A Development of Multi-response CADIS Method for the Optimization of Variance Reduction in Monte Carlo Simulation

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1. Introduction

Monte Carlo (MC) method is a stochastic approach that the results are obtained from the estimation of each particle transport simulation. MC method can directly simulate the particle simulation without modification of the Boltzmann transport equation; therefore, the accuracy of simulation results is superior to those of deterministic methods. However, it is well known that the calculation efficiency with MC method can be considerably lower for the deep penetration or large geometrical problems to reduce the stochastic error. In order to increase the simulation efficiency, variance reduction techniques have been introduced for the problems. The variance reduction method can be classified to three technical categories that are source, collision, and transport biasing [1-3]. All of the variance reduction techniques require specific parameters to control the transport probability. One of well-known methods to determine the optimized transport probability is called as the Consistent Adjoint Driven Importance Sampling (CADIS) method [4-5]. The CADIS method uses adjoint function to reduce the error of the response. This method can give high variance reduction efficiency on the single response in any problem. However, the CADIS method cannot properly reduce individual relative error for the cases, which have more than two responses. In this study, a multi-response CADIS method was derived by considering each position of the responses. Using the multi-response CADIS method, a radiation transport problem was estimated by applying it into the source angular biasing. The results were compared with those of the CADIS approach and the analog MC method.

2. Methods and Results

In stochastic theory, expected value of *g(x)* is expressed to Eq. (1).

$$G=\int g(x)f(x)dx \tag{1}$$

where $f(x)$ is probability density function (pdf) satisfying $f(x)\geq 0$ and $\int f(x)dx=1$ conditions. Also, the variance of *G* is obtained by using Eq. (2).

$$var(G)=\int g^2(x)f(x)dx-\left\{\int g(x)f(x)\right\}^2$$

$$=\int g^2(x)f(x)dx-G^2 \tag{2}$$

The variance reduction scheme is that the *f(x)* is changed to $\hat{f}(x)$ for reducing the variance of *G*. As the results, the average and variance with $\hat{f}(x)$ are given to Eqs. (3) and (4), respectively.

$$G=\int\left[\frac{g(x)f(x)}{\hat{f}(x)}\right]\hat{f}(x)dx \tag{3}$$

$$var(G)=\int\left[\frac{g^2(x)f^2(x)}{\hat{f}^2(x)}\right]\hat{f}(x)dx-\mathrm{G}^2 \tag{4}$$

To get the minimum variance for *G*, first term of RHS in Eq. (4) should be minimized. Therefore, determination of $\hat{f}(x)$ must be a key issue for the use of the efficient variance reduction. In Section 2.1, the introduction and the limitation for CADIS method were described. A multi-response CADIS method, which is to overcome the limitation of CADIS method, was proposed and derived in Section 2.2. Finally, for the verification of the multi-response CADIS method, a sample radiation transport problem was calculated with the proposed and CADIS methods in section 2.3.

2.1 Review of CADIS Method

In particle transport problems, response called as the tally results is obtained by Eq. (5).

$$R=\int\int\int\psi(\vec{\mathrm{r}},\widehat{\Omega},E)\sigma_d(\vec{\mathrm{r}},\widehat{\Omega},E)d\vec{r}d\widehat{\Omega}dE$$

$$=\int\psi(P)\sigma_d(P)dP \tag{5}$$

where $\psi(P)$ is particle flux at *P* phase-space and $\sigma_d(P)$ is object functions to get a response at *P*. In the time independent transport equation, transport term excepting the source term can be express by Eq. (6) using transport operator *H*.

$$\hat{\Omega}\cdot\nabla\psi+\Sigma_t\psi-\int dE'\int d\hat{\Omega}\,\Sigma_s(\vec{r},E'\to E,\hat{\Omega}'\to\Omega)\psi'$$

$$\equiv H\psi \tag{6}$$

Then, the transport equation is simply expressed as given in Eq. (7).

$$H\psi=q \tag{7}$$

where q is source density function. Also, the adjoint transport equation can be express by Eq. (8) [7].

$$\hat{\Omega}\cdot\nabla\psi^{+} + \Sigma_t\psi^{+} - \int dE'\int d\hat{\Omega}\ \Sigma_s(\vec{r},E'\rightarrow E,\hat{\Omega}'\rightarrow\Omega)\psi^{+'} = q^{+}$$

$$H^{+}\psi^{+} = q^{+} \qquad (8)$$

where H^+ is the adjoint function of H, ψ^+ is the adjoint function of ψ, and q^+ is the adjoint function of q. It is noted that Eq. (8) cannot be a self-adjoint function of Eq. (7) due to the particle transport relationship between forward and adjoint functions [7]. Therefore, those equations should be expressed as the following equation:

$$<\psi^{+}, H\psi> = <\psi, H^{+}\psi^{+}>$$

or

$$<\psi^{+}, q> = <\psi, q^{+}> \qquad (9)$$

where < > is an integration operator for all independent variables. The physical meaning of the adjoint flux (ψ^+) is the expected contribution to the specific response, and adjoint source (q^+) is the object function (σ_d). From the relationship given in Eq. (9), the Eq. (5) can be expressed as two expressions:

$$R = \int \psi(P)q^{+}(P)\ dP \qquad \text{(10-a)}$$

or

$$R = \int \psi^{+}(P)q(P)\ dP \qquad \text{(10-b)}$$

Then, with Eq. (10), the variance of the source probability density function for the source biasing, which is one of the variance reduction methods, can be rewritten to Eq. (11).

$$var(R) = \int \left[\frac{\psi^{+2}(P)q^{2}(P)}{\hat{q}^{2}(P)}\right]\hat{q}(P)dP - R^{2} \qquad (11)$$

The response R is the average value, and thus the value is fixed to a coefficient. To obtain the minimum variance of Eq. (11), the first term of RHS in Eq. (11) should be minimized by choosing modified pdf ($\hat{q}$). $\hat{q}$, which is the modified pdf for the variance reduction, is decide by importance sampling with Eq. (12) [8].

$$\hat{q} = \frac{\psi^{+}(P)q(P)}{\int\psi^{+}(P)q(P)dP} = \frac{\psi^{+}(P)q(P)}{R} \qquad (12)$$

In the biasing theory for using the variance reduction technique, the particle weight must be conserved as shown in Eq. (13). For example, in splitting event, a particle weight must be decreased as increasing the number of particles that is changed by the cell importance.

$$w(P)\hat{q}(P) = w_0(P)q(P) \qquad (13)$$

where $w(P)$ and $w_0(P)$ are biased and unbiased particle weights, respectively. Finally, the statistical weight of the source particle for the variance reduction is decided by substituting Eq. (12) into (13).

$$w(P) = \frac{\int\psi^{+}(P)q(P)dP}{\psi^{+}(P)} = \frac{R}{\psi^{+}(P)} \qquad (14)$$

If the R and $\psi^+(P)$ are obtained as using deterministic methods or the other approaches, the variance of Monte Carlo simulation can be optimized by this theory.

2.2 Proposal of Multi-response CADIS Method

As shown in Eqs. (10-14), the CADIS method does not consider the position of the response because the total response is introduced in Eq. (5). However, for general particle transport problems, responses having various positions are often required in a single MC simulation. For the cases, therefore, the total relative error can be efficiently reduced with CADIS method. However, it can fail to reduce the individual relative error at each response position. In this study, the relative error reduction method (defined as Multi-response CADIS method) was proposed with considering the positions of the response. First, the R_i, which is the response in i^{th} discrete region, is defined as the following equation.

$$R_{err,i} \equiv \int_{V_i}\frac{\sqrt{Var\left(R(\underline{r})\right)}}{R(\underline{r})}d\underline{r} \qquad (15)$$

where $\underline{r}$ is the position of the response. The purpose of the proposed method is that relative errors of the responses in the discrete region i are minimized, equally. Therefore, if the relative errors in discrete region i are equal to each other, the goal can be successfully achieved. Variance is a method to indicate the degree of differences among the values; hence, the relative errors, $R_{err,i}$, can be minimized by the following equation:

$$Min\left(\left(var\left[R_{err}\left(\hat{q}(P)\right)\right]\right)\right)$$

$$= Min\left(\frac{1}{N}\Sigma_{i=1}^{N}R_{err,i}^{2} - \left(\frac{1}{N}\Sigma_{i=1}^{N}R_{err,i}\right)^{2}\right) \qquad (16)$$

where $Min(f(x))$ is a function to fine a variable x which gives a minimum value of $f(x)$ and N is total number of response. The second term of RHS in Eq. (16) is a constant because it is an average value. Therefore, Eq. (16) can be derived to Eq. (17).

$$Min\left(\left(var\left[R_{err}\left(\hat{q}(P)\right)\right]\right)\right)$$

$$= Min\left(\Sigma_{i=1}^{N} R_{err,i}^2\left(\hat{q}(P)\right)\right) \qquad (17)$$

Substituting Eqs. (15) and (11) into Eq. (17), the $M\left(var\left(R_{err}\left(\hat{q}(P)\right)\right)\right)$ is expressed to Eq. (18).

$$Min(var[R_{err}(\hat{q}(P))])$$

$$= Min\left(\Sigma_{i=1}^{N}\left[\int \frac{q^2(P)\psi^{+2}_{i}(P)}{\hat{q}(P)R_i^2}dP\right] - N\right)$$

or

$$= Min\left(\Sigma_{i=1}^{N}\left[\int \frac{q^2(P)\psi^{+2}_{i}(P)}{\hat{q}(P)R_i^2}dP\right]\right) \qquad (18)$$

The value $\hat{q}(P)$ to give a minimum value of R_{err} can be calculated by using a Lagrange multiplier λ as used in the previous study [8].

$$L\left(\hat{q}(P)\right) =$$

$$\left[\Sigma_{i=0}^{N}\frac{q^2(P)\psi^{+2}_{i}(P)}{\hat{q}(P)R_i^2}\,dP + \lambda\int \hat{q}(P)dP\right] \qquad (19)$$

By partial differentiating the Eq. (19) with $\frac{\partial}{\partial\hat{q}(P)}$, and then the $var(R_{err})$ has a minimum value at $\frac{\partial L(\hat{q}(P))}{\partial\hat{q}(P)} = 0$. The minimized condition is given in Eq. (20).

$$-\Sigma_{i=0}^{N}\frac{q^2(P)\psi^{+2}_{i}(P)}{\hat{q}^2(P)R_i^2} + \lambda = 0 \qquad (20)$$

$\hat{q}(P)$ is the pdf, and thus $\int \hat{q}(P)dP$ should be 1. And, $q(P)$ and ψ^{+}(P) are positive values. Using the properties, the function to fine the $Min(var[R_{err}(\hat{q}(P))])$ can be derived to Eq. (21).

$$Min(var[R_{err}(\hat{q}(P))])$$

$$= \hat{q}(P) = \frac{q(P)\sqrt{\Sigma_{i=0}^{N}\psi^{+2}(P)/R_i^2}}{\int q(p)\sqrt{\Sigma_{i=0}^{N}\psi^{+2}_{i}(P)/R_i^2}\,dP} \qquad (21)$$

Also, the particle weights of the plural responses were calculated with Eq. (22) which is derived with Eq. (21) into Eq. (13).

$$w(P) = \frac{\int q(p)\sqrt{\Sigma_{i=0}^{N}\psi^{+2}_{i}(P)/R_i^2}\,dP}{\sqrt{\Sigma_{i=0}^{N}\psi^{+2}(P)/R_i^2}} \qquad (22)$$

2.3 Verification of Multi-response CADIS Method

For the verification of multi-response CADIS method, a simple shielding problem was assumed as shown Fig. 1. An isotropic point source (photon) having 1 MeV energy is located at the center of a room. The room inside is cubical shape, and each side has 100 cm length. The wall of the room is 50 cm thickness ordinary concrete (density=2.3g/cc). To get the response, the mesh tally (30 cm x 30cm x 10 cm unit length) is located at the right side of the room. This study is to confirm and verify the multi-response CADIS method, and thus the adjoint fluxes and responses were calculated by MCNPX code. Using the adjoint fluxes and responses, the radiation transport calculations were performed with proposed method and CADIS approach. Also, the results were compared with that of analog MC calculation.

Figures 2 - 4 show the results of the relative errors with 10^5, 10^6, and 10^7 particle transport histories, respectively. Figures 5 - 7 are the results of the fluxes. The results show that the relative errors using both CADIS and multi-response CADIS methods were reduced than those with analog MC calculation. The CADIS method gives best accuracy at center area for all cases; but it gives relatively lower accuracy in the other tally regions than those with proposed method. On the contrary, the multi-response CADIS method generally gives good accuracies in all tally regions. Figure 8 is the number of relative errors categorized by relative error bins. The results show that the multi-response CADIS method proposed in this study are successfully reduce the relative errors in all regions than the CADIS method.

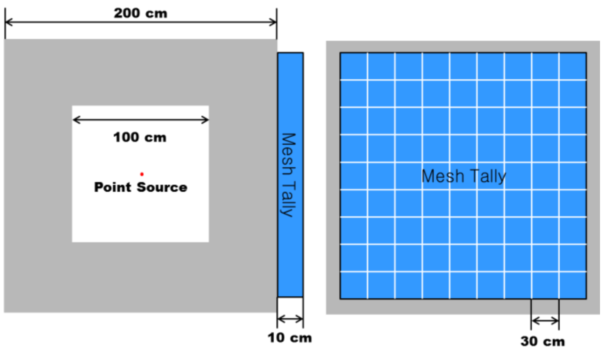


Fig. 1. Cross-sectional Drawing (Left) and Side View (Right) of Shielding Problem

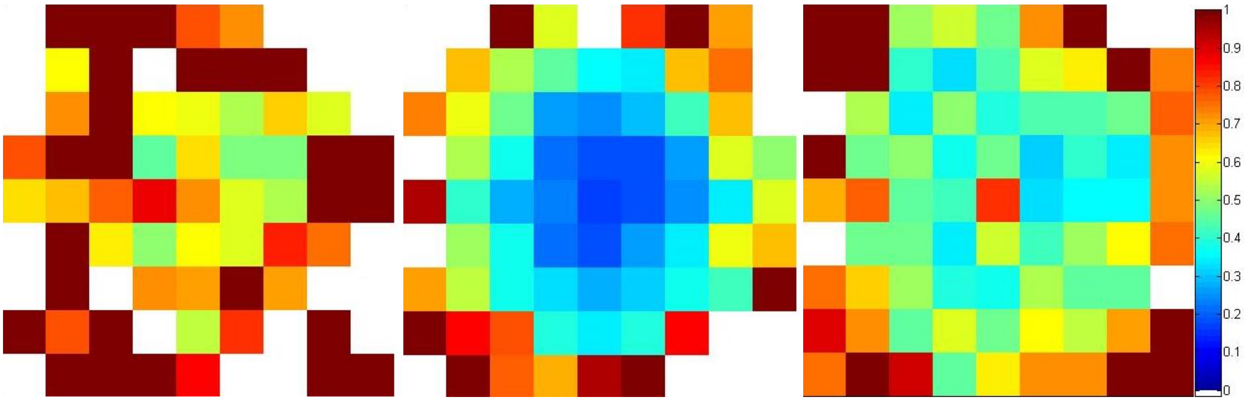


Fig. 2. Computed Relative Errors using No Biasing (Left), CADIS (Middle), and Multi-response CADIS (Right) Method for 10^5 Histories

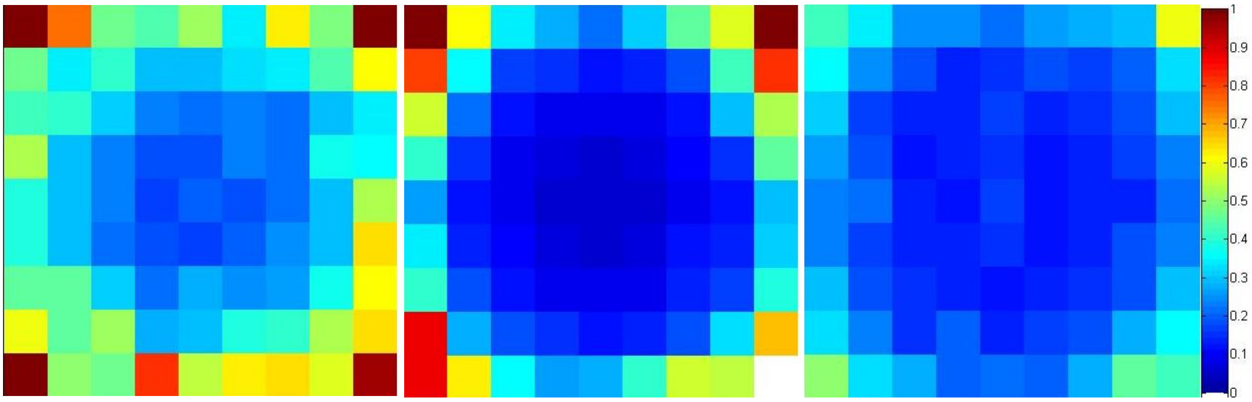


Fig. 3. Computed Relative Errors using Analog (Left), CADIS (Middle), and Multi-response CADIS (Right) Method for 10^6 Histories

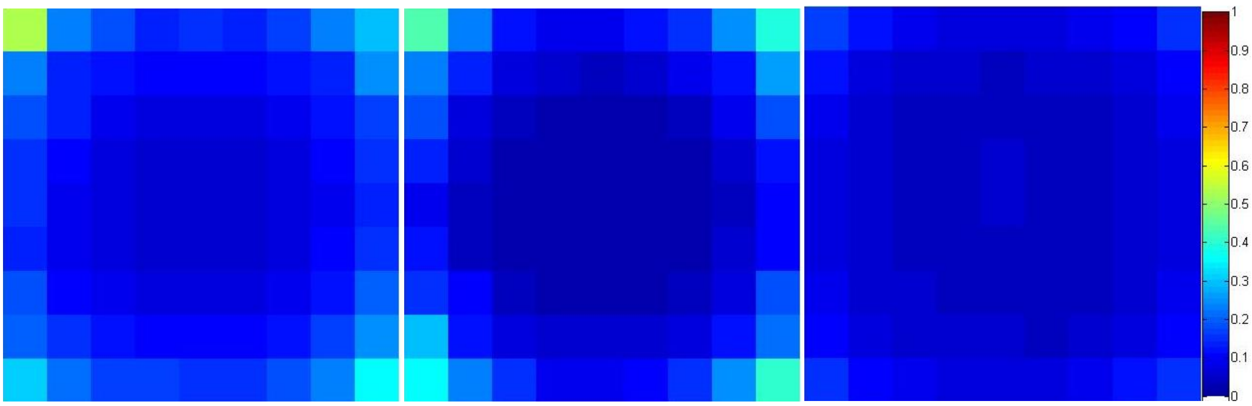


Fig. 4. Computed Relative Errors using Analog (Left), CADIS (Middle), and Multi-response CADIS (Right) Method for 10^7 Histories

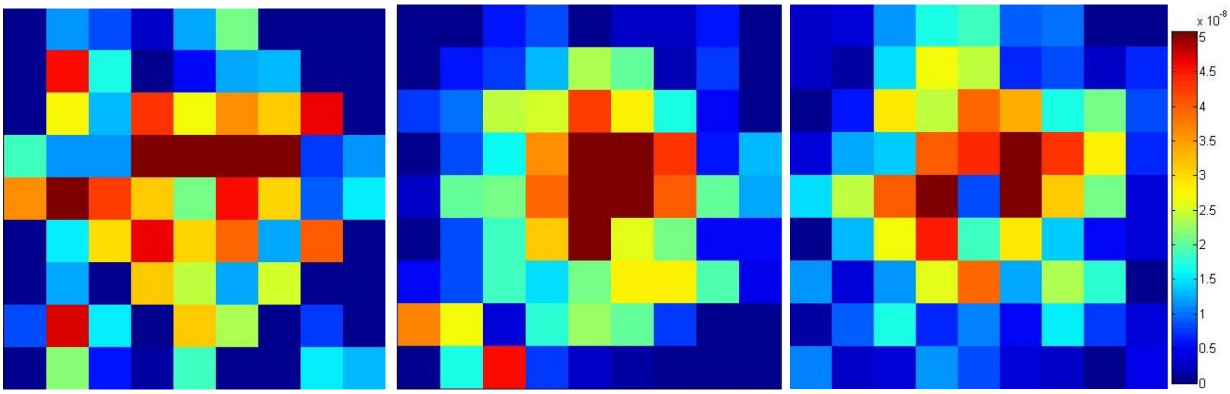


Fig. 5 Flux distribution using Analog (Left), CADIS (Middle), and Multi-response CADIS (Right) Method for 10^5 Histories

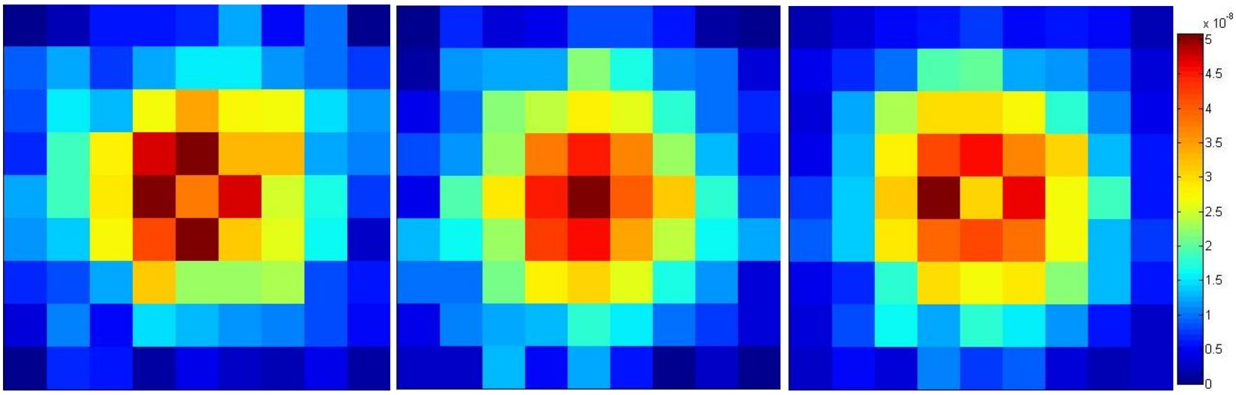


Fig. 6 Flux distribution using Analog (Left), CADIS (Middle), and Multi-response CADIS (Right) Methods for 10^6 Histories

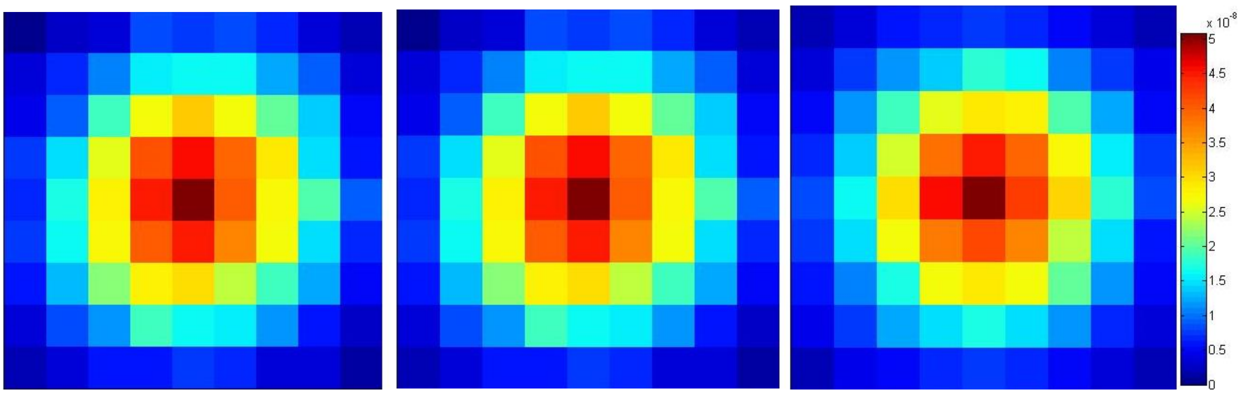
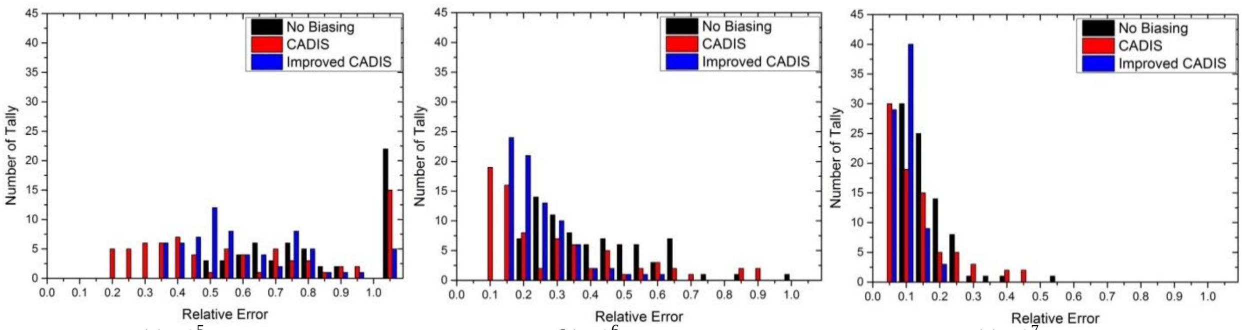


Fig. 7 Flux distribution using Analog (Left), CADIS (Middle), and Multi-response CADIS (Right) Methods for 10^7 Histories



(a) 10^5 Histories (b) 10^6 Histories (c) 10^7 Histories

Fig. 8. Number of Relative Errors in Each Error Boundary for Analog MC, CADIS, and Multi-Response CADIS Method

3. Conclusions

In this study, a multi-response CADIS method was proposed for minimizing relative errors in various tally regions. To reduce all relative errors for various responses, a weight decision equation was derived. For the verification of the proposed method, a shielding problem was set and the MC simulations were pursued. The results with the proposed method were compared with those estimated by CADIS and analog MC methods. The analysis shows that the relative error of each tally region can be successfully and efficiently reduced for overall regions than the other methods. It can be utilized for accurate calculation of various radiation transport problems, as well as to save the calculation time. Therefore, it is expected that the proposed method can contribute the improvement of expandability in Monte Carlo simulation.

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