factor g (large inclusion).

		Side 1	Side 2	Side 3	Side 4
DOS		1	1	1	1
DSM	$C=1$	0.147	0.130	0.134	0.141
DSM	$C=2$	0.159	0.140	0.146	0.151
DSM	$C=5$	0.167	0.147	0.153	0.156

Table 10 Second derivative of the surface flux with respect to Σ_c (large inclusion).

	Side 1	Side 2	Side 3	Side 4
DSM	4.53E-2 ^a	2.69E-2	3.88E-2	6.59E-2
$C=1$	(7.69E-6) ^b	(4.96E-6)	(7.00E-6)	(1.10E-5)
DOS	4.53E-2	2.69E-2	3.88E-2	6.60E-2
	(5.01E-6)	(3.58E-6)	(4.79E-6)	(6.65E-6)

^a Read as 4.53×10^{-2}

^b One standard deviation

Table 11 Second derivative of the surface flux with respect to Σ_s (large inclusion).

	Side 1	Side 2	Side 3	Side 4
DSM	1.84E-4 ^a	-1.28E-4	-8.14E-5	4.38E-5
$C=1$	(4.18E-6) ^b	(3.22E-6)	(3.79E-6)	(4.95E-6)
DOS	1.86E-4	-1.29E-4	-8.59E-5	4.48E-5
	(3.91E-7)	(2.44E-7)	(2.92E-7)	(4.39E-7)

^a Read as 1.84×10^{-4}

^b One standard deviation

Table 12 Second derivative of the surface flux with respect to the anisotropy factor g (large inclusion).

	Side 1	Side 2	Side 3	Side 4
DSM	1.75E+0 ^a	-1.29E+0	-7.64E-1	4.92E-1
$C=1$	(1.44E-2) ^b	(1.17E-2)	(1.41E-2)	(1.73E-2)
DOS	1.78E+0	-1.30E+0	-7.70E-1	5.15E-1
	(5.13E-3)	(3.38E-3)	(3.96E-3)	(5.68E-3)

^a Read as 1.75×10^0

^b One standard deviation

Table 13 Relative FOM of the second derivative with respect to Σ_c .

		Side 1	Side 2	Side 3	Side 4
DOS		1	1	1	1
DSM	$C=1$	0.145	0.448	0.287	0.145
DSM	$C=10$	21.9	30.1	10.8	7.61
DSM	$C=20$	47.5	60.6	15.5	11.9
DSM	$C=30$	57.2	71.0	15.9	12.6
DSM	$C=50$	58.4	70.2	14.3	11.7
DSM	$C=100$	36.9	43.5	8.59	7.15

Table 14 Relative FOM of the second derivative with respect to Σ_s .

		Side 1	Side 2	Side 3	Side 4
DOS		1	1	1	1
DSM	$C=1$	0.694	0.278	0.279	0.252
DSM	$C=10$	55.1	27.2	25.0	25.2
DSM	$C=20$	194	94.2	86.0	88.8
DSM	$C=30$	344	168	152	156
DSM	$C=50$	608	295	269	276
DSM	$C=100$	947	460	404	408
DSM	$C=500$	1030	491	244	211
DSM	$C=1000$	786	364	98.0	75.7

Table 15 Relative FOM of the second derivative with respect to the anisotropy factor g .

		Side 1	Side 2	Side 3	Side 4
DOS		1	1	1	1
DSM	$C=1$	1.00	0.959	0.956	1.09
DSM	$C=10$	11.5	9.12	10.8	11.3
DSM	$C=20$	21.9	20.4	18.7	20.4
DSM	$C=30$	29.0	29.5	27.2	28.8
DSM	$C=50$	41.6	39.6	37.7	40.7
DSM	$C=100$	48.1	47.3	41.1	48.7
DSM	$C=200$	34.4	33.3	31.7	34.5
DSM	$C=300$	25.3	24.6	23.7	26.2
DSM	$C=500$	16.2	14.9	14.1	15.6

Table 16 Comparison of relative FOM of Side 1 with respect to DOS between two inclusions.

Parameter α	Order	Size of inclusion	
		0.02×0.02 cm	0.05×0.05 cm
Σ_c	First	29.5 (500)*	20.1 (100)
Σ_s	First	47.2 (100)	26.6 (100)
g	First	92.9 (100)	64.6 (100)
Σ_c	Second	59.4 (40)	34.6 (20)
Σ_s	Second	1003 (500)	28.6 (100)
g	Second	48.1 (100)	12.7 (20)

*Factor C defined in Eq. (11)

Table A.1 Second derivative of the surface flux with respect to Σ_c (small inclusion).

	Side 1	Side 2	Side 3	Side 4
DSM	1.63E-7 ^a	1.28E-7	6.85E-7	1.34E-2
$C=30$	(5.28E-11) ^b	(4.79E-11)	(2.28E-10)	(1.34E-10)
DOS	1.62E-7	1.27E-7	6.85E-7	1.34E-6
	(7.92E-11)	(7.87E-11)	(2.09E-10)	(2.25E-10)

^a Read as 1.63×10^{-7}

^b One standard deviation

Table A.2 Second derivative of the surface flux with respect to Σ_s (small inclusion).

	Side 1	Side 2	Side 3	Side 4
DSM	-1.58E-9 ^a	-6.69E-10	-2.32E-9	7.03E-9
$C=1$	(1.99E-11) ^b	(1.70E-11)	(4.60E-11)	(6.66E-11)
DOS	-1.48E-9	-7.05E-10	-2.07E-9	7.29E-9
	(1.52E-10)	(1.37E-10)	(3.67E-10)	(4.98E-10)

^a Read as -1.58×10^{-9}

^b One standard deviation

Table A.3 Second derivative of the surface flux with respect to the anisotropy factor g (small inclusion).

	Side 1	Side 2	Side 3	Side 4
DSM	$-4.75\text{E-}5^{\text{a}}$	$4.84\text{E-}6$	$-3.44\text{E-}5$	$1.27\text{E-}4$
$C=100$	$(7.52\text{E-}7)^{\text{b}}$	$(5.93\text{E-}7)$	$(1.73\text{E-}6)$	$(2.91\text{E-}6)$
DOS	$-4.67\text{E-}5$	$3.00\text{E-}6$	$-3.44\text{E-}5$	$1.32\text{E-}4$
	$(3.49\text{E-}6)$	$(2.72\text{E-}6)$	$(7.97\text{E-}6)$	$(1.34\text{E-}5)$

^a Read as -4.75×10^{-5}

^b One standard deviation

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

CRedit authorship contribution statement

Toshihiro Yamamoto: Supervision, Methodology, Conceptualization, Investigation, Writing - original draft. **Hiroki Sakamoto:** Software, Validation, Formal analysis, Data curation, Writing - review & editing.