

A New Strategy on the Monte Carlo Eigenvalue Estimation Method Based on the Fission Matrix Using Fine-Coarse Mesh Division

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1. Introduction

The Monte Carlo (MC) method is a stochastic approach to estimate the particle transport behaviors with the simulation of each particle. When fissionable materials are included in MC neutron simulation, the fissionable materials can be potential neutron sources. Also, the MC simulation including the fissionable materials can be infinitely repeated when the multiplication factor of a system is exceeded to 1. To avoid the infinite repetition and to sample the fission neutron source positions, the MC power iteration method has been generally used. However, it is well-known that the power iteration method causes some problems about fission source convergence and real variance. In addition, for the MC simulation with the power iteration method, the simulation information in each cycle should be gathered to use them in the next cycle simulation. This leads calculation inefficiency in the parallel computation system because the communication time with each parallel computation system can cost with lots of the cycles. To overcome the problems, a lot of theories which are diagnostics [1-3] and acceleration methods [4-6] of the fission source convergence, estimation method of the real variance [7-9] have been studied. However, these methods cannot perfectly overcome the problems of the power iteration method. In a previous study [10], a fission matrix based eigenvalue estimation method was proposed using fixed source MC estimation method. However, the fission matrix based method has some critical limitations, which are the memory problem to generate an accurate fission matrix and the inefficiency to generate the fission matrix for small mesh sizes. In this study, to solve the problems, a new strategy to simulate the eigenvalue problems is proposed based on the fission matrix and adjoint fluxes with fine-coarse mesh divisions.

2. Methods and Results

In this section, the review of the MC eigenvalue simulation method is first introduced. Then, the proposed strategy is described in section 2.2.

2.1 Review of MC Eigenvalue Estimation Method

For the eigenvalue estimation, the neutron particle transport equation can be expressed as the follows:

$$\Omega \cdot \nabla \phi + \Sigma_t \phi = \int_{4\pi} \int_0^\infty \Sigma_s(r, \Omega', E' \rightarrow \Omega, E) \phi(r, \Omega', E') d\Omega' dE' \quad (1)$$

$$+ \frac{1}{k} \int_{4\pi} \int_0^\infty \frac{\chi}{4\pi} v \Sigma_f \phi'(r, \Omega', E') d\Omega' dE'$$

Eq. (1) can be simply expressed as the following equation:

$$T\phi = \frac{1}{k} \frac{\chi}{4\pi} s(r) \quad (2)$$

where,

$$T\phi = \Omega \cdot \nabla \phi + \Sigma_t \phi - \int_{4\pi} \int_0^\infty \Sigma_s(r, \Omega', E' \rightarrow \Omega, E) \phi(r, \Omega', E') d\Omega' dE'$$

$$s(r) = \int_{4\pi} \int_0^\infty v \Sigma_f \phi'(r, \Omega', E') d\Omega' dE'$$

Based on the Green's function [11], the flux at (r, Ω, E) can be estimated by Eq. (3).

$$\phi(r, \Omega, E) \quad (3)$$

$$= \frac{1}{k} \int_V \int_{4\pi} \int_0^\infty \frac{\chi(r_0, E_0)}{4\pi} S(r_0) G(r_0, \Omega_0, E_0 \rightarrow r, \Omega, E) dr_0 d\Omega_0 dE_0$$

where, $TG(r_0, \Omega_0, E_0 \rightarrow r, \Omega, E) = \delta(r - r_0) \delta(\Omega - \Omega_0) \delta(E - E_0)$ and T is the transport operator used in Eq. (2).

Then, with Eq. (3), the fission source density $S(r)$ in Eq. (2) can be expressed as the follows:

$$s(r) = \frac{1}{k} \int_V s(r_0) dr_0 \int_{4\pi} \int_0^\infty d\Omega dE v \Sigma_f \int_{4\pi} \int_0^\infty d\Omega_0 dE_0 \frac{\chi(r_0, E_0)}{4\pi} G(r_0, \Omega_0, E_0 \rightarrow r, \Omega, E) \quad (4)$$

If a fission kernel is defined as Eq. (5), the fission source density can be expressed to Eq. (6).

$$f(r_0 \rightarrow r) = \int_{4\pi} \int_0^\infty d\Omega dE v \Sigma_f \int_{4\pi} \int_0^\infty d\Omega_0 dE_0 \frac{\chi(r_0, E_0)}{4\pi} G(r_0, \Omega_0, E_0 \rightarrow r, \Omega, E) \quad (5)$$

$$s(r) = \frac{1}{k} \int_{V_f} f(r_0 \rightarrow r) s(r_0) dr_0 \quad (6)$$

In the general eigenvalue calculation, the fission source density is estimated with the equation (7) as known as the power iteration method.

$$s^t(r) = \frac{1}{k^{t-1}} \int_{V_f} f(r_0 \rightarrow r) s^t(r_0) dr_0 \quad (7)$$

where t is the number of iteration cycle, r_0 is a previous location, r is a current location, and k is the multiplication factor. It is practically impossible to simulate all of the positions r_0 and r . Therefore, in the general MC eigenvalue calculation with the power iteration method, initial sample locations $S(r_0)$ and multiplication factors k^0 are defined by the user. Then, using random process based on the Eq. (7), the new source distribution is obtained. This procedure should be repeated until the source distribution is converged. This power iteration method can be an effective solution with unknown fission source distribution. However, this

approach causes following problems; (1) fission source convergence and (2) real variance. The eigenvalue estimation should be performed in the convergence condition of the fission source distribution. However, the reference data of the fission source distribution is unknown. Hence, lots of studies performed to diagnostics of the fission source convergence [1-3]. Also, slow convergence problem of the fission source distribution is also known. The acceleration methods are studied in the previous studies [4-6]. Also, as shown in Eq. (7), the new source distribution is sampled from the previous source distribution. This means that the estimated error using MC simulation should be underestimated due to the correlation between the source distributions. The estimation of the real variance is noted at the previous studies [7-9].

To solve the fission source convergence and real variance problems in using the power iteration method, a fission matrix based MC method was proposed in a previous study [10]. Based on Eq. (7), fission matrix $F[i,j]$ based eigenvalue equation can be expressed as the follows:

$$S^t[j] = \frac{1}{k^{t-1}} F[i,j] S^{t-1}[i] \quad (8)$$

The fission matrix and source density matrix are defined as the follows:

$$F[i,j] = \frac{\int_{V_j} \int_{V_i} s(r_0) f(r_0 \rightarrow r) dr_0 dr}{\int_{V_j} s(r_0) dr_0} \quad (9)$$

$$S^t[i] = \int_{V_i} s^t(r) dr \quad (10)$$

If the V_i and V_j are very small (V_i and $V_j \rightarrow 0$), Eq. (8) gives a same result with that calculated by Eq. (7). In the previous study, it was assumed that the mesh is small enough to ignore the bias caused by mesh size. With the assumption, the eigenvalue can be calculated by Eq. (11) after enough power iteration with Eq. (8).

$$k^t = (S^t)^{-1} F S^{t-1} \quad (11)$$

This method uses the fixed sources to calculate the fission matrix; therefore, the problems about the fission source convergence and the real variance are not basically generated. However, this approach has some critical simulation problems. To calculate the accurate fission matrix, each mesh region V_i should be sufficiently small. This leads to the numerous number of mesh regions. If a system is divided to the 10^6 meshes, the fission matrix has $10^6 \times 10^6$ dimensions, which occupies 8×10^{12} bites (8 terabits) computation memories. This means that if a system is large, this method cannot be applied for the analysis. The physical meaning of the fission matrix $F[i,j]$ is that the fission neutron generation rate into j region from a neutron generated from i region. Therefore, if a system is divided to the 10^6 meshes, the fixed source estimation must be repeated to 10^6 times to calculate each fission matrix value with a sufficient number of particle

histories. This can lead a serious inefficiency on the estimating the MC eigenvalue problem.

2.2 Proposal on Fine-Coarse Mesh Division Strategy

In this study, to solve problem of the fission matrix based MC criticality calculation method, a fine-coarse mesh division strategy is proposed. As shown in Eq. (9), the accuracy of the fission matrix depends on the accurate $S(r_0)F(r_0 \rightarrow r)$ and $S(r_0)$ not only the mesh size V_i . This means that the very accurate mesh division for the fission matrix is not required for the fission matrix based MC eigenvalue calculation if both $S(r_0)F(r_0 \rightarrow r)$ and $S(r_0)$ are accurately estimated. Hence, we propose a strategy that a coarse mesh division is first performed for the fuel region based on Eqs. (8) – (10). To calculate accurate fission matrix for each coarse mesh, fine mesh division is pursued in each coarse mesh region. If the fine mesh size is small enough, Eqs. (9) and (10) can be approximated to Eqs. (11) and (12).

$$F[i,j] \approx \frac{\sum_{l=1}^n \sum_{k=1}^m S[i,k] f(r_i[k] \rightarrow r_j[l])}{\sum_{i=1}^m S[i,k]} \quad (11)$$

$$S[i] = \sum_{k=1}^m S[i,k] \quad (12)$$

where $r_i[k]$ is the region of the k^{th} fine mesh in i^{th} coarse mesh and $f(r_i[k] \rightarrow r_j[l])$ is the fission kernel from $r_i[k]$ region to $r_j[l]$ region. Based on the fine-coarse mesh division strategy, the MC eigenvalue simulation is performed as shown in Fig. 1. The details of the calculation procedure are given as the follows:

- Step 1) The source number density $S[i,k]$ in each fine-coarse is assumed to be uniform source.
- Step 2) Fixed source MC simulation is performed for each coarse mesh to estimate Eq. (13) with the information of the normalized source distribution with the Eq. (14). In the simulation, generation of neutron caused by fission reaction is suppressed. Instead of it, the number of fission neutrons started from i^{th} coarse mesh is counted for all fine meshes based on the track length estimation method. The results are stored in the computation memory.

$$\sum_k r_i[k] f(r_i[k] \rightarrow r_j[l]) = \frac{1}{N} \sum_c w_{i \rightarrow l, c} d_{i \rightarrow l, c} v_{l, c} \Sigma_{f, l, c} \quad (13)$$

$$r_i[k] = \begin{bmatrix} S[i,1] / S[i] \\ S[i,2] / S[i] \\ \dots \\ S[i,k] / S[i] \\ \dots \\ S[i,m] / S[i] \end{bmatrix} \quad (14)$$

where $r_i[k]f(r_i[k] \rightarrow r_j[l])$ is the fission contribution rate of neutrons produced from

the locations which are randomly sampled in $r_i[k]$ distribution to $r_j[l]$ fine mesh, N is the number of the particle transport started from the i^{th} coarse mesh, $w_{i \rightarrow l, c}$ is the weight of a particle started from i^{th} coarse mesh into the l^{th} fine mesh for c^{th} event, $d_{i \rightarrow l, c}$ is the trajectory track length started from i^{th} coarse mesh into the l^{th} fine mesh for c^{th} event, $\Sigma_{f, l, c}$ is the macroscopic fission cross section of l^{th} fine mesh for c^{th} event, and $\nu_{l, c}$ is the number of neutrons produced per fission in l^{th} fine mesh for c^{th} event. Then, fission matrix based on the coarse mesh with Eqs. (11) – (14) can be derived to Eq. (15).

$$F[i, j] = \sum_l \sum_k r_i[k] f(r_i[k] \rightarrow r_j[l]) \quad (15)$$

Also, to calculate the responses (such as flux or power distributions), forward adjoint fluxes $\sum_k \psi^+(r_i[k], \Omega_0, E_0 \rightarrow r, \Omega, E)$ are calculated during the fixed source simulations using scoring functions.

Step 3) Using the fission matrix calculated from the Eq. (15), the power iteration is pursued by Eq. (8). If the $S^t[i]$ and $S^{t-1}[i]$ satisfy the Eq. (16), the $S[i]$ is updated from the $S^t[i]$.

$$\frac{S^t[i] - S^{t-1}[i]}{S^{t-1}[i]} < e[i] \quad (16)$$

where $e[i]$ is the relative error criteria of the i^{th} coarse mesh to judge the convergence of the fission source density.

Step 4) Using the coarse mesh source number density $S[i]$ estimated in Step 3, the new source number density $S^t[i, k]$ in each fine mesh is calculated by Eq. (17).

$$S^t[i, k] = \sum_j S[j] \sum_l r_j[l] f(r_j[l] \rightarrow r_i[k]) \quad (17)$$

If the new source distribution meets the criteria given in Eq. (18), go to Step 5; otherwise, go to Step 2 with updating source number density using Eq. (19).

$$\frac{S[i, k] - S^t[i, k]}{S^t[i, k]} < e[i, k] \quad (18)$$

$$S[i, k] = S^t[i, k] \quad (19)$$

where $e[i, k]$ is the relative error criteria of the k^{th} fine mesh in i^{th} coarse mesh to judge the convergence of the fission source density.

Step 5) Using the coarse mesh source number density $S[i]$, multiplication factor is calculated by Eq. (11). Also, using the adjoint flux relation expressed in Eq. (20), the response can be calculated by Eq. (21). To express it as a matrix type, Eq. (21) can be rewritten to Eq. (22).

$$\langle \psi^+, q \rangle = \langle \psi, q^+ \rangle \quad (20)$$

$$R = \int_{V_r} \int_{4\pi} \sum_i S[i] \sum_k \psi^+(r_i[k], \Omega_0, E_0 \rightarrow r, \Omega, E) dr_r d\Omega_0 dE_0 \quad (21)$$

$$R = \psi^+[n] S[n] \quad (22)$$

where $\psi^+[n] = [\psi^+_1 \ \psi^+_2 \ \dots \ \psi^+_n]$, and ψ^+_i is the i^{th} adjoint flux (the expected contribution to the response from a particle of the $S[i]$ fission source locations).

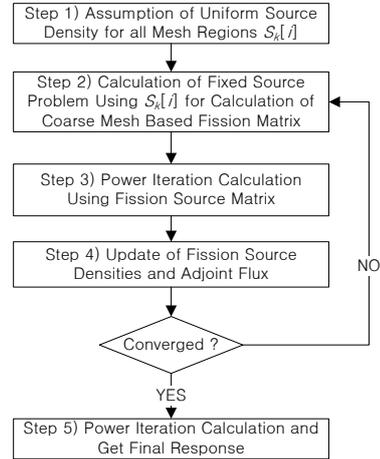


Fig. 1. Overall Algorithm on MC Eigenvalue Simulation Method Based on the Fine-Coarse Mesh Division Proposed in This Study

Because the fission matrix is calculated with fine-coarse meshes, which is not the continuous location, bias is existed in the fission matrix. Therefore, the bias caused by the fission source locations in each fine mesh should be included in the fission matrix. The $n \times n$ fission matrix including the biases can be expressed as given in Eq. (23).

$$F[n \times n] = \begin{bmatrix} F(r_1 \rightarrow r_1) + e_{11} & F(r_2 \rightarrow r_1) + e_{21} & \dots & F(r_n \rightarrow r_1) + e_{n1} \\ F(r_1 \rightarrow r_2) + e_{12} & F(r_2 \rightarrow r_2) + e_{22} & \dots & F(r_n \rightarrow r_2) + e_{n2} \\ \dots & \dots & \dots & \dots \\ F(r_1 \rightarrow r_n) + e_{1n} & F(r_2 \rightarrow r_n) + e_{2n} & \dots & F(r_n \rightarrow r_n) + e_{nn} \end{bmatrix} \quad (23)$$

where e_{ij} is the bias of the fission matrix element estimated in using the proposed method. Then, the bias term can be separated to Eq. (24).

$$F[n \times n] = F_R[n \times n] + E_b[n \times n] \quad (24)$$

where

$$F_R[n \times n] = \begin{bmatrix} F(r_1 \rightarrow r_1) & F(r_2 \rightarrow r_1) & \dots & F(r_n \rightarrow r_1) \\ F(r_1 \rightarrow r_2) & F(r_2 \rightarrow r_2) & \dots & F(r_n \rightarrow r_2) \\ \dots & \dots & \dots & \dots \\ F(r_1 \rightarrow r_n) & F(r_2 \rightarrow r_n) & \dots & F(r_n \rightarrow r_n) \end{bmatrix}$$

$$E_b[n \times n] = \begin{bmatrix} e_{11} & e_{21} & \dots & e_{n1} \\ e_{12} & e_{22} & \dots & e_{n2} \\ \dots & \dots & \dots & \dots \\ e_{1n} & e_{2n} & \dots & e_{nn} \end{bmatrix}$$

For the calculation of the multiplication factor, Eq. (11) can be rewritten to Eq. (25).

$$k^t = (S^t)^{-1} (F_R + E_b) S^{t-1} = (S^t)^{-1} F_R S^{t-1} + (S^t)^{-1} E_b S^{t-1} \quad (25)$$

In this study, it is assumed that the fine mesh has very small size. Then, in this research step, it is assumed that the each element of the bias matrix E_R is ~ 0 .

In the proposed method, the fission source density is calculated by fission matrix with the power iteration method; therefore, the MC uncertainties of the fission source density are not included. However, the fission matrix is calculated by MC method with the fixed sources. Thus, the fission matrix includes stochastic uncertainty. The stochastic error of the result calculated by proposed method can be expressed with Eqs. (26) and (27) for the multiplication factor and the other response, respectively.

$$\sigma_k = \sqrt{\sum_i \{S^p[i]\}^2 \sum_j \sigma^2[F(r_j \rightarrow r_i)] \{S^{p-1}[j]\}^2} \quad (26)$$

$$\sigma_R = \sqrt{\sum_i \sigma^2[\psi^+[i]] \{S[i]\}^2} \quad (27)$$

To optimize the calculation efficiency of the proposed method, CADIS approach [12] can be applied. Let the response R be the source distribution $S(r)$; then, it is clear that the fission matrix is the adjoint flux for the $S(r)$ response. If an alternative fission source generation density $s'(r_0)$ is introduced to Eq. (6), the new fission source density can be written to Eq. (28). Also, the variance in using $s'(r_0)$ is estimated with Eq. (29).

$$E[s(r)] = \int_{V_r} \left[\int_{V_r} dr \frac{f(r_0 \rightarrow r) s(r_0)}{V_T k \cdot s'(r_0)} \right] s'(r_0) dr_0 \quad (28)$$

$$\text{var}(s(r)) = \int_{V_r} \left[\int_{V_r} dr \frac{f(r_0 \rightarrow r) s(r_0)}{V_T k \cdot s'(r_0)} \right]^2 s'(r_0) dr_0 - E^2[s(r)] \quad (29)$$

The optimized $s'(r_0)$ can be decided by Eq. (30) which is derived to get the minimum variance of the source distributions from Eq. (29) [13]. Finally, the matrix form to apply it into our proposed method can be derived as shown in Eq. (31).

$$s'(r_0) = \frac{\int_{V_r} dr f(r_0 \rightarrow r) s(r_0)}{\int_{V_r} dr \int_{V_r} f(r_0 \rightarrow r) s(r_0) dr_0} \quad (30)$$

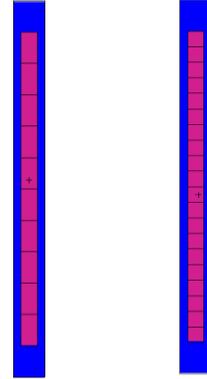
$$S'[i] = \frac{\sum_j F(i, j) S[j]}{\sum_i \sum_j F(i, j) S[i]} \quad (31)$$

where $S'[i]$ is the modified source number density at i^{th} coarse mesh for the optimization of the calculation efficiency. To optimize the calculation efficiency with Eq. (31), the particle history for each fixed source calculation at i^{th} coarse mesh should be decided as the fraction of $S'[i]$.

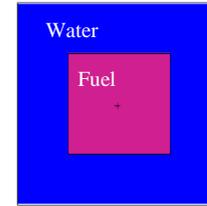
2.3 Feasibility Study and Analysis

For the verification of the proposed method, a benchmark problem was assumed and modeled by MCNPX code [14] as shown in Fig. 2. Using reflective boundary condition, an infinite arrangement was assumed. The details of the benchmark problem are given in Table I. Using the benchmark problem, three

calculations were pursued using the methods; (1) conventional power iteration method; (2) the proposed method with 10 coarse mesh division and 10 x 10 x 10 fine mesh division for each coarse mesh; (3) the proposed method with 20 coarse mesh division and 10 x 10 x 5 fine mesh division for each coarse mesh. For the estimation of the proposed method, it is assumed that the fission source is uniformly distributed at each initial cycle. The MCNP simulations were performed using MCNPX 2.7.0 code [14]. The ENDF-VI cross section library was used for the estimations. The details of the estimation conditions are given in Table II.



(a) Axial View for 10 (Left) and 20 (Right) Coarse Mesh Divisions



(b) Radial View

Fig. 2. Axial and Radial Views of the Benchmark Problem

Table I: Details of the Benchmark Problem

Group	Classification	Value	
Fuel	Geometry	Parallelepipedon (5 cm x 5 cm x 100 cm)	
	Density	10.96 g/cm ³	
	Atom Fraction	O-16:	0.666667
		U-234:	0.000090
U-235:		0.010124	
U-236:		0.000046	
Water	Geometry	Parallelepipedon (10 cm x 10 cm x 120 cm)	
	Density	1 g/cm ³	
	Atom Fraction	H-1:	0.666667
		O-16:	0.333333

Table II: Details of the Estimation Conditions for MCNP Simulation

Method	Classification	Value
Conventional Power Iteration Method (Case 1)	Source	KCODE / KSRC
	Inactive / Active Cycle	200 / 4,800
	Particle History per Cycle	50,000

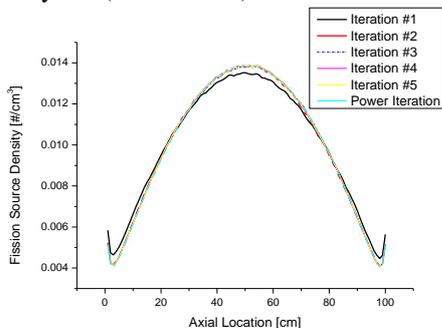
Proposed Method (Case 2)	Source	SDEF (Fixed Source)
	Particle History	1x10 ⁶ per Coarse Mesh
	Mesh Division	10 Coarse Meshes
Proposed Method (Case 3)	Source	SDEF (Fixed Source)
	Particle History	5x10 ⁵ per Coarse Mesh
	Mesh Division	20 Coarse Meshes

The multiplication factors calculated by each method and condition were given in Table III. Comparing with Case 3, the result of Case 2 has a low accuracy at the lower iteration number. The coarse mesh size is increased, and then the accuracy is highly affected by the distribution of the fission sources in fine meshes.

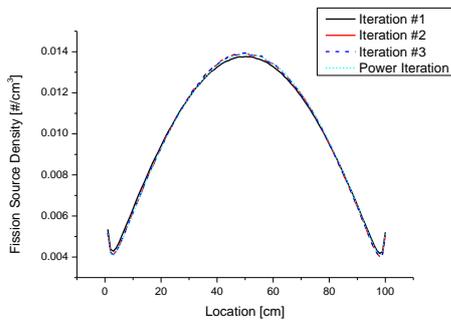
Table III: Results of k_{eff} for the Benchmark Problem

	Iteration #1	Iteration #2	Iteration #3	Iteration #4	Iteration #5
Case 1	1.13597 (0.00040)				
Case 2	1.13126 (0.00045)	1.13515 (0.00046)	1.13566 (0.00045)	1.13549 (0.00046)	1.13568 (0.00046)
Case 3	1.13509 (0.00045)	1.13598 (0.00045)	1.13600 (0.00045)	-	-

Fig. 3 shows the fission source distributions calculated by the proposed method and the conventional power iteration method. The results show that the fission source distributions give good agreements with the result calculated by the power iteration method excepting the Iteration #1 case. Analysis shows that the proposed method can get a high accuracy within few iteration cycles (about 2 or 3).



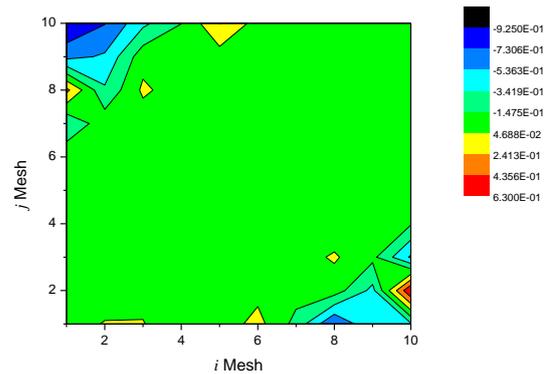
(a) Case 2



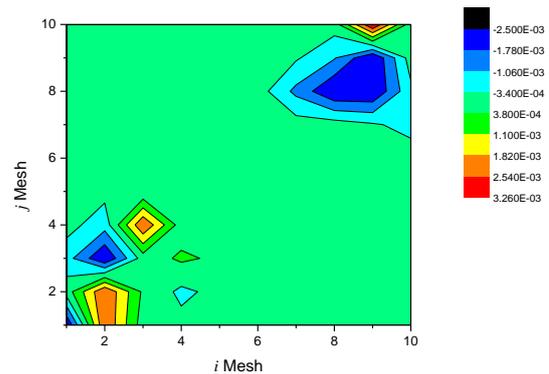
(b) Case 3

Fig. 3. Results of Fission Source Distributions for Each Case

For the confirmation, the relative differences of the fission matrix for Case 2 were calculated. Fig. 4 shows the relative difference maps of the fission matrix comparing with Iteration #3. The differences of the fission matrix at Iteration #1 were relatively high because of the assumption of the uniform distribution in each coarse mesh. Also, as shown in Fig. 4 (b), the relative differences were lowly estimated due to the applications of the fission source distribution (the fine mesh distribution) in each coarse mesh.



(a) Iteration #1



(b) Iteration #2

Fig. 4. Relative Difference Map of the Fission Matrix Comparing with Iteration #3 for Case 2

3. Conclusions

In this study, an alternative method for the MC eigenvalue calculation was proposed to substitute the MC power iteration method. The key idea of the proposed method is that the fuel region is divided to the coarse-fine meshes; then, the eigenvalue calculation is pursued using coarse mesh-based fission matrix with fixed source MC simulation. As a result, the eigenvalue calculation can be performed without the diagnostics of the source convergence and real variance problems occurred by using MC power iteration method. Also, the proposed method can solve the computation memory problem for the fission matrix generation. It is expected that if some additional studies are performed in the future, this method can be utilize for the general MC

eigenvalue calculation with having high accuracy and efficiency.

[14] D.B. Pelowitz, editor, MCNPX™ User's Manual, Version 2.7.0, LA-CP -11-00438, Los Alamos National Laboratory, 2011.

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