A Proposal on the Method of Real Uncertainty Estimation in Two Step Monte Carlo Simulation for Residual Radiation Analysis

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1. Introduction

There are many problems related to multi-step Monte Carlo (MC) calculation. Surface Source Reading (SSR) and Surface Source Writing (SSW) options in MCNP [1], MC depletion calculation, accelerator shielding analysis using secondary particle source term calculation, and residual particle transport calculation caused by activation are the examples of the simulations. In these problems, the average values estimated from the MC result in the previous step are used as sources of MC simulation in the next step. Hence, the uncertainties of the results in previous step are usually not considered for calculating that of next step MC simulation even though they are propagated as the stepwise progression. Therefore the real uncertainty considering the stepwise error propagation should be estimated to get reliable results from multi-step MC. Brute force technique using the multiple clones of input with different random seeds for each step MC is the most straightforward and accurate method to evaluate the real uncertainty. However, due to the computational cost to get the reliable results, a more efficient and accurate method is needed. To solve the problem, a method using the adjoint calculation in 2 step MC is proposed in Oak Ridge National Laboratory (ORNL) [2]. However, there are limitations in accuracy of the adjoint flux and lack of correlation degree between neutron fluxes in each cell. In this study, a new approach to calculate the real variance is proposed for improving the uncertainty estimation efficiency. Using the method, a real uncertainty in the simple activation problem was evaluated. The results were compared with those of the previous method (ORNL) and the brute force technique.

2. Methods and Results

In this section theoretical background and comparison results of the real uncertainty estimation methods are described; in section 2.1, theory and methodologies to evaluate the real uncertainty are introduced; in section 2.2, verification of the real uncertainty estimation method is pursued.

2.1 Proposal on the Theory and Methodologies

2.1.1 Error Propagation in 2 Step MC Calculations

The purpose of this study is to calculate the real uncertainty in 2nd step MC calculation (MC2) which includes the uncertainty developed from uncertainty of 1st MC calculation (MC1). The relationship between the real uncertainty and apparent uncertainty computed in MC2 is described as Eq. (1).

$$\sigma_r{}^2 = \sigma_a{}^2 + \sigma_h{}^2 \quad (1)$$

where σ_r is the real standard deviation (SD) in MC2, σ_a is the apparent SD in MC2, and σ_h is the hidden SD propagated from errors in MC1. In order to estimate the real uncertainty, a simple problem is assumed. In MC1, there are lots of detectors. The responses computed from MC1 become the sources, and a single detector is located for MC2. In this situation, the response in MC2 can be derived by Eq. (2)

$$R = \sum_i S_i C_i \quad (2)$$

where R is the response in MC2, S_i is the i^{th} source strength computed from i^{th} detector in MC1, and C_i is the expected contribution from particles distributed in S_i sources to R response. From Eq. (2), the SD of the R can be derived as shown in Eq. (3) using the error propagation formula.

$$\sigma_R{}^2 = \sum_i \left(\frac{\partial R}{\partial S_i}\right)^2 \sigma_{S_i}{}^2 + 2\sum_{i\neq j}\left(\frac{\partial R}{\partial S_i}\right)\left(\frac{\partial R}{\partial S_j}\right)\sigma_{S_iS_j} + \sum_i \left(\frac{\partial R}{\partial C_i}\right)^2 \sigma_{C_i}{}^2 + 2\sum_{i\neq j}\left(\frac{\partial R}{\partial C_i}\right)\left(\frac{\partial R}{\partial C_j}\right)\sigma_{C_iC_j} \quad (3)$$

where σ_R is the SD of the response in MC2, σ_{S_i} is the SD of the S_i, σ_{S_j} is the SD of the S_j, $\sigma_{S_iS_j}$ is the covariance between S_i and S_j, σ_{C_i} is the SD of the C_i, σ_{C_j} is the SD of the C_j , and $\sigma_{C_iC_j}$ is the covariance between C_i and C_j. If there was no uncertainty in S_i, the first and second term of RHS in Eq. (3) would equal to zero. However, in case of 2 step MC problem, S_i includes uncertainties because it is computed by Monte Carlo method (MC1). Thus, these two terms correspond to σ_h in Eq. (1), and this relationship can be expressed as Eq. (4).

$$\sigma_h{}^2 = \sum_i C_i{}^2 \sigma_{S_i}{}^2 + 2\sum_{i\neq j} C_i C_j \sigma_{S_iS_j} \quad (4)$$

If we can estimate σ_h by Eq. (4), σ_r can be evaluated by Eq. (1). In the following sections, the methods for solving Eq. (4) are proposed.

2.1.2 Error Estimation Method Using the Adjoint Calculation

In a previous study [2], they proposed an estimation method of Eq. (4) using the adjoint flux. Actually, the study were pursued to evaluate the lower bound of σ_h. Because each source strength in MC2 is calculated from responses in MC1, it varies dominantly by the number of particles incident on each detector from MC1 simulation. Therefore, when S_i increases, the neighboring source strength also increases because it is originated from the increased number of incident particles ($\sigma_{S_iS_j} > 0$). However, the sources located far away from each other have low dependency ($\sigma_{S_iS_j} \cong 0$). This shows that there is no negative correlation between the source strengths in MC2, thus the 2nd term of RHS in Eq. (4) is bigger than zero. By this process, this term can be assumed to be zero, and only the lower bound of σ_h is estimated as followed in Eq. (5).

$$\sigma_h = \sqrt{\sum_i {C_i}^2 {\sigma_{S_i}}^2} \tag{5}$$

The C_i can be further expanded into Eq. (6).

$$C_i = \int C_i(E) f_i(E) dE \tag{6}$$

where $C_i(E)$ is the contribution energy spectrum of S_i to R, and $f_i(E)$ is the probability density function of source energy spectrum in MC2. Because the meaning of $C_i(E)$ is the adjoint flux, Eq. (5) can be arranged by applying Eq. (6) and substituting $C_i(E)$ for $\emptyset_i^+(E)$ as given in Eq. (7).

$$\sigma_h = \sqrt{\sum_i \left\{\int \emptyset_i^+(E) f_i(E)\right\}^2 {\sigma_{S_i}}^2} \tag{7}$$

According to Eq. (7), if the $\emptyset_i^+(E)$ is computed from the adjoint calculation in MC2, the lower bound of the σ_h can be estimated. However, because $\emptyset_i^+(E)$ is usually inaccurate due to the limitation of deterministic approach, it should be refined by comparing the response evaluated from Eq. (2) using $\emptyset_i^+(E)$ to that computed from MC2 simulation.

2.1.3 Proposed Method Using Forward-Adjoint Calculation and Union Tally

In contrast with conventional solution using the adjoint flux, a methodology to get the result of C_i by the forward calculation in MC2 is proposed in this study. The lower bound of σ_h can be estimated using the proposed method without any additional calculation in MC2. First, the Eq. (4) can be modified into Eq. (8) by multiplying and dividing the S_i and S_j.

$${\sigma_h}^2 = \sum_i (S_iC_i)^2 (\frac{\sigma_{S_i}}{S_i})^2 + 2\sum_{i\neq j} (S_iC_i)(S_jC_j)\frac{\sigma_{S_iS_j}}{S_iS_j} \tag{8}$$

The physical meaning of S_iC_i is the response originated from S_i; therefore, it can be estimated from the MC forward calculation. Also, the energy spectrum of the adjoint flux is reflected in the MC particle transport process. Hence, there is no need to refine the inaccurate adjoint flux. As a result, this approach has an advantage over the previous one in evaluating the 1st term of RHS in Eq. (8). Also, to obtain σ_h, the covariance between the source strengths, the 2th term of RHS in Eq. (8) should be quantified. In this study, an evaluation method for $\sigma_{S_iS_j}$ is developed by defining a union tally. If we calculate not only the individual source strength (S_i, S_j), but also the sum (S_i+S_j) defined as the union tally in MC1, the average and relative error of each calculation can be evaluated. Using the error propagation formula, the relationship between the uncertainties of three tallies can be represented by Eq. (9), and the covariance between S_i and S_j can be estimated by Eq. (10).

$${\sigma_U}^2 = {\sigma_{S_i}}^2 + {\sigma_{S_j}}^2 + 2\sigma_{S_iS_j} \tag{9}$$

$$\sigma_{S_iS_j} = ({\sigma_U}^2 - {\sigma_{S_i}}^2 - {\sigma_{S_j}}^2)/2 \tag{10}$$

where U means the union tally summing S_i+S_j, and σ_U is SD of the union tally. After applying the Eq. (10) to Eq. (8), the proposed estimation method finally can be derived as followed in Eq. (11).

$${\sigma_h}^2 = \sum_i (S_iC_i)^2 \left(\frac{\sigma_{S_i}}{S_i}\right)^2 + \sum_{i\neq j} (S_iC_i)(S_jC_j)\frac{{\sigma_U}^2 - {\sigma_{S_i}}^2 - {\sigma_{S_j}}^2}{S_iS_j} \tag{11}$$

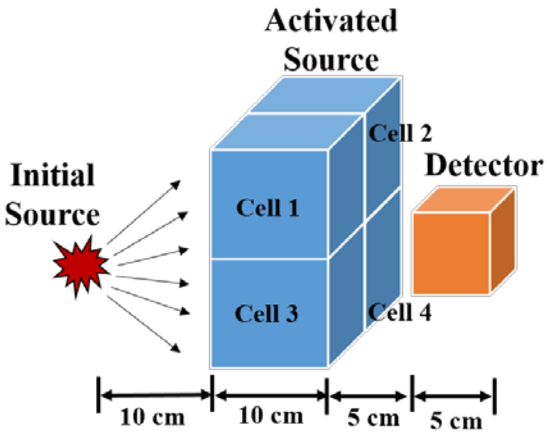
2.2 Verification of the Real Uncertainty Estimation Methods

For the verification of the proposed estimation method, two activation problems were assumed and evaluated by using MCNPX 2.7.0 code with JENDL/HE-2007 [3] and JENDL-4.0 [4] neutron cross-section libraries and mcplib84 photon cross-section library. It was assumed that a neutron source in MC1 is a point source having the energy of 14 MeV and strength of 2×10^{10} particles/sec, and there are 2 types of detectors which consist of 4 and 8 cubic cells entirely composed of ^{59}Co. After a long neutron irradiation, a ^{60}Co is produced by (n, γ) reaction and its production rate is the equal to the activation rate density as shown in Eq. (12).

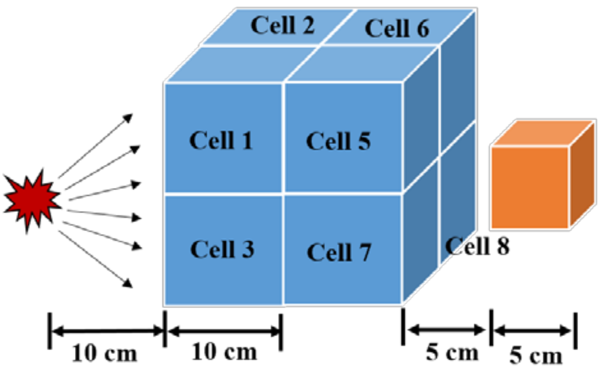
$$A(\vec{r}) = \int \Sigma(E) \emptyset_n(\vec{r}, E) dE \tag{12}$$

where $A(\vec{r})$ is the activity per volume of the ^{60}Co, $\Sigma(E)$

is the macroscopic cross section for (n, γ) reaction and $\emptyset_n(\vec{r}, E)$ is the neutron flux. Because it is the radioactive nuclide, it emits the residual radiations as it decays. Hence, in MC2 simulation, the 1.17 MeV and 1.33 MeV photons emitted from ^{60}Co were used as sources, and the single volumetric detector is defined. F8 FT RES tally option is used to calculate the production rate of ^{60}Co, and F4 tally was used in MC2 simulation. The schematic descriptions for the benchmark problems are shown in Fig. 1.



(a) 4-Cell Problem



(b) 8-Cell Problem

Fig. 1. The Overview of the Benchmark Problem

The result of the real uncertainty estimated from the brute force technique was used as the reference value. 101 random seeds for each step of MC simulation were used. And, by the statistical processing, σ_r were estimated with 90% confidence interval. Then, it was compared with that of other estimation methods. The previous method was pursued by calculating the adjoint flux using Denovo [5] in SCALE MAVRIC sequence [6]. The adjoint parameters were determined by comparing the adjoint fluxes with those evaluated from MONACO [7]. They were determined to 47 energy group/S_8 (8 quadrature set)/P_3/2cm mesh size for both benchmark problems. To estimate the uncertainty with the proposed method, separate transport method (ST method) was performed. To fix the total calculation cost, the particle histories are proportionally allocated to individual source strength. The covariance was calculated by adding 'T' tally option in MC1 simulation. Here is the covariance matrix of 8-cell benchmark problem in Fig. 2.

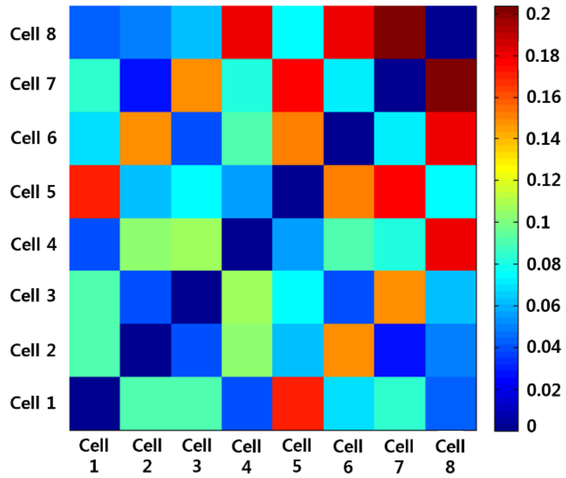


Fig. 2. Correlation Coefficient Matrix of the Benchmark Problem

The results estimated by the three methods are given in Table I. In 4-cell problem, both the previous and proposed methods are on the 90 % confidence interval of the real SD. However in 8-cell problem, the result estimated by using the adjoint based method does not agree within 90 % confidence interval. This shows that the proposed method has a good accuracy for the analysis of the uncertainty propagation. Also, the covariance data is calculated during the MC1 simulation without any additional calculation; therefore, it gives a large efficiency for complex systems.

Table I: Comparison of the Real SD Results (σ_R) Estimated from Each Method for 2 Benchmark Problems

Case	Real Standard Deviation (σ_R)		
	Reference	Prev.	Prop.
	Brute Force Technique (90% conf. Intv.)	Adjoint Cal.	ST & Union
4*	128.67 (115.39, 145.75)	121.38	128.59
8*	57.477 (51.545, 65.109)	50.304	56.849

* 90% Confidence Interval
* 4-Cell, 8-Cell Benchmark Problem

3. Conclusions

In this study, a new method using the forward-adjoint calculation and the union tally is proposed for the estimation of real uncertainty. For the activation benchmark problems the responses and real uncertainties were estimated by using the proposed method. And, the results were compared with those estimated by the brute force technique and the adjoint-based approach. The result shows that the proposed approach gives an accurate result comparing with the reference results. Also, it is expected that it will have a high efficiency for complex systems because the covariance data can be calculated during the MC step 1 simulation without any additional calculations. The developed method will contribute to increasing the accuracy and reliability for estimation of the real uncertainty in various 2 step MC problems.

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