A Proposal of the Stochastic Error Estimation Method for the Sampling Based Sensitivity and Uncertainty Analysis in Monte Carlo Eigenvalue Calculation

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1. Introduction

The sampling based sensitivity and uncertainty (S/U) analysis method [1] is a stochastic approach to get the uncertainties of the reactor characteristics using the sets of randomly sampled cross sections. XSUSA [2] is a representative code using the stochastic approach for the sampling based S/U analysis. Due to the characteristic of the stochastic methodology, the result of the sampling based S/U estimation always accompanies the stochastic errors. In addition, if the Monte Carlo method is used as a tool of transport analysis, the stochastic error of the uncertainty result can be propagated by the two stochastic uncertainty parameters, which are the Monte Carlo stochastic error and the input uncertainty caused by the sampling based approach. Usually, to reduce the Monte Carlo stochastic uncertainty, the stochastic errors are enough reduced using lots of the particle history per each calculation. In this study, an estimate method of the stochastic uncertainty on the S/U analysis using the Monte Carlo method is proposed to confirm the effect of the Monte Carlo stochastic errors to the S/U result.

2. Methods and Results

The sampling based S/U analysis is performed as the following procedure: 1) a number of cross section sets are generated with the random sampling of the cross section using the covariance data, 2) the transport calculations with each sampled cross section are pursued using a transport code, and 3) the uncertainty of the responses calculated by the transport code is analyzed. In the analysis procedure, if the Monte Carlo code is used for the S/U analysis, each response has a stochastic uncertainty. As a result, the stochastic error can affect the result of S/U analysis. In this study, a method to evaluate and separate the stochastic uncertainty caused by using Monte Carlo simulation method is proposed.

2.1 Analysis Method

Let α is an input uncertainty parameter. Then, we can get a single output response $R(\alpha)$ from each transport simulation. The sampling based S/U analysis is performed with sets of the cross sections as follows:

$$\alpha_k = [\alpha_{k1}, \alpha_{k2}, \alpha_{k3}, ..., \alpha_{kI}]; \ (k = 1, 2, ..., n) \quad (1)$$

$$R(\alpha_k) = [R_1(\alpha_k), R_2(\alpha_k), ..., R_J(\alpha_k)]; \ (k = 1, 2, ..., n) \quad (2)$$

where I is the number of parameter types for a transport simulation, k is a set of random sampling, and n is the number of random samples. Generally, the standard deviation of the responses in Eq. (2) is evaluated for the S/U analysis. With considering the Monte Carlo stochastic uncertainty, the standard deviation of the responses can be expressed by Eq. (3).

$$\overline{\sigma_R}^2 + \overline{\sigma_{MC}}^2 = \overline{\sigma_T}^2 \quad (3\text{-}1)$$

$$\overline{\sigma_R} = \sqrt{\overline{\sigma_T}^2 - \overline{\sigma_{MC}}^2} \quad (3\text{-}2)$$

where $\overline{\sigma_R}$ is an average standard deviation of the responses caused by the input uncertainty, $\overline{\sigma_{MC}}$ is an averaged standard deviation of Monte Carlo stochastic uncertainties for the responses, $\overline{\sigma_T}$ is an averaged total standard deviation of the responses including both input uncertainty and Monte Carlo stochastic uncertainty. Using the Monte Carlo method, the $\overline{\sigma_T}$ is calculated, of which the stochastic uncertainty is included. Therefore, the response uncertainty caused by the randomly sampled cross sections can be estimated by Eq. (3-2). To calculate the uncertainty of the $\overline{\sigma_R}$, a well-known uncertainty propagation equation was introduced as shown in Eq. (4).

$$\sigma_f^{\ 2} \approx \left|\frac{\partial f}{\partial a}\right|^2 \sigma_a^{\ 2} + \left|\frac{\partial f}{\partial b}\right|^2 \sigma_b^{\ 2} + 2\left|\frac{\partial f}{\partial a}\right|\left|\frac{\partial f}{\partial b}\right| \mathrm{cov}[a,b] \quad (4)$$

where f is a function which has the variables a and b; $f(a,b)$. Using Eqs. (3-2) and (4), the uncertainty of the standard deviation of the response, $\sigma[\overline{\sigma_R}]$, can be derived to the following equation:

$$\sigma[\overline{\sigma_R}] \simeq \sqrt{\frac{\overline{\sigma_T}^2}{\overline{\sigma_T}^2 - \overline{\sigma_{MC}}^2}\sigma^2[\overline{\sigma_T}] + \frac{\overline{\sigma_{MC}}^2}{\overline{\sigma_T}^2 - \overline{\sigma_{MC}}^2}\sigma^2[\overline{\sigma_{MC}}] + 2\frac{\overline{\sigma_T}\cdot\overline{\sigma_{MC}}}{\overline{\sigma_T}^2 - \overline{\sigma_{MC}}^2}\mathrm{cov}[\overline{\sigma_T}, \overline{\sigma_{MC}}]} \quad (5)$$

where $\sigma[\overline{\sigma_T}]$ is a standard deviation of the average uncertainty including both response uncertainty and Monte Carlo stochastic uncertainty, $\sigma[\overline{\sigma_{MC}}]$ is a standard deviation of the averaged Monte Carlo stochastic uncertainty, and $\mathrm{cov}[\overline{\sigma_T}, \overline{\sigma_{MC}}]$ is a covariance between $\overline{\sigma_T}$ and $\overline{\sigma_{MC}}$. The uncertainty parameters, which are $\overline{\sigma_{MC}}$, $\sigma[\overline{\sigma_{MC}}]$, and $\overline{\sigma_T}$, can be easily estimated from the response results. However, the parameters $\sigma[\overline{\sigma_T}]$ and $\mathrm{cov}[\overline{\sigma_T},\overline{\sigma_{MC}}]$ cannot be directly calculated from the results of the responses. Here, we introduced the estimation strategies for the parameters. The $\overline{\sigma_T}^2$ is the average over the square of each deviation $\{R(\alpha) - \overline{R}\}^2$; therefore, the distribution of the square of the deviation follows the gamma distribution. Also, it is well known that the sampling distribution of the gamma distribution follows the central limit theory. Thus, the standard error of the gamma distribution (the standard deviation of the responses) can be estimated as given in Eq. (6).

$$\overline{\sigma} \sim N(\sigma, \frac{\sigma^2[\sigma]}{n}) \tag{6}$$

In this study, the $\sigma[\overline{\sigma_T}]$ and $\sigma[\overline{\sigma_{MC}}]$ is calculated as shown in Fig. 1. First, the responses are grouped with n number of sub-groups. As a result, each group has m responses. Then, the standard deviation of each group can be estimated. The standard deviation of the group standard deviations from the n groups is can be simply calculated. Finally, using the central limit theorem, the uncertainty $\sigma[\overline{\sigma_T}]$ and $\sigma[\overline{\sigma_{MC}}]$ can be calculated with Eqs. (7) and (8).

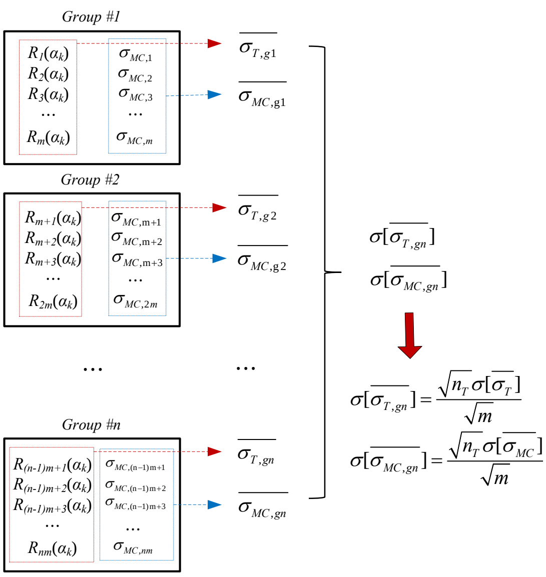


Fig. 1. Proposed strategy for the calculation of $\sigma[\overline{\sigma_T}]$ and $\sigma[\overline{\sigma_{MC}}]$

$$\sigma[\overline{\sigma_T}] = \frac{\sqrt{m}\cdot\sigma[\overline{\sigma_{T,gn}}]}{\sqrt{n_T}} \tag{7}$$

$$\sigma[\overline{\sigma_{MC}}] = \frac{\sqrt{m}\cdot\sigma[\overline{\sigma_{MC,gn}}]}{\sqrt{n_T}} \tag{8}$$

Also, the covariance in Eq. (5) can be calculated as shown in Fig. 2. As the same way with Fig. 1, the results are grouped, and the covariance of the group standard deviations is estimated. The relationship between the $\mathrm{cov}[\overline{\sigma_{T,gn}},\overline{\sigma_{MC,gn}}]$ and $\mathrm{cov}[\overline{\sigma_T},\overline{\sigma_{MC}}]$ are given in Eq. (9). Hence, the covariance $\mathrm{cov}[\overline{\sigma_T},\overline{\sigma_{MC}}]$ can be directly calculated from the estimation of $\mathrm{cov}[\overline{\sigma_{T,gn}},\overline{\sigma_{MC,gn}}]$.

$$\begin{aligned}\mathrm{cov}[\overline{\sigma_{T,gn}},\overline{\sigma_{MC,gn}}] &= \mathrm{cov}[\frac{\sum\overline{\sigma_T}}{m},\frac{\sum\overline{\sigma_{MC}}}{m}] \\ &= \frac{\mathrm{cov}[\sum\overline{\sigma_T},\sum\overline{\sigma_{MC}}]}{m^2} \\ &= \sum\sum\frac{\mathrm{cov}[\overline{\sigma_T},\overline{\sigma_{MC}}]}{m^2} \\ &= \frac{m^2\,\mathrm{cov}[\overline{\sigma_T},\overline{\sigma_{MC}}]}{m^2} = \mathrm{cov}[\overline{\sigma_T},\overline{\sigma_{MC}}]\end{aligned} \tag{9}$$

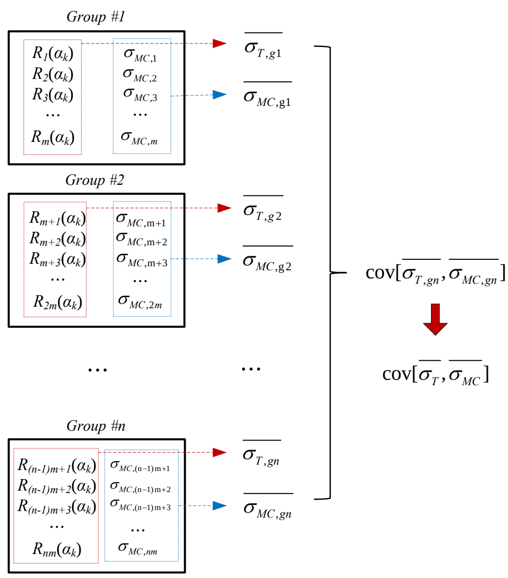


Fig. 2. Proposed strategy for the calculation of $\mathrm{cov}[\overline{\sigma_T},\overline{\sigma_{MC}}]$

2.2 Evaluation and Analysis

For the estimation and verification of the proposed method, 44 group cross section and covariance data from ENDF-VII.1 cross section library were generated using NJOY code [3]. Then, random sampling of both U-235 and U-238 cross sections using covariance data was pursued for the reactions which are MT number #1, #2, #4, #18, and #102 (total, elastic, (n,n'), fission, and absorption reactions), respectively [4]. For three benchmark problems, multiplication factors using each randomly sampled cross section were estimated by McCARD Monte Carlo code [5]. The details of the benchmark problems are given in Fig. 3 and Table I. Also, the simulation conditions for each eigenvalue calculation are given in Table II.

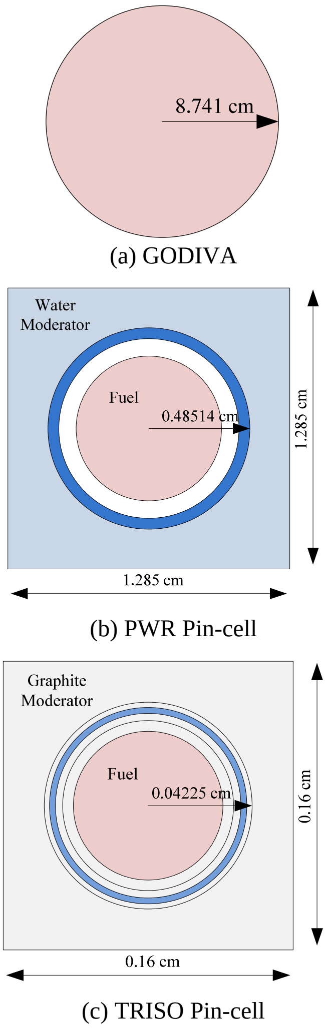


Fig. 3. Radial Views of the Benchmark Problems

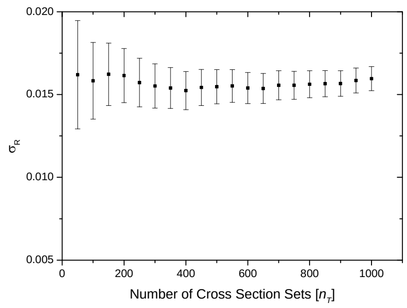
Table I: Details of Benchmark Problems

Problem Name	Classifi-cation	Variable	Value
GODIVA	Geometry	Radius of Uranium Sphere	8.741 cm
	Density	U-sphere Density	18.74 g/cc
	Material	U-235 [mass fraction]	94.73 %
		U-238 [mass fraction]	5.27%
PWR Pin-cell	Geometry	Radial Arrangement	Infinite
		Radius of Fuel Cylinder	0.41275 cm
		Radius of Inner Cladding	0.42164 cm
		Radius of Outer Cladding	0.48514
		Height	Infinite
		x-max. of Water Moderator	0.6425 cm
		x-min. of Water Moderator	-0.6425 cm
		y-max. of Water Moderator	0.6425 cm
		y-min. of Water Moderator	-0.6425 cm
	Density	Fuel	10.176 g/cc
		Gap	0.001 g/cc
		Cladding	6.55 g/cc
		Water	0.7 g/cc
	Material	U-234 in Fuel [mass fraction]	0.0237 %
		U-235 in Fuel [mass fraction]	14.9618 %
		U-238 in Fuel [mass fraction]	66.1645 %
		O-16 in Fuel [mass fraction]	11.8500 %
		O-16 in Gap [mass fraction]	100 %
		Natural Zr in Cladding [mass fraction]	100 %
		H-1 in Water [mass fraction]	11.19 %
		O-16 in Water [mass fraction]	88.81 %
		B-10 in Water [mass fraction]	0.02 %
		B-11 in Water [mass fraction]	0.08 %
TRISO Pin-cell	Geometry	Radius of Fuel Sphere	0.02125 cm
		Radius of Buffer	0.03125 cm
		Radius of Inner PyC	0.03475 cm
		Radius of SiC	0.03825 cm
		Radius of Outer PyC	0.04225 cm
		x-max. of Graphite Moderator	0.08 cm
		x-min. of Graphite Moderator	-0.08 cm
		y-max. of Graphite Moderator	0.08 cm
		y-min. of Graphite Moderator	-0.08 cm
		z-max. of Graphite Moderator	0.08 cm
		z-min. of Graphite Moderator	-0.08 cm
	Density	Density of Fuel Sphere	10.5 g/cc
		Density of Buffer	1 g/cc
		Density of Inner PyC	1.9 g/cc
		Density of SiC	3.2 g/cc
		Density of Outer PyC	1.9 g/cc
		Density of Graphite Moderator	1.9 g/cc
	Material	U-235 in Fuel Sphere [atomic fraction]	5.22 %
		U-238 in Fuel Sphere [atomic fraction]	28.07 %
		O-16 in Fuel Sphere [atomic fraction]	50.07 %
		C-Nat in Fuel Sphere [atomic fraction]	16.64 %
		C-Nat in Buffer [atomic fraction]	100 %
		C-Nat in PyC [atomic fraction]	100 %
		Si-28 in SiC [atomic fraction]	46.08 %
		Si-29 in SiC [atomic fraction]	2.34 %
		Si-30 in SiC [atomic fraction]	1.55 %
		C-Nat in SiC [atomic fraction]	50.03 %
		C-Nat in Graphite Moderator [atomic fraction]	100 %

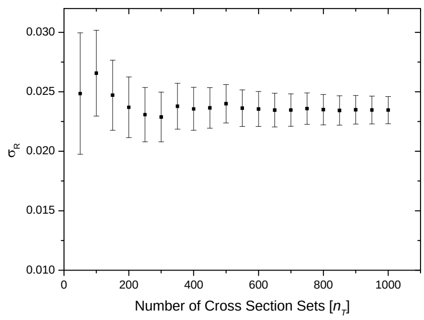
Table II: Simulation Conditions for the Calculation Cases

Case No.	Problem Name	Num. of Responses	Active Cycles	Particle History
1-1	GODIVA #1	1,000	10,000	350
1-2	GODIVA #2	1,000	1,000	350
1-3 /1-4	GODIVA #3	300	100	350
2-1	PWR Pin-cell #1	1,000	5,000	300
2-2	PWR Pin-cell #2	1,000	500	300
2-3 /2-4	PWR Pin-cell #3	300	100	300
3-1	TRISO Pin-cell #1	1,000	2,000	100
3-2	TRISO Pin-cell #2	1,000	390	100
3-3 /3-4	TRISO Pin-cell #3	300	190	100

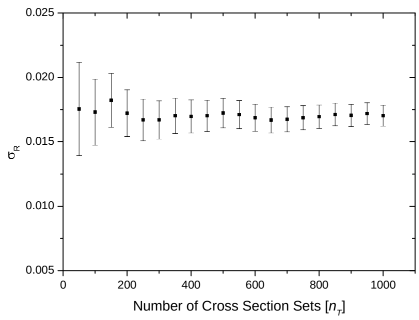
Fig. 4 is the results of the S/U analysis with 95 % confidence interval for Cases 1-1, 2-1, and 3-1 as increasing the number of cross section sets. The results show that the S/U results have a good agreement with each other within the 95 % confidence interval.



(a) GODIVA Problem (Case 1-1)



(b) PWR Pin-cell Problem (Case 2-1)



(C) TRISO Pin-cell Problem (Case 3-1)

Fig. 4. S/U Results of Responses (k_{eff}) with 95% Confidence Interval as Increasing the Number of Cross Section Sets

Table III are the results of $\overline{\sigma_R}$, $\sigma[\overline{\sigma_R}]$, and $\overline{\sigma_{MC}}$ for the benchmark problems with Table II condition. It was evaluated that all results of the S/U analysis give good agreements within the 95% confidence interval for each problem. The analysis on the agreements within the 95% confidence interval shows that the proposed method can effectively calculate the standard errors of the S/U analysis results. In addition, the analysis results show that the effect of the Monte Carlo stochastic error on the S/U analysis result is much smaller than that of the number of the cross section sets.

Table III: Results of S/U analyses and stochastic errors

Case No.	$\overline{\sigma_R}$	$\sigma[\overline{\sigma_R}]$	$\overline{\sigma_{MC}}$
1-1	0.015961	0.000366	0.000324
1-2	0.015947	0.000382	0.001024
1-3	0.015590	0.000799	0.003228
1-4	0.017197	0.000930	0.003259
2-1	0.022488	0.000539	0.000519
2-2	0.022254	0.000578	0.001643
2-3	0.020162	0.001049	0.003712
2-4	0.023951	0.001211	0.003678
3-1	0.017032	0.000406	0.001730
3-2	0.017273	0.000463	0.003920
3-3	0.016344	0.000818	0.005668
3-4	0.018383	0.000843	0.005645

3. Conclusions

In this study, an evaluation method of the stochastic error on the result of the sampling based S/U analysis with Monte Carlo simulation is proposed. Using the properties of the sample distribution, the evaluation method was derived. The S/U analysis and their uncertainties were evaluated for the three benchmark problems for the verification of the proposed method. The results show that all S/U analysis results give good agreements within the 95 % confidence intervals for each other. It is expected that the proposed method can contribute to improve the accuracy of the sampling based S/U analysis as well as the enhancing the calculation efficiency.

Acknowledgement

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