An Analysis on the Calculation Efficiency of the Responses Caused by the Biased Adjoint Fluxes in Hybrid Monte Carlo Simulation

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1. Introduction

To accelerate Monte Carlo calculation in the problems which spend a lot of calculation time, hybrid methods were introduced. The hybrid method in this simulation field is a technique to increase the calculation efficiency by optimizing the parameters of variance reduction techniques (VRT). One of the VRTs employs adjoint functions to generate source biasing and weight window parameters. This technique is known as Consistent Adjoint Driven Importance Sampling (CADIS) method [1] and it is implemented in SCALE code system. In the CADIS method, adjoint transport equation has to be solved to determine deterministic importance functions. Using the CADIS method, a problem was noted that the biased adjoint flux estimated by deterministic methods can affect the calculation efficiency and error [2]. The biases of adjoint function are caused by the methodology, calculation strategy, tolerance of result calculated by the deterministic method and inaccurate multi-group cross section libraries. In this paper, a study to analyze the influence of the biased adjoint functions into Monte Carlo computational efficiency is pursued.

2. Method and Result

2.1 Overview of CADIS Method

It has long been recognized that the adjoint function has physical significance as a measure of the importance of a particle to objective functions. In CADIS method, the adjoint function was applied to increase the calculation efficiency. The forward and adjoint forms of the transport equation can be expressed as follows:

$$H\psi = q \tag{1}$$

$$H^{+}\psi^{+} = q^{+} \tag{2}$$

where H and H^{+} are forward and adjoint transport operators, ψ and ψ^{+} are forward and adjoint functions, and q and q^{+} are forward and adjoint sources. The relation between forward and adjoint transport equation is given to Eqs. (3) and (4).

$$\left\langle \psi^{+}, H\psi \right\rangle = \left\langle \psi, H^{+}\psi^{+} \right\rangle \tag{3}$$

$$\left\langle \psi^{+}, q \right\rangle = \left\langle \psi, q^{+} \right\rangle \tag{4}$$

In the adjoint transport equation, let q^{+} be σ_d which is the object function; then, Eq. (4) is corresponding to the response R as given in Eq. (5).

$$R = \left\langle \psi, q^{+} \right\rangle = \left\langle \psi, \sigma_d \right\rangle = \left\langle \psi^{+}, q \right\rangle \tag{5}$$

The idea of CADIS method is started from biasing the distribution of the sources to reduce variance of detector response to get minimum value. Applying the biased source distribution at phase space P, $\hat{q}(P)$, the response and variance can be estimated by Eqs. (6) and (7), respectively.

$$R = \int_P dP q(P)\psi^{+}(P) = \int_P dP \frac{q(P)\psi^{+}(P)}{\hat{q}(P)} \hat{q}(P) \tag{6}$$

$$\mathrm{var}(R) = \int_P dP \left[\frac{q(P)\psi^{+}(P)}{\hat{q}(P)} \right]^2 \hat{q}(P) - R^2 \tag{7}$$

To preserve the number of particles in phase space between analog and non-analog simulation, the statistical weight of the source particles must be conserved as the follows:

$$w(P)\hat{q}(P) = w_0(P)q(P) \tag{8}$$

where $w(P)$ and $w_0(P)$ are biased and unbiased particle weights. Using mathematical derivations, finally, the biased particle weight optimized by the CADIS method [2] is given as the follows:

$$w(P) = \frac{\int q(P)\psi^{+}(P)dP}{\psi^{+}(P)} = \frac{R}{\psi^{+}(P)} \tag{9}$$

Using Eqs. (6) and (9), the variance reduction was performed by CADIS method. To determine the optimized values, the adjoin function $\psi^{+}(P)$ must be evaluated. Generally, the adjoint functions are calculated using some deterministic methods; therefore, the biases are accompanied.

2.2 Proposal of the Method to Estimate the Influence of the Biased Adjoint Flux

Eq. (5) describes the ways to calculate the responses using either forward flux or adjoint flux. To consider the error caused by the biased adjoint fluxes, the biased adjoint flux ψ^{*} is defined as given in the following equation:

$$\psi^{*}(P) = \psi^{+}(P) + \delta\psi_t^{+}(P) + \delta\psi_s^{+}(P) \tag{10}$$

where $\delta\psi_t^{+}(P)$ is the bias of the adjoint flux caused by the tolerance of the deterministic calculation, and $\delta\psi_s^{+}(P)$ is the bias of the adjoint flux caused by the systematic error of the deterministic method. If the biased adjoint flux is inserted into Eq. (9), Eq. (11) is derived using Eqs. (7) and (8). It requires that there is no change of the expected values using the biased adjoint flux; however, the variance is changed as given in Eq. (11).

$$\mathrm{var}(R) = \int_P dP\left[q(P)\psi^+(P)\right]^2 \frac{R}{w_0(P)q(P)\{\psi^+(P)+\delta\psi_t^+(P)+\delta\psi_s^+(P)\}} - R^2 \quad (11)$$

Also, the variance using the unbiased adjoint flux can be expressed to Eq. (12).

$$\mathrm{var}(R) = \int_P dP\left[q(P)\psi^+(P)\right]^2 \frac{R}{\psi^+(P)w_0(P)q(P)} - R^2 \quad (12)$$

If Eq. (11) is subtracted by Eq. (12), the difference of the variances by applying the biased adjoint flux can be derived as the follows:

$$\mathrm{Diff}[\mathrm{var}(R)] = \int_P dP\left[q(P)\psi^+(P)\right]^2 \frac{R}{\psi^+(P)w_0(P)q(P)} \frac{\delta\psi_t^+(P)+\delta\psi_s^+(P)}{(\psi^+(P)+\delta\psi_t^+(P)+\delta\psi_s^+(P))} \quad (13)$$

As known that the variance calculated by Eq. (12) has a minimum value; therefore, it shows that the biased adjoint flux gives the inefficiency by increasing the variance as given in Eq. (13).

2.3 Evaluation and Analysis

For the verification of the proposed equation, a benchmark problem is assumed. The benchmark problem consists of a 1 m x 1 m x 1 m slab of concrete with single source and detector. The 5 MeV neutron source (1 Bq) is located at a straight line which passes through center of shielding material and is away 50 cm from the slab. The detector is located for 50 cm at the other side of the source. Then, with the given condition, adjoint function was calculated in SCALE code . Using MONACO module [3], the Monte Carlo simulation was performed in SCALE code. To give the different biases to the adjoint fluxes, the adjoint functions were calculated with tolerance 0.001; 0.0001; 0.00001. The calculation results of 200 batches (each batch has 50,000 histories) are given as shown in Fig. 1 and Table I.

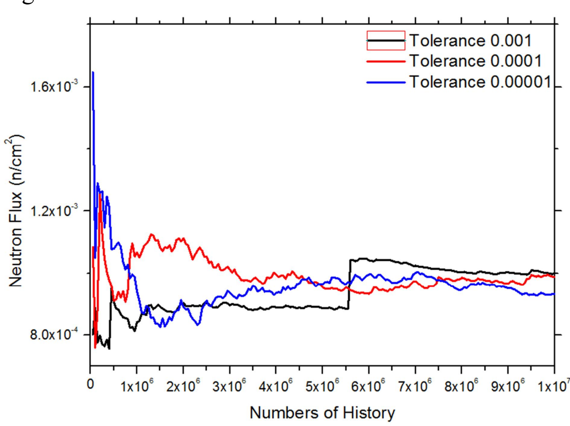

Fig. 1. Responses (Flux) as Applying the Biased Adjoint Fluxes

Table I: Summary of the Results after 10^7 NPS

Tolerance Error	0.001	0.0001	0.00001
Neutron Flux (n/cm^2)	9.999E-04	9.878E-04	9.320E-04
Calculation time (min)	60.1	22.16	19.88
Relative error	0.0901	0.04797	0.05629
FOM (/min)	1.93E+00	1.76E+01	1.60E+01

As shown in Fig. 1, the result for the case of tolerance 0.001 seems to be fast converged until 2x10^6 particle history. However, when it was continually run more than 2x10^6 particle history, the result and FOM given in Fig. 2 were suddenly fluctuated. It was analyzed that the adjoint fluxes estimated with 0.001 tolerance have a large biases in some local regions while major regions were relatively well evaluated. As a result, the particles having high weight caused by biased adjoint fluxes scored to the tally region and the fluctuations of the tally results and FOM were generated. The analysis shows that the biased adjoint fluxes highly affect the calculation efficiency and fluctuations of the results; therefore, the difference of the variance referred in Eq. (13) should be properly estimated and verified for the efficient use of the variance reduction techniques.

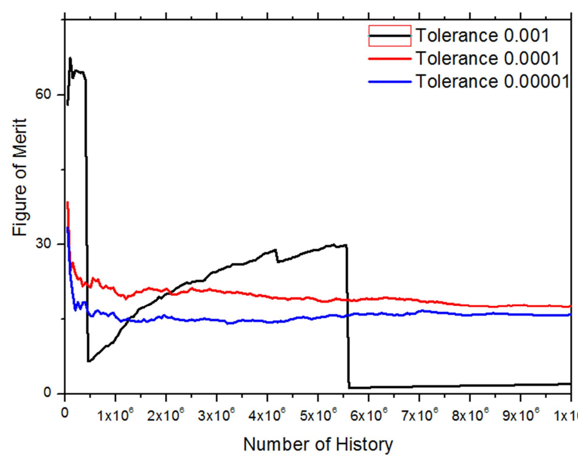

Fig. 2. Comparison of FOMs as Applying the Biased Adjoint Fluxes.

3. Conclusion

In this study, a method to estimate the calculation efficiency was proposed for applying the biased adjoint fluxes in the CADIS approach. For a benchmark problem, the responses and FOMs using SCALE code system were evaluated as applying the adjoint fluxes. The results show that the biased adjoint fluxes significantly affects the calculation efficiencies. Also, it shows that the accuracy depends on not only the tolerance of the results but also the systematic error caused by the applied deterministic methods. This study will contribute to construct the strategy that is how the adjoint flux should be accurately estimated for the hybrid Monte Carlo simulation.

As the future work, it is planned that the relationship between the biased adjoint fluxes and efficiency of the Monte Carlo simulation will be derived.

Acknowledgments

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