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

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1. Introduction

The sensitivity and uncertainty (S/U) methodology [1] in deterministic tools [2,3] has been utilized for quantifying uncertainties of nuclear design parameters induced by those of nuclear data. The S/U analyses which are based on multi-group cross sections 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 section. The multi-group covariance data required for S/U analysis have been produced by nuclear data processing codes such as ERRORJ [4] or PUFF [5] from the covariance data in evaluated nuclear data files. However in the existing nuclear data processing codes, an asymptotic neutron flux energy spectrum, not the exact one, has been applied to the multi-group covariance generation since the flux spectrum is unknown before the neutron transport calculation. It can cause an inconsistency between the sensitivity profiles and the covariance data of multi-group cross section especially in resolved resonance energy region, because the sensitivities we usually use are resonance self-shielded while the multi-group cross sections produced from an asymptotic flux spectrum are infinitely-diluted [6].

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 depression by resonance 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 that produced from the existing covariance processing code ERRORR in NJOY99 [7].

2. Multi-group covariance tally method

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

2.1 Mathematical Derivation of Multi-group Covariance Tally Algorithm.

Before estimating the covariance of the multi-group cross sections, let us define the multi-group cross section of reaction type r and energy group G of isotope i, $x^i_{r,G}$, as

$$x^i_{r,G} = \frac{1}{\phi_G}\int_{E_G}^{E_{G-1}} x^i_r(E)\phi(E)dE \quad (1)$$
,

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

where $\phi(E)$ is the flux spectrum, E_G is the lower energy bound of group G.

Then the multi-group covariance for $x^i_{r,G}$ and $x^{i'}_{r',G'}$, $\mathrm{cov}\left[x^i_{r,G}, x^{i'}_{r',G'}\right]$, is estimated by the following equation as applied in ERRORR,

$$\mathrm{cov}\left[x^i_{r,G}, x^{i'}_{r',G'}\right] = \frac{1}{\phi_G\phi_{G'}}\int_{E_{G-1}}^{E_G}\int_{E_{G'-1}}^{E_{G'}} \mathrm{cov}\left[x^i_r(E), x^{i'}_{r'}(E')\right]\phi(E)\phi(E')dEdE'. \quad (3)$$

In this study, the double integration in Eq. (3) is converted into a single one by utilizing sampling method to estimate the multi-group covariance in the ongoing MC simulation. If $\phi(E')$ is regarded as a probability density function for sampling an energy, the double integration in Eq. (3) can be expressed as,

$$\mathrm{cov}\left[x^i_{r,G}, x^{i'}_{r',G'}\right] = E\left[\frac{1}{\phi_G}\int_{E_{G-1}}^{E_G} \mathrm{cov}\left[x^i_r(E), x^{i'}_{r'}(\tilde{E})\right]\phi(E)dE\right], \quad (4)$$

where $E[]$ is the expectation operator and $\tilde{E}$ is the sampled energy from the probability distribution. The flux spectrum $\phi(E')$ for sampling an energy, $\tilde{E}$, is prepared from the previous fission source simulation.

2.2 Procedure of Multi-group Covariance Tally

First, from the MC history simulation for the $(j$-$1)$ th fission source, an energy may be selected by $E_{(j-1)\tilde{k}}$ corresponding to track $\tilde{k}$ satisfying,

$$\sum_{k=1}^{\tilde{k}-1} w_{(j-1)k} l_{(j-1)k} \Big/ \sum_{k=1}^{N_{j-1}} w_{(j-1)k} l_{(j-1)k} \le \xi < \sum_{k=1}^{\tilde{k}} w_{(j-1)k} l_{(j-1)k} \Big/ \sum_{k=1}^{N_{j-1}} w_{(j-1)k} l_{(j-1)k}, \quad (5)$$

where $w_{(j-1)k}$ and $l_{(j-1)k}$ denote the neutron weight and the track length, respectively, of track k of (j-1) th fission source. ξ is a random number having the uniform distribution in the range of [0,1).

Then the multi-group covariance for energy group G and G', $\mathrm{cov}\left[x^{i}_{r,G}, x^{i'}_{r',G'}\right]$, can be calculated in the *j*-th fission source simulation as

$$< \mathrm{cov}[x^{i}_{r,G}, x^{i'}_{r',G'}] >= \left\langle \frac{\sum_{k=1,E_{jk}\in G}^{N_j} w_{jk} l_{jk} \,\mathrm{cov}\left[x^{i}_{r}(E_{jk}), x^{i'}_{r'}(E_{(j-1)\tilde{k}})\right]}{\sum_{k=1,E_{jk}\in G}^{N_j} w_{jk} l_{jk}} \right\rangle, \quad (6)$$

where the operator < > means the average over all the neutron histories in the MC simulations. The neutron weight , track length, $w_{jk} l_{jk}$, and corresponding energy, E_{jk}, are stored for the next fission source, (*j*+1) th source, simulation.

3. Numerical Result

The proposed multi-group covariance tally algorithm has been implemented in a Seoul National University MC code, McCARD, and tested for multi-group covariance generation in TMI-1 PWR pin-cell problem, one of the OECD benchmarks for Uncertainty Analysis Modeling (UAM) [8]. Table I shows that the numerical results of ERRORR are compared to that of multi-group covariance tally by McCARD. A mid-life PWR flux spectrum defined by Electric Power Research Institute (EPRI) [9], built-in weight function in ERRORR, is applied to the ERRORR calculation. Old version of JENDL4.0 library of uranium-235 is used for covariance data since the covariance data of resonance parameter have been removed in the new version. The calculations were conducted in the Los Alamos National Lab (LANL) 30-group structure. MC calculations are performed for 15 active cycles and 1000 histories per cycle.

Table I: Uncertainty of Multi-group Capture Cross Section

Energy Group	Upper Energy Bound [eV]	Multi-group XS [barn]	Uncertainty (RSD) of Multi-group XS	
			ERRORR	McCARD Cov Tally
1	0.1520	62.188	2.06%	2.01% ±0.05%
2	0.4140	37.024	2.66%	2.55% ±0.23%
3	1.1300	10.076	2.04%	2.22% ±0.09%
4	3.0600	8.589	1.75%	2.22% ±0.24%
5	8.3200	24.048	0.60%	0.87% ±0.08%
6	22.600	42.628	0.79%	0.74% ±0.10%
7	61.400	25.991	0.88%	0.76% ±0.14%

4. Conclusions

In this study, the multi-group covariance tally algorithm for generation of multi-group covariance data from continuous-energy neutron flux spectrum in MC transport calculations have been developed. In order to calculate the multi-group covariance estimation in the ongoing MC simulation, mathematical derivations for converting the double integration equation into a single one by utilizing sampling method have been introduced along with the procedure of multi-group covariance tally. The developed multi-group covariance tally algorithm has been implemented in McCARD, then some numerical calculations have been conducted for test.

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