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Nth-order Multi-Response CADIS Method for Optimizing Variance Reduction Parameter in Monte Carlo Simulation

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Abstract - *The Monte Carlo method has been used to solve particle transport problems including nuclear reactor analysis, radiation shielding, and the others related to the nuclear research field. Generally, the Monte Carlo method produces lower efficiency than deterministic methods. To increase the efficiency in the Monte Carlo simulation, a lot of variance reduction techniques (VRT) have been developed. In these days, the hybrid Monte Carlo methods were introduced to automatically apply VRT parameters. For a single response, consistent adjoint driven importance sampling (CADIS) method is well derived. For the multiple responses, Forward Weight CADIS (FW-CADIS) presents the best efficiencies among global variance reduction method. In this study, N^{th}-order Multi-Response CADIS (N-CADIS) method was proposed to optimize the relative errors for multiple responses using a concept that minimizing the sum of n^{th} order weighted relative error for the individual response can achieve uniformly low uncertainty. To evaluate and compare the efficiency of the N-CADIS method, a shielding problem was estimated. The mean based and tail-based penalty FOMs using N-CADIS method was improved by factor 2.03 and 1.46 compared to FW-CADIS. However, the computational time for FOM values does not include deterministic calculation time to estimate weight map. Therefore, it was concluded that if a deterministic transport code to estimate n^{th} order adjoint values is developed, the proposed N-CADIS method can show improved efficiency.*

I. INTRODUCTION

The Monte Carlo method has been used to solve particle transport problems including nuclear reactor analysis, radiation shielding, and the others related to the nuclear research field. Generally, the Monte Carlo method produces lower efficiency than deterministic methods. To increase the efficiency in the Monte Carlo simulation, a lot of variance reduction techniques (VRT) have been developed [1] as controlling the particle transport behaviors. Generally, parameters used to apply the VRT in the Monte Carlo simulation should be properly determined to accelerate the calculation efficiency. In the initial stage of VRT, some additional simulations using Monte Carlo method were utilized for deciding the parameters of VRTs [2]. The computational scheme using the Monte Carlo method, however, caused another estimation inefficiency; therefore, some other approaches have been studied. Those problems were successfully solved by hybrid Monte Carlo method to decide the VRT parameters. The consistent adjoint driven importance sampling (CADIS) method [3, 4] is one of the hybrid methods deriving the zero variance Monte Carlo scheme for a single response. However, the variances of multiple responses cannot be properly reduced by the CADIS method [5]. To achieve the low and uniform uncertainties in all multiple responses as well as having high efficiency, several methods were introduced [5-9]. The forward weighted CADIS (FW-CADIS) method presents one of the best efficiencies among global variance reduction method. FW-CADIS method uses an assumption that the uniform density of Monte Carlo particle in the multiple responses can lead to a uniformly low uncertainty of them. In our previous study, Multi-Response CADIS (MR-CADIS) method [10] was proposed with a concept that the VRT parameters are decided to minimize the sum of square relative error for multiple responses. In this study, N^{th}-order Multi-Response CADIS (N-CADIS) method was proposed to get the uniformly low uncertainty

II. BACKGROUND OF PREVIOUS STUDIES

The CADIS, FW-CADIS, and MR-CADIS methods are reviewed in this section to provide background.

1. Optimization for Single Response

A. Overview of CADIS method

In this section, the derivation method of CADIS is introduced to provide the background for FW-CADIS, MR-CADIS and N-CADIS methods.

The single response in Monte Carlo particle transport can be express by following integral equation

$$R = \int \sigma_d(P)\psi(P)\, dP \quad (1)$$

where σ_d is objective function to convert the particle flux into a response, ψ is particle flux and P is phase-space including position, angle and energy space. The time independent transport equation with transport operator is given by follows:

$$\hat{\Omega} \cdot \nabla\psi(P) + \Sigma_t(P)\psi(P) - \int\int \Sigma_s(\vec{r}, E' \to E, \hat{\Omega}' \to \hat{\Omega})$$
$$\psi(\vec{r}, \hat{\Omega}', E')d\hat{\Omega}'dE' = H\psi(P) = q(P) \quad (2)$$

where $\Sigma_t(P)$ total macroscopic cross section, $\Sigma_s(\vec{r}, E' \to E, \hat{\Omega}' \to \hat{\Omega})$ is scattering cross section from $(\vec{r}, \hat{\Omega}', E')$ to $(\vec{r}, E, \hat{\Omega})$, and $q(P)$ is source. Also, the adjoint form of Eq. (2) can be expressed as Eq. (3).

$$-\hat{\Omega} \cdot \nabla\psi^+(P) + \Sigma_t(P)\psi^+(P) - \int\int \Sigma_s(\vec{r}, E \to E', \hat{\Omega} \to \hat{\Omega}')$$
$$\psi^+(\vec{r}, \hat{\Omega}', E')d\hat{\Omega}'dE' = H^+\psi^+(P) = q^+(P) \quad (3)$$

where $\psi^+(P)$ = adjoint flux and $q^+(P)$ = adjoint source corresponding with objective function in Eq. (1). The relationship between Eqs. (2) and (3) is not self-adjoint [11]. Hence, the forward and adjoint transport equations only have following identity with vacuum boundary condition:

$$< \psi^+, H\psi > = < \psi, H^+\psi^+ >$$
$$or < \psi^+, q > = < \psi, q^+ > \quad (4)$$

where, < > is an integration operator for phase space. Using Eq. (4), the response of Eq. (1) can be expressed as follows:

$$R = \int \psi(P)q^+(P)dP$$
$$or \qquad R = \int \psi^+(P)q(P)dP \quad (5)$$

In stochastic theory, the variance of response in Eq. (1) is obtained by Eq. (6) using integration formulation.

$$Var(R) = \int {\psi^+}^2(P)q(P)dP - R^2 \quad (6)$$

When the biased sampling probability is used in VRTs, the variance of response is differently estimated as follows:

$$Var(R) = \int \left[\frac{{\psi^+}^2(P)q^2(P)}{\hat{q}^2(P)}\right] \hat{q}(P)dP - R^2 \quad (7)$$

where $\hat{q}(P)$ is a modified sampling probability to supersede the $q(P)$. The modified source, which has a minimum variance, is derived by using importance sampling [12] as following equation:

$$\hat{q}(P) = \frac{\psi^+(P)q(P)}{\int \psi^+ q(P)dP} = \frac{\psi^+(P)q(P)}{R} \quad (8)$$

If this modified source is inserted into Eq. (7), the variance, then, becomes zero, formulaically. Therefore, it is called zero variance scheme. To apply the modified sampling function, the Monte Carlo particle weight is converted by the following equation:

$$w(P)\hat{q}(P) = w_0 q(P) \quad (9)$$

where $w_0(P)$ is the analog Monte Carlo particle weight and $w(P)$ is the particle weight converted by a ratio of sampling density ($q(P)/\hat{q}(P)$). The optimized particle weight at source sampling is derived by substituting Eq. (8) into Eq. (9) as follows:

$$w(P) = \frac{\int \psi^+ q(P)dP}{\psi^+(P)} = \frac{R}{\psi^+(P)} \quad (10)$$

2. Optimization for Multiple Responses

A. Overview of FW-CADIS Method

In the CADIS method, the multiple adjoint sources and responses are treated by single value as following equations:

$$q^+(P) = \sum_i^N q_i^+(P) \quad (11)$$

$$R = \sum_i^N R_i \quad (12)$$

where q_i^+ is adjoint source for *i*th response and R_i is *i*th response.

As a result using Eqs. (11) and (12), only the variance of average response is reduced with the CADIS method. Thus, some responses having large error among the multiple responses cannot be properly considered. To accomplish uniformly low relative error for each response, an assumption, which is uniform Monte Carlo particle density [6] in responses, was applied in the FW-CADIS method. Using the concept, the adjoint source can be written as follows:

$$q^{+\prime}(P) = \sum_i^N \frac{q_i^+(P)}{R_i} \quad (13)$$

The FW-CADIS method uses Eq. (13) to get the optimal weights based on the CADIS methodology. Then, the adjoint fluxes are expressed as Eq. (14).

$$\psi^+(P) \to \sum_{i=1}^N \frac{\psi_i^+(P)}{R_i} \quad (14)$$

where ψ_i^+ is adjoint flux generated from i^{th} adjoint source and N is the number of responses in a system. Also, the response in FW-CADIS method is written as follows:

$$R = \int_P \psi^+(P) q(P) dP \ \rightarrow \int_P \sum_{i=1}^{N} \frac{\psi_i^+(P)}{R_i} q(P)\, dP \quad (15)$$

Also, the weight at P phase-space was derived by substituting Eqs. (13) and (14) into Eq. (10) as follows:

$$w(P) = \frac{\int_P q(P) \sum_{i=1}^{N} \frac{\psi_i^+(P)}{R_i} dP}{\sum_{i=1}^{N} \frac{\psi_i^+(P)}{R_i}} \quad (16)$$

B. Overview of MR-CADIS Method

To get the uniform and low uncertainty, a weight to minimize the sum of squared relative error was derived in MR-CADIS method. The relative error of i^{th} response is defined as follows:

$$R_{err}(R_i) = \frac{\sqrt{Var[R_i^2]}}{R_i} \quad (17)$$

The modified sampling probability function can be obtained by the following function:

$$Min\left[\sum_{i=1}^{N} R_{err,i}^2\big(\hat{q}(P)\big)\right] \quad (18)$$

where the function $Min[f(x)]$ is to get a variable (x) for minimizing $f(x)$. Eq. (18) is rewritten by substituting Eqs. (7) and (17) into Eq. (18) as follows:

$$Min\left[\sum_{i=1}^{N} \int_P \frac{q^2(P) \psi_i^{+2}(P)}{\hat{q}(P) R_i^2} dP - N\right]$$

$$= \ Min\left[\sum_{i=1}^{N} \int_P \frac{q^2(P) \psi_i^{+2}(P)}{\hat{q}(P) R_i^2} dP\right] \quad (19)$$

N (the number of responses) on the left-hand side of Eq. (19) is eliminated because it does not have any meaning for finding minimum value. The modified source probability to satisfy Eq. (19) is obtained by using Lagrange multiplier λ [13] as follows:

$$L\big(\hat{q}(P)\big) = \left[\sum_{i=1}^{N} \int_P \frac{q^2(P) {\psi^+}_i^2(P)}{\hat{q}(P) R_i^2} dP + \lambda \int_P \hat{q}^2(P)\, dP\right] \quad (20)$$

The desired source probability can be obtained at $\frac{\partial L(\hat{q}(P))}{\partial \hat{q}(P)} = 0$ with following properties: (1) $\int \hat{q}(P) dP = 1$, and (2) $\psi^+(P) > 0$. The source probability to satisfy the above conditions is derived as following equation:

$$\hat{q}(P) = \frac{q(P) \sqrt{\sum_{i=1}^{N} \frac{\psi_i^{+2}(P)}{R_i^2}}}{\int_P q(P) \sqrt{\sum_{i=1}^{N} \frac{\psi_i^{+2}(P)}{R_i^2}} dP} \quad (21)$$

The particle weight of MR-CADIS is, then, written by substitute Eq. (21) into Eq. (9) as follows:

$$w(P) = \frac{\int_P q(P) \sqrt{\sum_{i=1}^{N} \frac{\psi_i^{+2}(P)}{R_i^2}} dP}{\sqrt{\sum_{i=1}^{N} \frac{\psi_i^{+2}(P)}{R_i^2}}} \quad (22)$$

III. Proposal of N-CADIS Method

To optimize the uncertainty for multiple response systems, the MR-CADIS methods was deduced by assumption, which is minimizing the sum of squared relative error as shown Eq. 18. If reducing the relative error of a specific responses is very difficult compared with others responses, this assumption can make inefficiency such as low-flux area because a cost to reducing the relative error of low-flux area is higher than that for high flux area. In this study, to obtain uniform uncertainty, n^{th} order weighted relative error, which was defined in Eq. (23), $R_{err}^{n^{th}}$, was used instead of squared relative error in MR-CADIS method.

$$R_{err}^{n^{th}} \equiv \frac{E(x^n) - E(x)^n}{E(x)^n} \quad (23)$$

where $E(x)$ is the expected value of the x and n is not zero using this equation, the sum of n^{th} order weighted relative error for multiple responses can be express as following equation:

$$\sum_{i=1}^{N} R_{err,i}^{n^{th}} = \sum_{i=1}^{N} \frac{E_i(x^n) - E_i(x)^n}{E_i(x)^n} \quad (24)$$

where $R_{err,i}^{n^{th}}$ is n^{th} order weighted relative error for an i^{th} response, $E(x)$ is the expected value of the x for the i^{th} response. The Eq. (24) means that a response having highest error has dominant value when n are set high order. Thus, uniform relative errors can be obtained by minimizing the sum of n^{th} order weighted relative error. Using source sampling biasing, the Eq. (24) can be rewritten to Eq. (25)

$$\sum_{i=1}^{N} R_{err,i}^{n^{th}} = \sum_{i=1}^{N} \frac{\int_P \left[\frac{q^n(P)\psi_i^{+n}(P)}{\hat{q}^n(P)}\right] \hat{q}(P)dP - R_i^n}{R_i^n}$$

or

$$\sum_{i=1}^{N} R_{err,i}^{n^{th}} = \sum_{i=1}^{N} \left[\int_P \frac{q^n(P)\psi_i^{+n}(P)}{\hat{q}^{n-1}(P)R_i^n}\, dP\right] - N \quad (25)$$

In the same manner of Eq. (18-19), the modified PDF $\hat{q}$ to minimize $\sum_{i=1}^{N} R_{err,i}^{n^{th}}$ can be calculated by following equations:

$$Min\left[\sum_{i=1}^{N} \int_P \frac{q^n(P)\psi_i^{+n}(P)}{\hat{q}^{n-1}(P)R_i^n} dP - N\right] \quad (26a)$$

where N is constant, which is the number of response. Thus, The N does not affect to find the minimum value. Therefore, the N in Eq.(26a) can be re-expressed as follows:

$$Min\left[\sum_{i=1}^{N} \int_P \frac{q^n(P)\psi_i^{+n}(P)}{\hat{q}^{n-1}(P)R_i^n} dP\right] \quad (26)$$

To find $\hat{q}$ for minimizing Eq. (25), Lagrange multiplier λ was used as following equation:

$$L(\hat{q}(P)) = \left[\sum_{i=1}^{N} \int_P \frac{q^{\mathrm{n}}(P)\psi^{+\mathrm{n}}_{i}(P)}{\hat{q}^{n-1}(P)R_i^{\mathrm{n}}} dP + \lambda \int_P \hat{q}^n(P)\, dP\right] (27)$$

The desired $\hat{q}$ can be found when a partial differential equation of Eq. (27) is equal to zero as follows:

$$\frac{\partial \mathrm{L}(\hat{\mathrm{q}})}{\partial \hat{\mathrm{q}}} = -(\mathrm{n}-1)\Sigma_{\mathrm{i}=1}^{\mathrm{N}} \left[\int_p \frac{q^{\mathrm{n}}(P)\psi^{+\mathrm{n}}_{i}(P)}{\hat{q}^n(P)R_i^{\mathrm{n}}} dP\right] + \lambda \int dP = 0 \ (28a)$$

or

$$-(n-1)\Sigma_{i=1}^{N} \left[\frac{q^{\mathrm{n}}(P)\psi^{+\mathrm{n}}_{i}(P)}{\hat{q}^n(P)R_i^{\mathrm{n}}}\right] + \lambda = 0 \quad (28b)$$

or

$$\hat{q}(P) = \frac{(n-1)^{\frac{1}{n}}}{\lambda^{\frac{1}{n}}} \sum_{i=1}^{N} \frac{q^n(P)\psi_i^{+n}(P)}{R_i^n} \quad (28c)$$

The value of $\lambda^{\frac{1}{n}}$ can be found by using following properties: $\int \hat{q}(P)dP$ = 1 and $\psi^{+}(P) > 0$

$$\lambda^{\frac{1}{n}} = (n-1)^{\frac{1}{n}} \left(\int_p \sum_{i=1}^{N} \frac{q^n(P)\psi_i^{+n}(P)}{R_i^n} dP\right)^{\frac{1}{n}} \quad (29)$$

Then, the modified pdf $\hat{q}$ can be derived as Eq. (30) by substituting Eq. (29) into Eq. (28c) and rearranging

$$\hat{q}(P) = \frac{q(P)\left(\sum_{i=1}^{N} \frac{\psi_i^{+n}(P)}{R_i^n}\right)^{\frac{1}{n}}}{\int_p q(P)\left(\sum_{i=1}^{N} \frac{\psi_i^{+n}(P)}{R_i^n}\right)^{\frac{1}{n}} dP} \quad (30)$$

Finally, the weight function to minimize the sum of n^{th} order weighted relative error for multiple responses was derived by substituting Eq. (30) into Eq. (9) as shown follows:

$$w(P) = \frac{\int_P q(P)\left(\sum_{i=1}^{N} \frac{\psi_i^{+\mathrm{n}}(P)}{R_i^n}\right)^{\frac{1}{n}} dP}{\left(\sum_{i=1}^{N} \frac{\psi_i^{+\mathrm{n}}(P)}{R_i^{\mathrm{n}}}\right)^{\frac{1}{\mathrm{n}}}} \quad (31)$$

In Eq. (31), when *n'* are set by 1, it becomes FW-CADIS method; and, if *n'* is set by 2, Eq. it becomes MR-CADIS method.

IV. EVALUATION AND COMPARISON

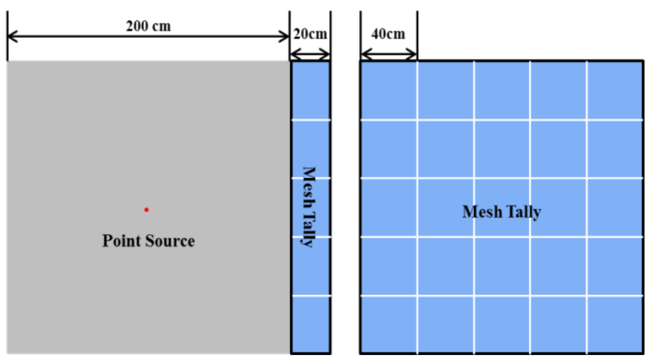
The FW-CADIS method is well applicated in SCALE6 [14] and ADVANTG [15] code. To obtain the weight by the FW-CADIS method using those code, only two deterministic calculation were required as follows: (1) a forward calculation to get values for multiple responses R_i in Eq. (16); (2) an adjoint calculation using adjoint sources devided by forward response. In the case of the MR-CADIS and N-CADIS method, the n^{th} order responses R_i^n in Eq. (31) can calculated by general deterministic calculation. However, n squared adjoint flux ψ_i^{+n} cannot be efficiently calculated by existent deterministic transport code. For applying the N-CAIDS method in realistic problem, deterministic tansport code must be developed to get n squared adjoint fluxes. In this time, development of a deterministic transport code for the N-CADIS is difficult for us to achieve. Thus, in this study, the weight function Eq. (31) was modifed to Eq. (32) using weight function of the CADIS method to easily apply the proposed method.

$$w(P) = \frac{\int_P q(P)\left(\sum_{i=1}^{N} \frac{1}{w_i'^n(P)}\right)^{\frac{1}{n}} dP}{\left(\sum_{i=1}^{N} \frac{1}{w_i'^n(P)}\right)^{\frac{1}{n}}} \quad (32)$$

where $w_i'(P)$ is a weight function for i^{th} response estimated by the CADIS method, Eq. (10). To get the adjoint flux and response from each response for weight equation, DENOVO, which is module to calculate forward and adjoint fluxes using S_N method in SCALE 6 [14], was used with 5 cm × 5 cm × 5 cm uniform meshes, 16 quadrature set and 10^{-5} tolerance for criterion the flux conversion. The Monte Carlo calculation was performed by MCNPX 2.7 [16] using weight window VRT.

1. Calculation Model

To understand the performance of N-CADIS method, a shielding problem was set as shown in Fig. 1. The concrete shielding block having 200 cm × 200 cm × 200 cm with 2.3 g/cm^3 density was used, and isotopic point gamma source having 1 MeV energy is located in the center of the concrete box. The Response function is set to the flux. It is recorded in the 40 cm × 40 cm × 20 cm unit mesh as shown in Fig. 1.



(a) Radial View (b) Axial View

Fig. 1 Schematic Drawing of the Shielding Problem

2. Results Comparison

To compare the efficiency with the methods, two kinds of figure of merit (FOM) [17] were used. First, mean based FOM is given as follows:

$$FOM_{mean} = \frac{1}{\bar{R}^2 T} \quad (24)$$

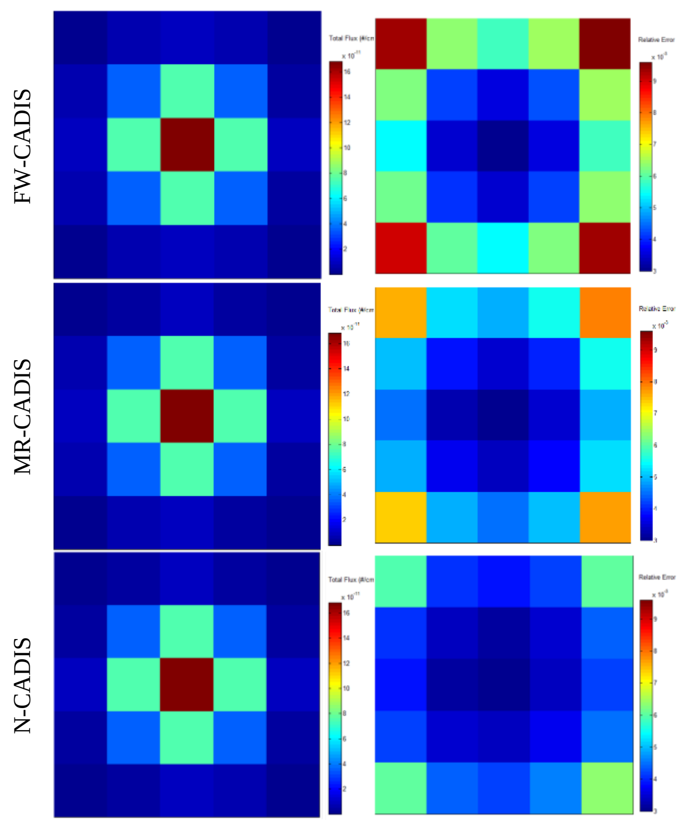
$$\bar{R} = \frac{1}{N}\sum_{i}^{N} R_{i,err} \quad (25)$$

where T is the computational time and $R_{i,err}$ is the relative error for i^{th} response. In this study, computational time does not include deterministic transport calculation time. therefore, only Monte Carlo simulation time was used. Second, tail based penalty FOM is given as follows:

$$FOM_{tail} = \frac{1}{[\bar{R}^2 + \left(\frac{\kappa_R}{3}\right)^{\frac{1}{4}} \sigma_R]T} \quad (26)$$

where κ_R is kurtosis to express the shape of relative error distribution and σ_R is relative uncertainty of variance for multiple responses. For result of N-CADIS method, order *n* was set to 10 because higher order can make infinite value when estimating weight value. The computational time of MCNPX simulation was set by 100 min to clearly compare the calculation efficiencies.

Fig. 2 is the maps of total flux and relative error. The gamma fluxes calculated by each method show good agreement within 2 sigma level. However, the relative errors at the corner of mesh tally calculated by the N-CADIS method show the lowest value compared to those of other methods. Table I is the detail information for the result. The FOM_{mean} of the result estimated by the N-CADIS method was increased by factor 1.87 and 1.36 compared to those of FW-CADIS and MR-CADIS, respectively. Also, the FOM_{tail} from N-CADIS was improved by the factor 2.03 and 1.46, respectively.



(a) Total Flux (B) Relative Error

Fig.2 Total Flux and Relative Error Distribution using FW-CADIS, MR-CADIS and N-CADIS method

Table I Relative Error and FOM values From FW-CADIS, MR-CADIS and N-CADIS method

	FW-CADIS	MR-CADIS	N-CADIS	Ratio (N-CADIS /FW-CADIS)	Ratio (N-CADIS /FW-CADIS)
Maximum Relative Error	0.96×10^{-2}	0.79×10^{-2}	0.63×10^{-2}	0.66	0.80
Average Relative Error	0.58×10^{-2}	0.49×10^{-2}	0.42×10^{-2}	0.72	0.86
FOM_{mean}	301.67	415.59	565.48	1.87	1.36
FOM_{tail}	203.46	282.50	413.55	2.03	1.46

V. CONCLUSION

In this study, the N-CADIS method was proposed to optimize the relative errors for multiple responses using a concept that minimizing the sum of n^{th} order weighted relative error for the individual response can achieve uniformly low uncertainty. To evaluate and compare the efficiency of the N-CADIS method, a shielding problem was estimated. The mean based and tail-based penalty FOMs using N-CADIS method was improved by factor 2.03 and 1.46 compared to FW-CADIS. However, the computational time for FOM values does not include deterministic calculation time to estimate weight map. Therefore, it was concluded that if a deterministic code to estimate n^{th} order squared adjoint particle transport is developed, the proposed N-CADIS method can create improved efficiency.

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