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An Application of the N-CADIS Method to Optimize Variance Reduction Parameters for Multiple Responses

Do Hyun KIM, Jong Kyung KIM*
Department of Nuclear Engineering, Hanyang University, 222, Wangsimni-ro, Seongdong-gu, Seoul 04763, Korea
**Corresponding author: jkkim1@hanyang.ac.kr*

1. Introduction

In past few decades, the Monte Carlo (MC) method has been widely used to solve radiation transport problems. It is well known that the MC method generally gives better accurate results than those of the deterministic method. On the other hand, an efficiency of the MC method is generally lower than that of the deterministic method. To improve the inefficiency of the MC method, variance reduction (VR) techniques have been introduced [1]. The main difficulty to apply VR techniques lies in the decision of VR parameters. In single response problems, the Consistent Adjoint Driven Importance Sampling (CADIS) can successfully produce those parameters [2]. It gives mathematically a zero variance solution and is referred to as hybrid MC in that it obtains adjoint fluxes from a deterministic method.

In the multiple response problems such as dose distribution and multiple detector problems, the CADIS method cannot usually give proper VR parameters to get a uniformly low variance. For these problems, several hybrid methods have been developed. It is noted that the Forward-Weighted CADIS (FW-CADIS) method can give the best efficiency among them [3]. In our previous study, the Multi-Response CADIS (MR-CADIS) method is developed [4]. The efficiency of MC calculation using the MR-CADIS method is higher than that of FW-CADIS. However, it is noted that the overall efficiency of the MR-CADIS including the deterministic and MC calculation was inefficient because it requires numerous deterministic calculation depending on the number of responses [5]. Also, in our previous study, the Nth-order Multi-response CADIS (N-CADIS) is developed for the same goal as the FW-CADIS method [6]. However, the problems, which are required many adjoint calculations, is not solved yet. In this study, a modified adjoint transport process to avoid many deterministic calculations was proposed. To verify the proposed process, results were compared with the FW-CADIS method.

2. Methods and Results

2.1.1 VR Theory in MC Method

In the MC method, the expected value G of function g is given as following the integral form:

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

where, $f(x)$ is the probability density function (PDF), which satisfies $\int f(x)dx = 1$ and $f(x) > 1$ for a continuous random variable x. Also, the variance is expressed by

$$Var[G] = \int [g^2(x)] f(x) dx - G^2 \,. \tag{2}$$

Using VR technique means using a modified PDF $\hat{f}(x)$ instead of the original PDF $f(x)$. The expectation value and variance using VR techniques can be expressed as follows:

$$G_{VR} = \int [g(x) f(x) / \hat{f}(x)] \hat{f}(x) dx \,, \tag{3}$$

$$Var_{VR}[G] = \int [\frac{g^2(x) f^2(x)}{\hat{f}^2(x)}] \hat{f}(x) dx - G^2 \,. \tag{4}$$

In the VR technique, the expectation value is not changed. However, the variance can be reduced by choosing the modified PDF $\hat{f}(x)$. Hence, selecting $\hat{f}(x)$ is a key for the VR techniques.

2.1.2 CADIS Method

The response using the integral form of the Boltzmann transport equation, which corresponds with Eq. (1) is given as follows:

$$R = \int_P \psi(P) \sigma_d(P) dP = \int_P \psi(P) q^+(P) dP \,, \tag{5}$$

where P is a phase-space including position, angle and energy spaces, ψ is the particle flux, σ_d is some objective functions, q is the source density function and the variables with '$^+$' signify the adjoint variables.

The Boltzmann transport equation is not a self-adjoint. Thus, the forward and adjoint transport equations follow adjoint identity:

$$\left\langle \psi^+, H\psi \right\rangle = \left\langle \psi, H^+\psi^+ \right\rangle \,, \tag{6}$$

where the bracket $\langle \; \rangle$ indicates an integration over all independent variables and H is the transport operator.

The response R can be re-expressed using Eq. (6) as follows:

$$R = \int_P \psi^+(P) q(P) dP \,. \tag{7}$$

For the VR techniques, this response and its variance can be written by using a modified PDF $\hat{q}(P)$ as follows:

$$R = \int_P \left[\frac{\psi^+(P) q(P)}{\hat{q}(P)} \right] \hat{q}(P) dP \tag{8}$$

$$Var_{VR}[R] = \int_P \left[\frac{\psi^{+2}(P) q^2(P)}{\hat{q}^2(P)} \right] \hat{q}(P) dP - R^2 \,. \tag{9}$$

Using importance sampling [6], the optimized $\hat{q}(P)$ to minimize is given by

$$\hat{q}(P) = \frac{\psi^+(P)q(P)}{\int_P \psi^+(P)q(P)dP} \quad . \tag{10}$$

If Eq. (10) puts into Eq. (9), the variance becomes zero. Thus, it can theoretically lead to minimum variance.

To apply the VR techniques, the weight of MC particle must be corrected by following relationship:

$$w(P)\hat{q}(P) = w_0(P)q(P) \quad . \tag{11}$$

where $w_0(P)$ is the initial MC particle weight, which is generally set to 1, and $w(P)$ is the alternative MC particle weight. Substituting Eq. (10) into Eq. (11) and rearranging, the weight equation of the CADIS method is derived as follows:

$$w(P) = \frac{\int_P \psi^+(P)q(P)dP}{\psi^+(P)} = \frac{R}{\psi^+(P)} \quad . \tag{12}$$

2.1.3 FW-CADIS Method

For the multiple responses, the response and adjoint source of the CADIS method can be expressed by

$$R = \sum_{i=1}^{N} R_i \tag{13}$$

and

$$q^+(P) = \sum_{i=1}^{N} q_i^+(P) \quad , \tag{14}$$

where N is the total number of responses; R_i and $q^+(P)$ are a response and an adjoint source of the *i-th* response, respectively. For the multiple responses, the FW-CADIS method employs an alternative adjoint source weighted by the inverse of the forward response as follows:

$$q^+_{FW-CADIS} = \sum_{i=1}^{N} q_i^+(P) / R_i \quad . \tag{15}$$

Then, the adjoint fluxes can be re-expressed as

$$\psi^+_{FW-CADIS} = \sum_{i=1}^{N} \psi_i^+(P) / R_i \quad , \tag{16}$$

where $\psi_i^+(P)$ is the adjoint flux generated by *i-th* adjoint source. By substituting Eq. (16) into Eq. (12), the weight equation of the FW-CADIS method can be expressed as follows:

$$w_{FW-CADIS}(P) = \frac{\int_P q(P) \sum_{i=0}^{N} \psi_i^+(P) / R_i dP}{\sum_{i=0}^{N} \psi_i^+(P) / R_i} \quad . \tag{17}$$

2.1.4 MR-CADIS Method

For uniformly low variance, the MR-CADIS method uses the objective function for a biased PDF, which minimizes the sum of the squared relative error, as the following form:

$$\hat{q}_{MR-CADIS}(P) = Min\left[\sum_{i=1}^{N} R_{err}^2(\hat{q}(P))\right] , \tag{18}$$

where: $R_{err}(R_i) \equiv \sqrt{Var(R_i)} / R_i$;

$Var(R_i) = \int_P \psi^2(P) q_i^+(P) dP - R^2 = E(R_i^2) - E^2(R_i)$;

$R_{err}^2(R_i) = \dfrac{E(R_i^2) - E^2(R_i)}{E^2(R_i)}$.

$Min[f(x)]$ returns a variable x for the minimum $f(x)$.

The solution of Eq. (18) is following form [3]:

$$\hat{q}_{MR-CADIS}(P) = \frac{q(P)\sqrt{\sum_{i=1}^{N} \psi^{+^2}(P) / R_i^2}}{\int_P q(P)\sqrt{\sum_{i=1}^{N} \psi^{+^2}(P) / R_i^2 dP}} \quad . \tag{19}$$

Substituting Eq. (19) into Eq. (11) and rearranging, the weight equation of the MR-CADIS method given by

$$w_{MR-CADIS}(p) = \frac{\int_P q(P)\sqrt{\sum_{i=1}^{N} \psi^{+^2}(P) / R_i^2 dP}}{\sqrt{\sum_{i=1}^{N} \psi^{+^2}(P) / R_i^2}} \quad . \tag{20}$$

2.1.5 N-CADIS Method

In the MR-CADIS method, the relative errors will not be uniformly distributed because the efforts for reducing the relative error are different depending on the responses. In the N-CADIS method, to give more weight to responses which have higher relative errors, the *n-th* order weighted relative error (NWRE) was introduced as follows:

$$R_{err}^{n-th} \equiv \frac{E(R_i^n) - E^n(R_i)}{E^n(R_i)} = \frac{E(R_i^n)}{E^n(R_i)} - 1 \quad . \tag{21}$$

It returns a relatively high value for the response with a higher relative error. Using NWRE, the objective function for a biased PDF of the N-CADIS method is expressed as follows:

$$\hat{q}_{N-CADIS}(P) = Min\left[\sum_{i=1}^{N} R_{err}^{n-th}(R_i)\right] \quad . \tag{22}$$

The solution of Eq. (22) is given by [5]

$$\hat{q}_{N-CADIS}(P) = q(P)\left[\frac{\left(\sum_{i=1}^{N} \psi_i^{+^n}(P) / R_i^n\right)^{\frac{1}{n}}}{\int_P q(P)\left(\sum_{i=1}^{N} \psi_i^{+^n}(P) / R_i^n\right)^{\frac{1}{n}} dP}\right] \quad . \tag{23}$$

Also, the weight equation can be written by substituting Eq. (23) into Eq. (11) as follows:

$$w_{N-CADIS}(P) = \frac{\int_P q(P)\left(\sum_{i=1}^{N} \psi_i^{+^n}(P) / R_i^n\right)^{\frac{1}{n}} dP}{\left(\sum_{i=1}^{N} \psi_i^{+^n}(P) / R_i^n\right)^{\frac{1}{n}}} \quad . \tag{24}$$

The summation terms $\left(\sum_{i=1}^{N} \psi^{+^n}(P) / R_i^n\right)^{\frac{1}{n}}$ of Eq. (24) take the same form of the p-norm. It gives the maximum value when the order n set to infinity. Thus, Eq. (24) can be re-expressed by using $Max[f_i(x)]$ as following equation:

$$w_{N-CADIS}(P) = \lim_{n\to\infty} \frac{\int_P q(P)\left(\sum_{i=1}^{N} \psi_i^{+^n}(P)/R_i^n\right)^{\frac{1}{n}} dP}{\left(\sum_{i=1}^{N} \psi_i^{+^n}(P)/R_i^n\right)^{\frac{1}{n}}}. \quad (25)$$

Then,

$$w_{N-CADIS}(P) = \frac{\int_P q(P) Max\left(\psi_i^{+}(P)/R_i\right) dP}{Max\left(\psi_i^{+}(P)/R_i\right)}. \quad (26)$$

2.2 Application of the N-CADIS Method

To obtain the weight of the N-CADIS method, this method requires adjoint calculations that equal the number of adjoint sources. It can lead to inefficiencies, especially problems such as distribution problems. To overcome this inefficiency, transport equation or transport process should be improved.

The difference of weight function between the FW-CADIS and N-CADIS method is the terms, which use $\sum_{i=0}^{N}\psi^{+}(P)/R_i$ or $Max\left(\psi_i^{+}(P)/R_i\right)$ as shown in Eq. (17) and Eq. (26). Therefore, to apply the N-CADIS method, values other than the maximum should be removed. In this study, the following strategy was used for the adjoint calculation process in the deterministic method.

i. Cell-centered Adjoint Flux:

$$\psi_{cen}^{+} = \begin{cases} C\left[\psi_{in}^{+}\right], & C\left[\psi_{in}^{+}\right] \ge C\left[q^{+}\right] \\ C\left[q^{+}\right], & C\left[\psi_{in}^{+}\right] < C\left[q^{+}\right] \end{cases}, \quad (27)$$

where ψ_{in}^{+} is incoming adjoint flux and $C[\ ]$ is a function to calculate cell-centered adjoint flux.

ii. Outgoing Adjoint Flux:

$$\psi_{out}^{+} = \begin{cases} O\left[\psi_{in}^{+}\right] + O\left[q^{+}\right], & O\left[\psi_{in}^{+}\right] \ge O\left[q^{+}\right] \\ O\left[q^{+}\right], & O\left[\psi_{in}^{+}\right] < O\left[q^{+}\right] \end{cases}, \quad (28)$$

where ψ_{out}^{+} is outgoing adjoint flux and $O[\ ]$ is a function to calculate outgoing adjoint flux. In the case that the flux generated from the incoming flux is larger than that generated from the source, the flux was not modified to maintain the flux that comes from the other energy bins. ADVANTG code was modified by using this strategy.

2.3 Verification

2.3.1 Simple Stick Problem

To validate the proposed strategy, a simple stick problem was selected as shown in Fig.1. It consists of concrete with 2.3 g/cm^3 density. For a deterministic calculation, this model was uniformly divided into 10 parts. A volume neutron source, which has the Watt fission spectrum, is located on the left end part. For the deterministic calculation, BPLUS library was used and the tolerance to check conversion was set to 10^{-10} to reduce the error of the deterministic method. The other calculation conditions were set to the default option.

Fig. 2 shows a ratio between the sum $\psi_i^{+}(P)/R_i$ and the maximum $\psi_i^{+}(P)/R_i$ which are the same as the FW-CADIS and the N-CADIS method, respectively. Also, Fig. 3 shows a ratio between the sum $\psi_i^{+}(P)/R_i$ by using the modified transport process (N-CADIS-M) and maximum $\psi_i^{+}(P)/R_i$. The results show that the overall difference using the proposed strategy was properly reduced and the maximum difference was decreased from 8.44 to 2.29.

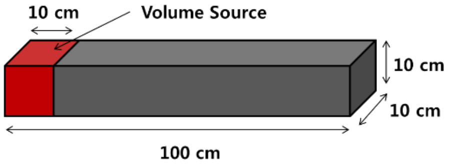


Fig. 1. Calculation model for a simple stick problem

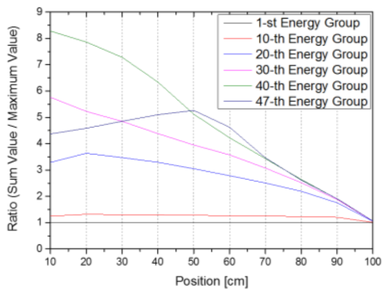


Fig.2 The ratio between the sum $\psi_i^{+}(P)/R_i$ and the maximum $\psi_i^{+}(P)/R_i$

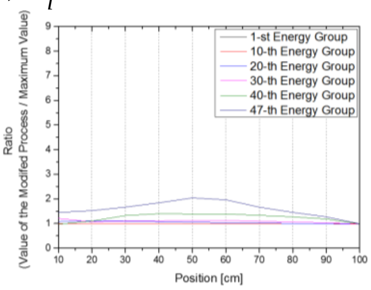


Fig.3 The ratio between the sum $\psi_i^{+}(P)/R_i$ from the modified transport process and maximum $\psi_i^{+}(P)/R_i$

2.3.2 Hollow Concrete Cube Problem

To evaluate the performance of the N-CADIS-M method, the hollow concrete cube problem was used as shown in Fig.4. A void space with 50 cm × 50 cm × 50 cm is located on the center of the box and a point neutron source with the Watt fission spectrum is located at the center of the void space. The concrete shielding with a density of 2.3 g/cm^3 was used, with a thickness of 50, 100, and 200 cm. The mesh tally with a 10 cm × 10 cm × 10 cm uniform size for the whole cube was used. The MC calculation was performed by MCNPX code with the weight window and source biasing VR techniques.

Fig 6 shows the relative error map at 60 minutes of the MC calculation time for the case of 100 cm thick shielding problem. The relative error from the N-CADIS-M was generally lower than that from the FW-CADIS method. Table I contains information for the result of this calculation.

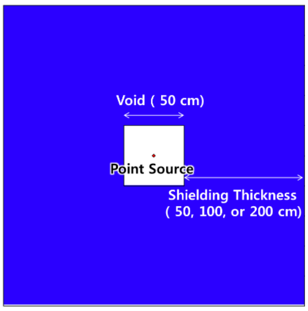
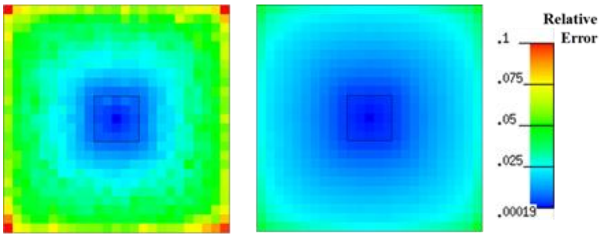


Fig. 5 Calculation model for the hollow cube problem



FW-CADIS N-CADIS-M

Fig. 6 The relative error distribution obtained by using the FW-CADIS and N-CADIS-M methods for the case of 100 cm shielding thickness problem

For the N-CADIS-M method, an additional calculation at the adjoint transport step is needed for selecting the maximum value. However, all of the deterministic calculation time decreases because the number of iterations for the adjoint transport sweep was decreased. For some energy bins, the transport sweep does not converge. Therefore, it seems that the N-CADIS-M method needs more careful statistical checks. In this problems, The FOM_{ave} and FOM_{max} values from the N-CADIS-M method are higher than those from FW-CADIS method.

3. Conclusions

The N-CADIS method was derived by minimizing the sum of the NWRE, which gives a weighted value for a response having higher variance. However, the N-CADIS method needs many adjoint calculations depending on a number of the adjoint sources. To overcome this inefficiency, in this study, a strategy to apply the N-CADIS method was proposed by modifying the adjoint transport process of ADVANTG code. To verify the proposed process, a hollow cube problem was simulated. The FOM_{ave} and the FOM_{max} values were increased about 2.55 ~ 7.84 and 3.89 ~ 15.63 times, respectively. Therefore, it is expected that the N-CADIS method can effectively apply to multiple response problems.

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REFERENCES

[1] A. Haghighat, Monte Carlo Methods for Particle Transport, CRC Press Taylor & Francis Group, Boca Raton, FL, 2014.
[2] J. C. Wagner and A. Haghighat, Automated Variance Reduction of Monte Carlo Shielding Calculations Using the Discrete Ordinates Adjoint Function, Nuclear Science Engineering, Vol. 128.2 p. 186-208, 1998.
[3] J. C. Wagner, E. P. Douglas and W. M. Scott, FW-CADIS Method for Global and Regional Variance Reduction of Monte Carlo Radiation Transport Calculations, Nuclear Science and Engineering, Vol. 176.1, 37-57, 2014.
[4] D. H. Kim, and et al., A Proposal on Multi-response CADIS Method to Optimize Reduction of Regional Variances in Hybrid Monte Carlo Simulation, Annals of Nuclear Energy, Vol. 104 p. 282-290, 2017.
[5] D. E. Peplow, A Comparison of the FW CADIS and MR CADIS Variance Reduction Methods, Transaction of America Nuclear Society, Vol. 116 p. 540-543, 2017
[6] D. H. Kim, C. H. Shin and S. H. Kim, Nth-order Multi-Response CADIS Method for Optimizing Variance Reduction Parameter in Monte Carlo Simulation, M&C 2017 - International Conference on Mathematics & Computational Methods Applied to Nuclear Science & Engineering, Jeju, Korea, April 16-20, 2017

Table I: Results from the FW-CADIS and N-CADIS-N method for the hollow concrete cube problem

Shielding Thickness	Methods	MC Time [Min]	Deterministic Calculation Time [Min]	Variance of Relative Error	FOM_{ave}** (MC FOM)	FOM_{max}*** (MC FOM)
50 cm	FW-CADIS	10.2	5.62	2.64×10^{-4}	53.0 (112)	4.75 (7.41)
	N-CADIS-M	10.0	4.93	8.63×10^{-5}	135 (202)	18.48 (27.6)
	Ratio*	-	-	0.33	2.55 (1.80)	3.89 (3.72)
100 cm	FW-CADIS	59.9	19.13	3.93×10^{-4}	5.79 (7.65)	0.307 (0.405)
	N-CADIS-M	60.1	17.50	7.00×10^{-5}	25.0 (32.3)	3.21 (4.14)
	Ratio*	-	-	0.18	4.32 (4.22)	10.46 (10.22)
200 cm	FW-CADIS	200	61.76	1.27×10^{-3}	0.453 (0.594)	0.016 (0.0204)
	N-CADIS-M	200	60.23	1.40×10^{-4}	3.39 (4.41)	0.25 (0.332)
	Ratio*	-	-	0.11	7.84 (7.42)	15.63 (16.27)

*: N-CADIS-M / FW-CADIS; **: FOM value using average relative error; ***: FOM value using maximum relative error