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Multi-Group Covariance Data Generation from Continuous-Energy Monte Carlo Transport Calculations

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1. Introduction

In reactor physics field, uncertainty quantification of nuclear design parameters induced by nuclear data is an important issue. The Sensitivity and uncertainty (S/U) methodology [1] in deterministic tools [2,3] has been utilized for the uncertainty quantification. For a multi-group cross section based code, the S/U analysis can be conducted by an simple error propagation formula with the sensitivities of nuclear design parameters to multi-group cross sections and the covariance of multi-group cross sections, multi-group covariance. Recently the Monte Carlo(MC) S/U analysis method [4,5] with the continuous-energy cross section libraries has been developed for uncertainty quantification of the effective multiplication factor *k*. However it still utilizes the multi-group covariance data.

Conventionally, the multi-group covariance data required for S/U analysis have been produced by nuclear data processing codes such as ERRORJ [6] or PUFF [7] from the covariance data in Evaluated Nuclear Data Files (ENDF). However in the existing nuclear data processing codes, an asymptotic flux spectrum has been applied to the multi-group covariance data generation as an assumption since the exact flux spectrum is unknown before the neutron transport calculation. So the self-shielding effect cannot be reflected in the multi-group covariance generation. It can cause an inconsistency between the sensitivity profiles from reactor physic codes and the multi-group covariance data from nuclear data processing codes especially in resolved resonance energy region as pointed out previous research [8].

In order to generate the self-shielded multi-group covariance data from a real flux spectrum, we present a method based on the multi-group covariance tally in the continuous-energy Monte Carlo (MC) transport calculations. By utilizing MC transport calculations, the continuous-energy neutron flux spectrum with the depressions around resonances can be applied to the multi-group covariance processing. In this paper the methodology for multi-group covariance tally in MC transport calculations is introduced. Then the numerical results are compared to those of conventional covariance processing code ERRORR in NJOY99 [9].

2. Multi-Group Covariance Tally

In this section, the methodology for multi-group covariance tally in MC transport calculation is described.

2.1 Mathematical derivation of multi-group covariance for the tally in MC transport calculation.

2.1.1 Definition of multi-group covariance.

First, let us define the multi-group cross section of reaction type *r* and energy group *G* of isotope *i*, $x_{r,G}^{i}$, which conserves reaction rate as

$$x_{r,G}^{i} = \frac{1}{\phi_G}\int_{E_G}^{E_{G-1}} x_r^i(E)\phi(E)dE \tag{1}$$

$$\phi_G = \int_{E_G}^{E_{G-1}} \phi(E)dE \tag{2}$$

where

$x_r^i(E)$ = cross section at energy *E*,

$\phi(E)$ = flux spectrum at energy *E* and

E_G = lower energy bound of group G.

Then the multi-group covariance, covariance of $x_{r,G}^{i}$ and $x_{r',G'}^{i'}$, $\mathrm{cov}[x_{r,G}^{i} x_{r',G'}^{i'}]$ can be expressed by the following equation as applied in ERRORR,

$$\begin{aligned}&\mathrm{cov}\left[x_{r,G}^{i}, x_{r',G'}^{i'}\right]\\ &= \frac{1}{\phi_G\phi_{G'}}\int_{E_G}^{E_{G-1}}\int_{E_{G'}}^{E_{G-1}} \mathrm{cov}\left[x_r^i(E), x_{r'}^{i'}(E')\right]\phi(E)\phi(E')dEdE'.\end{aligned} \tag{3}$$

Note that Eq. (3) ignores the correlation between cross section and flux spectrum which can be called indirect effect.

As you can see in Eq. (3), multi-group covariance calculation requires a double integration with flux weighting. In MC simulation, it is difficult to deal with the double integration directly. Thus it is needed to convert the double integration in Eq. (3) into a single one. For this work, the description of point-energy covariance data given by ENDF will be followed

2.1.2 Description of ENDF covariance data

ENDF provides the point-energy covariance data as the forms of File 32 and File 33. The File 32 contains covariance of resonance parameter to represent covariance of cross section in short-range while File 33 covers long-range one in discrete forms. Thus ENDF covariance data for point-energy cross sections can be expressed as follows.

$$\begin{aligned}&\mathrm{cov}\left[x_r^i(E),x_{r'}^{i'}(E')\right]\\&=\mathrm{cov}_{\mathrm{MF32}}\left[x_r^i(E),x_{r'}^{i'}(E')\right]+\mathrm{cov}_{\mathrm{MF33}}\left[x_r^i(E),x_{r'}^{i'}(E')\right]\end{aligned}\quad(4)$$

where

$\mathrm{cov}_{\mathrm{MF32}}[]$ = covariance calculated from File 32 and

$\mathrm{cov}_{\mathrm{MF33}}[]$ = covariance calculated from File 33.

For the covariance of point energy cross sections from File 32, $\mathrm{cov}_{\mathrm{MF32}}[x_r^i(E),x_{r'}^{i'}(E')]$, it should be expressed in terms of the covariance of resonance parameters which are provided by File 32. By the error propagation formula, it can be expressed as

$$\begin{aligned}&\mathrm{cov}_{\mathrm{MF32}}\left[x_r^i(E),x_{r'}^{i'}(E')\right]\\&=\sum_m\sum_{m'}\left(\frac{\partial x_r^i(E)}{\partial\Gamma_m^i}\right)\left(\frac{\partial x_{r'}^{i'}(E')}{\partial\Gamma_{m'}^{i'}}\right)\mathrm{cov}[\Gamma_m^i,\Gamma_{m'}^{i'}]\end{aligned}\quad(5)$$

where

Γ_m^i = m-th resonance parameter of isotope i.

$\mathrm{cov}[\Gamma_m^i,\Gamma_{m'}^{i'}]$=covariance of resonance parameters

The sensitivity of the cross section to the resonance parameter in Eq. (5), $\partial x_r^i(E)/\partial\Gamma_m^i$, can be calculated by a numerical differentiation as applied in ERRORJ

$$\frac{\partial x_r^{\mathrm{res},i}(E)}{\partial\Gamma_m^i}=\frac{x_r^i(\Gamma_m^i+\Delta\Gamma_m^i,E)-x_r^i(\Gamma_m^i-\Delta\Gamma_m^i,E)}{2\Delta\Gamma_m^i}.\quad(6)$$

where

$\Delta\Gamma_m^i=0.01\Gamma_m^i$ is selected in this study.

Before expressing the covariance from File 33, it should be noted that File 33 provides the group-wise relative covariance data although it is supposed to be treated as point energy covariance. The relative covariance given by File 33 is

$$\mathrm{rcov}_{\mathrm{MF33}}\left[x_r^i(E_g),x_{r'}^{i'}(E_{g'})\right]\quad(7)$$

where

$\mathrm{rcov}[X,Y]=\mathrm{cov}[X,Y]/(E[X]E[Y])$

$E[\ ]$ = expectation operator and

$E\in(E_g,E_{g-1}]$, $E'\in(E_{g'},E_{g'-1}]$

Then, the point energy covariance from File 33 can be expressed as,

$$\begin{aligned}&\mathrm{cov}_{\mathrm{MF33}}\left[x_r^i(E),x_{r'}^{i'}(E')\right]\\&=x_r^i(E)\cdot x_{r'}^{i'}(E')\cdot\mathrm{rcov}_{\mathrm{MF33}}\left[x_r^i(E_g),x_{r'}^{i'}(E_{g'})\right]\end{aligned}\quad(8)$$

In order to separate the multi-group covariance by ENDF covariance data, Eq.(4) is inserted into Eq.(3) as follows ,

$$\begin{aligned}&\mathrm{cov}\left[x_{r,G}^i,x_{r',G'}^{i'}\right]\\&=\mathrm{cov}_{\mathrm{MF32}}\left[x_{r,G}^i,x_{r',G'}^{i'}\right]+\mathrm{cov}_{\mathrm{MF33}}\left[x_{r,G}^i,x_{r',G'}^{i'}\right]\end{aligned}\quad(9)$$

$$\begin{aligned}&\mathrm{cov}_{\mathrm{MF32}}\left[x_{r,G}^i,x_{r',G'}^{i'}\right]\\&=\frac{1}{\phi_G\phi_{G'}}\int_{E_G}^{E_{G-1}}\int_{E_{G'}}^{E_{G-1}}\mathrm{cov}_{\mathrm{MF32}}\left[x_r^i(E),x_{r'}^{i'}(E')\right]\\&\qquad\times\phi(E)\phi(E')dEdE'\end{aligned}\quad(10)$$

$$\begin{aligned}&\mathrm{cov}_{\mathrm{MF33}}\left[x_{r,G}^i,x_{r',G'}^{i'}\right]\\&=\frac{1}{\phi_G\phi_{G'}}\int_{E_G}^{E_{G-1}}\int_{E_{G'}}^{E_{G-1}}\mathrm{cov}_{\mathrm{MF33}}\left[x_r^i(E),x_{r'}^{i'}(E')\right]\\&\qquad\times\phi(E)\phi(E')dEdE'\end{aligned}\quad(11)$$

2.1.3 Derivation of multi-group covariance from File 32 without double integration

Insertion of Eq.(5) into Eq.(10) yields,

$$\begin{aligned}&\mathrm{cov}_{\mathrm{MF32}}\left[x_{r,G}^i,x_{r',G'}^{i'}\right]\\&=\frac{1}{\phi_G\phi_{G'}}\int_{E_G}^{E_{G-1}}\int_{E_{G'}}^{E_{G'-1}}\sum_m\sum_{m'}\left(\frac{\partial x_r^i(E)}{\partial\Gamma_m^i}\right)\left(\frac{\partial x_{r'}^{i'}(E')}{\partial\Gamma_{m'}^{i'}}\right)\\&\qquad\times\mathrm{cov}[\Gamma_m^i,\Gamma_{m'}^{i'}]\phi(E)\phi(E')dEdE'\\&=\sum_m\sum_{m'}\mathrm{cov}[\Gamma_m^i,\Gamma_{m'}^{i'}]\left(\frac{1}{\phi_G}\int_{E_G}^{E_{G-1}}\frac{\partial x_r^i(E)}{\partial\Gamma_m^i}\phi(E)dE\right)\\&\qquad\times\left(\frac{1}{\phi_{G'}}\int_{E_{G'}}^{E_{G'-1}}\frac{\partial x_{r'}^{i'}(E')}{\partial\Gamma_{m'}^{i'}}\phi(E')dE'\right)\end{aligned}\quad(12)$$

From the derivation in Eq.(12), the double integration in Eq.(10) is reduced to a single integration,

$$\frac{\partial x_{r,G}^i}{\partial\Gamma_m^i}=\frac{1}{\phi_{G'}}\int_{E_{G'}}^{E_{G'-1}}\frac{\partial x_{r'}^{i'}(E')}{\partial\Gamma_{m'}^{i'}}\phi(E')dE'\quad(13)$$

2.1.4 Derivation of multi-group covariance from File 33 without double integration

Insertion of Eq. (8) into Eq. (11) yields

$$\begin{aligned}&\mathrm{cov}_{\mathrm{MF33}}\left[x_{r,G}^i,x_{r',G'}^{i'}\right]\\&=\frac{1}{\phi_G\phi_{G'}}\int_{E_G}^{E_{G-1}}\int_{E_{G'}}^{E_{G'-1}}x_r^i(E)\cdot x_{r'}^{i'}(E')\\&\quad\times\mathrm{rcov}_{\mathrm{MF33}}\left[x_r^i(E_g),x_{r'}^{i'}(E_{g'})\right]\times\phi(E)\phi(E')dEdE'\\&=\frac{1}{\phi_G\phi_{G'}}\sum_{g\in G}\sum_{g'\in G'}\int_{E_g}^{E_{g-1}}\int_{E_{g'}}^{E_{g'-1}}x_r^i(E)\cdot x_{r'}^{i'}(E')\\&\quad\times\mathrm{rcov}_{\mathrm{MF33}}\left[x_r^i(E_g),x_{r'}^{i'}(E_{g'})\right]\times\phi(E)\phi(E')dEdE'\\&=\sum_{g\in G}\sum_{g'\in G'}\mathrm{rcov}_{\mathrm{MF33}}\left[x_r^i(E_g),x_{r'}^{i'}(E_{g'})\right]\\&\quad\times\left(\frac{1}{\phi_G}\int_{E_g}^{E_{g-1}}x_r^i(E)\phi(E)dE\right)\left(\frac{1}{\phi_{G'}}\int_{E_{g'}}^{E_{g'-1}}x_{r'}^{i'}(E')\phi(E')dE'\right)\end{aligned}\quad(14)$$

where

$$\int_{E_G} dE = \sum_{g \in G} \int_{E_g}^{E_{g-1}} dE .$$

Note that relative covariance of g and g' is constant within energy group interval.

From the derivation in Eq.(14), the double integration in Eq.(11) is reduced to a single integration,

$$\frac{\phi_{g'} x^{i'}_{r',g'}}{\phi_{G'}} = \frac{1}{\phi_G} \int_{E_g}^{E_{g-1}} x^i_r(E)\phi(E)dE \qquad (15)$$

2.2 Algorithm for multi-group covariance tally

In this proposed method, it is required to calculate the terms in Eq. (13) and Eq. (15) on MC simulation. In the conventional MC tally algorithm, integrated values of microscopic reaction rate and neutron flux within given energy range can be numerically evaluated by the track length estimator. Similarly, the terms in Eq.(13) and Eq.(15) can also be calculated as follows

$$\frac{\partial x^i_{r,G}}{\partial \Gamma^i_m} = \frac{1}{\phi_G} \int_{E_G} \frac{\partial x^i_r(E)}{\partial \Gamma^i_m} \phi(E)dE = \left\langle \frac{\sum_{k=1, E_{jk} \in G}^{N_j} w_{jk} l_{jk} \frac{\partial x^i_r(E_{jk})}{\partial \Gamma^i_m}}{\sum_{k=1, E_{jk} \in G}^{N_j} w_{jk} l_{jk}} \right\rangle \qquad (16)$$

$$\frac{\phi_g x^i_{r,g}}{\phi_{G'}} = \frac{1}{\phi_G} \int_{E_g} x^i_r(E)\phi(E)dE = \left\langle \frac{\sum_{k=1, E_{jk} \in g}^{N_j} w_{jk} l_{jk} x^i_r(E_{jk})}{\sum_{k=1, E_{jk} \in G}^{N_j} w_{jk} l_{jk}} \right\rangle \qquad (17)$$

where

k = track index,
j = history index,
w_{jk} = neutron weight of k-th track of j-th history,
l_{jk} = track length of k-th track of j-th history.
E_{jk} = neutron energy of k-th track of j-th history.
operator < > = average over all neutron histories

Then multi-group covariance can be calculated by Eq. (12) and Eq. (14).

3. Numerical Results

The proposed multi-group covariance tally algorithm has been implemented in a Seoul National University MC code, McCARD [10], and tested for several cases. All of the calculations were conducted in the SCALE 44-group structure [11] and ENDF of ^{238}U in JEDNL 3.3 [12] which contains File 32 is used for raw covariance data.

3.1 Uniform and 1/E flux distribution

For the proposed method, it requires several subroutines such as reconstruction of resonance cross section or calculation of sensitivity to resonance parameters. In order to validate the proposed method, multi-group covariance with uniform and 1/E flux distribution are estimated by the proposed method and compared with the results from NJOY.

Table I, II show the numerical results of uncertainty of multi-group cross section with uniform and 1/E flux distribution respectively by the proposed method(MC Cov Tally), and they are compared to the results of ERRORR in NJOY99. From these tables, it is noted that the two modules are identical when self-shielding effect is not considered. Also, It is observed that the shape of asymptotic flux spectrum has little impact on multi-group covariance in this energy group structure although the spectrum is change to uniform to 1/E.

Table I. Uncertainty of Multi-Group Capture Cross Section of U-238 from JENDL-3.3 with Uniform Flux

Energy Group	Upper Energy Bound [eV]	Multi-Group XS [barn]	Uncertainty (RSD) of Multi-Group XS [%]		
			ERRORR	MC Cov Tally	
				Mean	SD
1	0.0030	14.864	1.88	1.88	0.00
2	0.0075	6.0950	1.88	1.88	0.00
21	1.7700	0.48108	2.31	2.31	0.00
22	3.0000	0.48346	2.73	2.73	0.00
23	4.7500	0.81972	3.25	3.25	0.00
24	6.0000	3.0024	4.20	4.22	0.00
25	8.1000	409.19	2.03	2.04	0.01
26	10.000	0.77453	3.43	3.43	0.01

Table II. Uncertainty of Multi-Group Capture Cross Section of U-238 from JENDL-3.3 with 1/E Flux

Energy Group	Upper Energy Bound [eV]	Multi-Group XS [barn]	Uncertainty (RSD) of Multi-Group XS [%]		
			ERRORR	MC Cov Tally	
				Mean	SD
1	0.0030	14.864	1.88	1.88	0.00
2	0.0075	6.0950	1.88	1.88	0.00
21	1.7700	0.48108	2.30	2.30	0.00
22	3.0000	0.48346	2.70	2.70	0.00
23	4.7500	0.81972	3.24	3.24	0.00
24	6.0000	3.0024	4.19	4.21	0.00
25	8.1000	409.19	2.03	2.01	0.01
26	10.000	0.77453	3.46	3.45	0.01

3.2 TMI-1pin cell problem

The proposed method has been tested for a TMI-1 pin cell problem [13], a OECE/NEA benchmark problem for

Uncertainty Analysis in Modeling (UAM). In order to compare the result with that of ERRORR, a mid-life Light Water Reactor (LWR) spectrum defined by Electric Power Research Institute (EPRI) [14], built-in flux spectrum in ERRORR, is applied to the ERRORR calculation as an asymptotic flux spectrum. Note that multi-group covariance generated by ERRORR are infinitely diluted since EPRI flux spectrum is the asymptotic spectrum. MC calculations are performed for 100 active cycles and 1000 histories per cycle.

Table III shows the numerical results of uncertainty of multi-group cross section in TMI-1 pin cell problem compared to those of ERRORR. From this table, it is noted that self-shielding effect make some differences in the multi-group covariance estimation.

Table III. Uncertainty of Multi-Group Capture Cross Section of U-238 from JENDL-3.3 in TMI-1 problem

Energy Group	Upper Energy Bound [eV]	Multi-Group XS [barn]	Uncertainty (RSD) of Multi-Group XS [%]		
			ERRORR	MC Cov Tally	
				Mean	SD
1	0.0030	14.864	1.88	1.88	0.00
2	0.0075	6.0950	1.88	1.88	0.00
21	1.7700	0.48108	2.30	2.31	0.00
22	3.0000	0.48346	2.70	2.70	0.00
23	4.7500	0.81972	3.24	3.32	0.00
24	6.0000	3.0024	4.19	4.14	0.00
25	8.1000	409.19	2.03	4.27	0.00
26	10.000	0.77453	3.46	3.33	0.00
27	30.000	61.994	6.15	4.25	0.01
28	100.00	44.546	1.79	2.56	0.00
29	550.00	10.893	0.76	2.84	0.01
30	3000.0	2.2595	0.40	12.06	0.11

6. Conclusions

In this study, the MC multi-group covariance tally algorithm for multi-group covariance data generation from continuous-energy MC transport calculation has been developed. In order to calculate the multi-group covariance estimation in the MC simulation, some mathematical derivations for reducing double integration into single one are introduced. The developed multi-group covariance tally algorithm has been implemented in McCARD, then some numerical calculations have been conducted for test. It is observed in TMI-1 pin problem that self-shielding effect makes a difference in multi-group covariance generation.

The proposed method has an advantage that the exact self shielding effect can be reflected in the multi-group covariance evaluation when compared to the conventional nuclear data processing code. It is expected that self shielded multi-group covariance data can be provided by this method for more accurate S/U analysis.

References

1. Cacuci DG, *Sensitivity and Uncertainty Analysis, Volume I: Theory*, Chapman & Hall/CRC, (2003).
2. Kodeli I, "SUSD3D: A Multi-Dimensional, Discrete-Ordinates Based Cross Section Sensitivity and Uncertainty Analysis Code System," RSICC Code Package: CCC-695 (2000).
3. Rearden BT, *TSUNAMI-3D: Control Module for Three-Dimensional Cross-Section Sensitivity and Uncertainty Analysis for Criticality*, SCALE 5.1 Manual, Vol. I, Sect. C9, ORNL/TM-2005/39, Oak Ridge National Laboratory (2006).
4. Park HJ, Joo HG, Shim HJ, Kim CH, "Effect of Cross Section Uncertainties on Criticality Benchmark Problem Analysis by McCARD," *Journal of the Korean Physical Society*, **59**, *2*, 1252 (2011).
5. Shim HJ, Kim CH, "Adjoint Sensitivity and Uncertainty Analyses in Monte Carlo Forward Calculations," *J. Nucl. Sci. Technol.*, **48**, *12*, 1453 (2011).
6. Chiba G, "ERRORJ: Covariance Processing Code System, Version 2.2," RSICC Code Package: PSR-526 (2005).
7. Dunn ME, "PUFF-III: A Code for Processing ENDF Uncertainty Data into Multigroup Covariance Matrices," ORNL/TM-1999/235, Oak Ridge National Laboratory (2000).
8. Chiba G, Tsuji M, Narabayashi T, "Resonance Self-Shielding Effect in Uncertainty Quantification of Fission Reactor Neutronics Parameters," *Nucl. Eng. Technol.*, **46**, *3*, 281 (2014).
9. MacFarlane RE, Muir DW, "NJOY99.0 Code System for Producing Pointwise and Multigroup Neutron and Photon Cross Sections from ENDF/B Data," PSR-480/NJOY99.0, Los Alamos National Laboratory (2000).
10. Shim HJ et al., "McCARD: Monte Carlo Code for Advanced Reactor Design and Analysis," *Nucl. Eng. Technol.*, 44, *2*, 161 (2012).
11. "ZZ SCALE6.0/COVA-44G, 44-group cross-section covariance matrix library extracted from SCALE6.0," NEA Data Bank, USCD-1236/02, (2009).
12. Shibata K, et al. "Japanese evaluated nuclear data library version 3 revision-3: JENDL-3.3," *J. Nucl. Sci. Technol.*, **39**, *11*, 1125 (2002).
13. Ivanov K, Avramova M, Kamerow S, Kodeli I, Sartori E, Ivanov E, Cabellos O, "Benchmark for Uncertainty Analysis in Modeling (UAM) for Design, Operation and Safety Analysis of LWRs, Volume I: Specification and Support Data for the Neutronics Cases (Phase I)," NEA/NSC/DOC and OECD Nuclear Energy Agency (2012).
14. MacFarlane RE, "ENDF/B-V Cross-Section Library for Reactor Cell Analysis," Electric Power Research Institute report EPRI NP-3418 (1984).