Implementation of Cross Section Random Sampling Code System for Direct Sampling Method in Continuous Energy Monte Carlo Calculations

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1. Introduction

In the conventional nuclear reactor development, the uncertainty of the nuclear core design and analysis code is evaluated and provided by comparing calculated values with measured. Generally, this uncertainty is calculated under conservative conditions. Recently, the Best Estimate Plus Uncertainty (BEPU) method has been widely investigated and utilized for the uncertainty quantification (UQ). In the BEPU method, the uncertainty provides a combination of the best-estimate models under realistic conditions. The best estimate results are calculated by the average values and their uncertainties, which can be calculated by the uncertainties from various inputs.

There are two approaches for the uncertainty analysis in the BEPU method. One is the Sensitivity/Uncertainty (S/U) analysis method [1] based on the perturbation techniques and the other is the Direct Sampling Method (DSM) [2,3] by random samplings (RS) of input parameters according to their covariance data.

In this study, we developed the McCARD/MIG [4] cross section RS code system for DSM in continuous energy MC calculations. This code system was applied to the Godiva and TMI-1 PWR pin problem for UQ analysis.

2. Methods and Results

2.1 Direct Sampling Method (DSM)

The mean value of the uncertain input parameter, u_i, and the covariance between u_i and u_j uncertain input parameters are defined by

$$\overline{u^i} \cong \frac{1}{K}\sum_{k=1}^{K} u_k^i, \tag{1}$$

$$\mathrm{cov}[u_i, u_j] \cong \frac{1}{K-1}\sum_{k=1}^{K}(u_i^k - \overline{u_i})(u_j^k - \overline{u_j}). \tag{2}$$

where K and k are the number of input parameters and the input index. Suppose that $\mathbf{C}_u$ is the covariance matrix defined by cov[u_i, u_j] and that a lower triangular matrix **B** is known through the *Cholesky* decomposition of $\mathbf{C}_u$, then we have

$$\mathbf{C}_u = \mathbf{B}\cdot\mathbf{B}^T \tag{3}$$

where $\mathbf{B}^T$ is the transpose matrix of **B**. Then, if $\mathbf{C}_u$ is symmetrical and positive definite, one can obtain a sample set by:

$$\mathbf{X}^i = \overline{\mathbf{X}} + \mathbf{B}\cdot\mathbf{Z} \tag{4}$$

where $\overline{\mathbf{X}}$ is the mean vector defined by the mean values from Eq. (1), and **Z** is a random normal vector calculated directly from a random sampling of the standard normal distribution using the *Box-Muller* method.

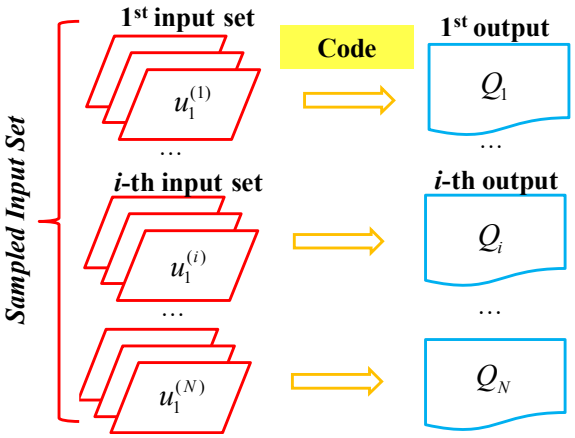

Fig. 1. Diagram for direct sampling method scheme

In the DSM, a nuclear core design parameter Q for each sampled input set can be calculated by the code or function, as shown in Fig. 1. Finally, the uncertainty of Q can be calculated by the sampled input set as below:

$$\sigma(Q) \cong \sqrt{\frac{1}{N-1}\sum_{k=1}^{N}(Q_i^k - \overline{Q_i})}. \tag{5}$$

To estimate the confidence interval of Q, bootstrapping (BS) method [5] was applied. For the BS method, the N number of Q were resampled with replacement one thousands of times.

2.2 McCARD/MIG code system for Cross Section Random Sampling

To establish the UQ analysis code system based on the continuous energy McCARD MC code, we used the MIG program. The latest MIG code, MIG 1.6, is capable of performing multiple-correlated sampling to estimate uncertainties of nuclear reactor core design

parameters by means of the DSM. Figure 2 shows the flowchart of the McCARD/MIG UQ analysis code system by cross section RS. Using the raw covariance matrix, MIG produces the cross section ratio input sets by random multiple-correlated sampling. Using the sampled cross section input sets, McCARD performs direct sampling core calculations.

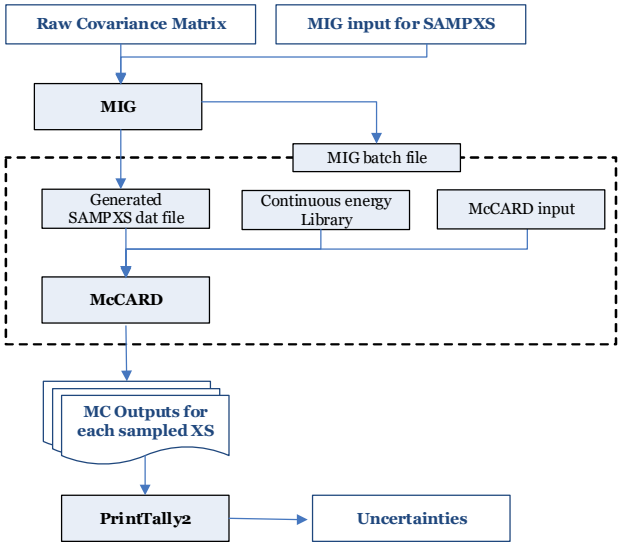

Fig. 2. Flowchart of McCARD/MIG UQ analysis code system by cross section random sampling

Figures 3 and 4 show the correlation coefficient matrix of ^{235}U ν (mt452) from raw cross section covariance data and 100 random samples by MIG. The raw cross section covariance matrix was generated by the NJOY code using the ENDF/B-VII.1 evaluated nuclear data library. The LANL 30 energy group structure was used. Figures 5 and 6 show the correlation coefficient matrix of ^{235}U considering three different cross section types (capture, elastic and inelastic scattering). Overall, the correlation coefficients sampled by MIG agree well with those from the raw cross section covariance.

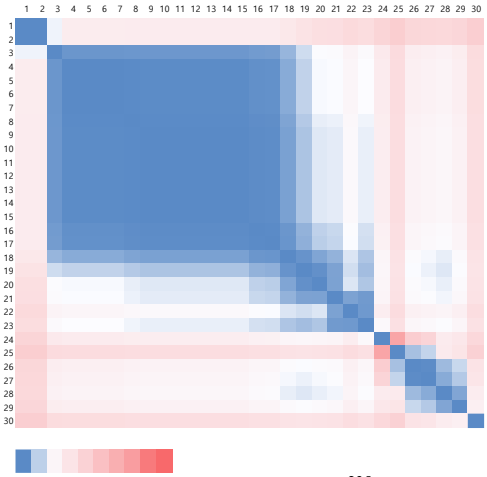

Fig. 3. Correlation coefficient matrix of ^{235}U ν (mt452) from raw cross section covariance data

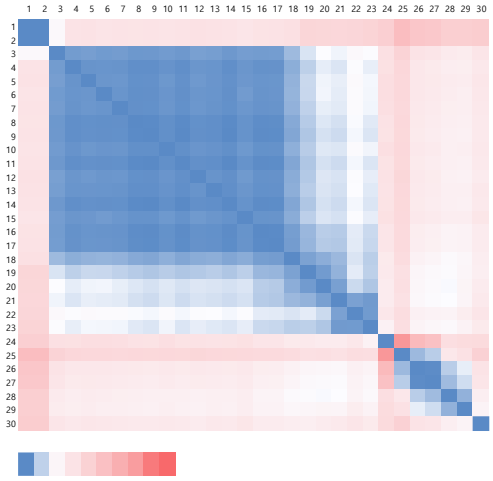

Fig. 4. Correlation coefficient matrix of ^{235}U ν (mt452) from 100 random samples by MIG

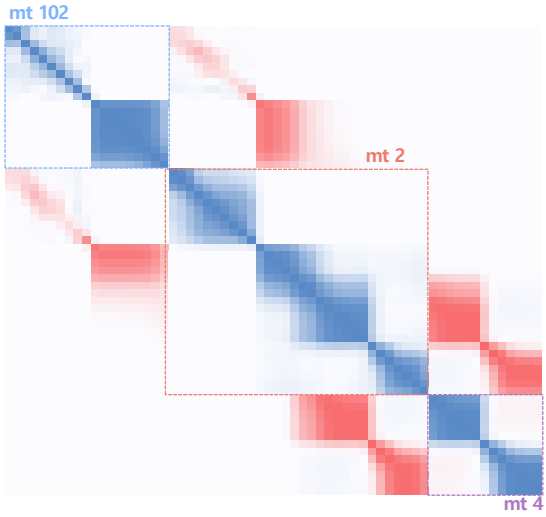

Fig. 5. Correlation coefficient matrix of ^{235}U considering three cross section types from raw cross section covariance data

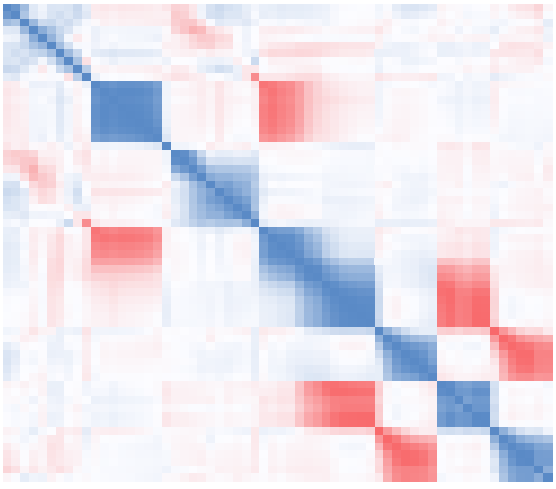

Fig. 6. Correlation coefficient matrix of ^{235}U including three cross section types from 100 random samples by MIG

2.3 Uncertainty Quantification in k for Godiva and TMI-1 PWR pin problem

Tables I and II provide a comparison of the uncertainties by the S/U analysis by the McCARD MC perturbation modules and DSM analysis by the McCARD/MIG UQ analysis code system for the Godiva and TMI-1 PWR pin problem [6]. As the covariance data of the cross section, the ENDF/B-VII.1 data for ^{235}U and ^{238}U were used on the assumption that only these two major actinides have cross-section uncertainties. In these calculations, we considered the correlations between (n,γ), elastic scattering, inelastic scattering cross sections, and independently sampled the cross sections for the other reaction types (i.e. *ν* and fission). For the DSM, 100 MC runs were conducted for each case. For the Godiva and TMI-1 pin problem, the statistical uncertainty in *k* for a single MC calculation was less than 0.02% and 0.03%, respectively. The results by S/U method were taken from the reference [6,7].

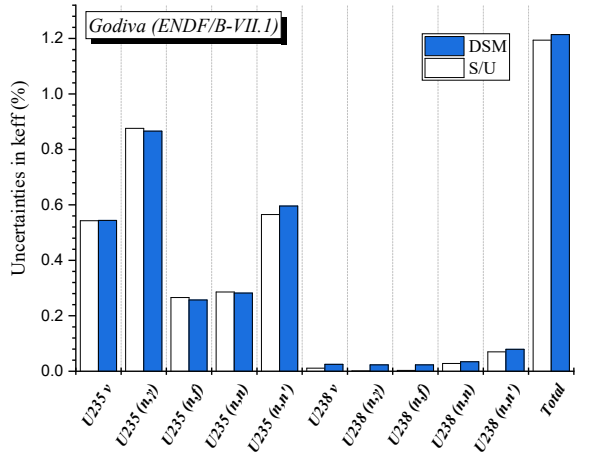

Fig. 7. Comparison between the uncertainties in k_{eff} by DSM and by S/U UQ analysis for the Godiva

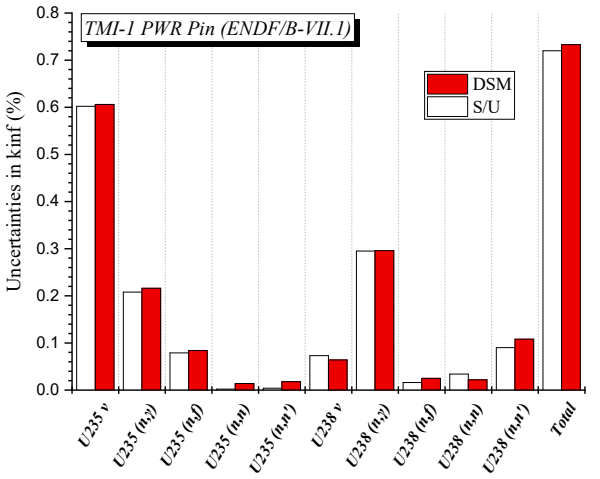

Fig. 8. Comparison between the uncertainties in k_{inf} by DSM and by S/U UQ analysis for the TMI-1 pin problem

Table I: Uncertainties in k_{eff} for the Godiva

Nuclide	XS Type for Covariance	*Uncertainties (%) in k_{eff} (ENDF/B-VII.1)*	
		S/U	**DSM**※ (100 samples)
^{235}U	ν, ν	0.543	0.544
	(n,γ), (n,γ)	0.876	0.866
	(n,f), (n,f)	0.266	0.257
	(n,n), (n,n)	0.286	0.282
	(n,n'), (n,n')	0.565	0.596
^{238}U	ν, ν	0.011	0.025
	(n,γ), (n,γ)	0.001	0.023
	(n,f), (n,f)	0.003	0.023
	(n,n), (n,n)	0.028	0.034
	(n,n'), (n,n')	0.070	0.079
Total		1.194	1.214±0.086

※ The statistical uncertainty for each k_{eff} in DSM is less than 0.02%

Table II: Uncertainties in k_{inf} for the TMI-1 pin problem

Nuclide	XS Type for Covariance	*Uncertainties (%) in k_{inf} (ENDF/B-VII.1)*	
		S/U	**DSM**※ (100 samples)
^{235}U	ν, ν	0.602	0.606
	(n,γ), (n,γ)	0.208	0.216
	(n,f), (n,f)	0.079	0.084
	(n,n), (n,n)	0.002	0.014
	(n,n'), (n,n')	0.004	0.018
^{238}U	ν, ν	0.073	0.064
	(n,γ), (n,γ)	0.295	0.296
	(n,f), (n,f)	0.016	0.025
	(n,n), (n,n)	0.034	0.022
	(n,n'), (n,n')	0.090	0.108
Total		0.720	0.733±0.071

※ The statistical uncertainty for each k_{eff} in DSM is less than 0.03%

The confidence intervals of the total uncertainties were calculated by the BS method using 1,000 repeated samplings. The uncertainties in *k* by the S/U and DSM analysis were in good agreement as shown in Figs. 7 and 8.

3. Conclusions

In this study, we successfully implemented the cross section RS modules for the DSM in continuous energy Monte Carlo Calculations into the McCARD and MIG v1.6 codes, and established the McCARD/MIG UQ analysis code system for the DSM. From the UQ results for Godiva and TMI-1 PWR pin problem, the results by the DSM agreed well with those by the S/U method and confirmed that this code system works well.

Owing to the versatility of the RS capability by MIG, the McCARD/MIG UQ analysis code system can be widely applied to all sorts of MC analysis.

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