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A new propagation analysis of statistical uncertainty in multi-group cross sections generated by Monte Carlo method

Jae Yong Lee, Jong Kyung Kim *

Department of Nuclear Engineering, Hanyang University, 222 Wangsimni-ro, Seongdong-gu, Seoul 04763, Republic of Korea

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ABSTRACT

There are many studies on the Monte Carlo method to generate multi-group cross sections. However, there are not enough studies about the propagation of statistical uncertainty in multi-group cross sections. The purpose of this study is to generate Monte Carlo-based multi-group cross sections for the deterministic code and to evaluate the uncertainty of reactor physics parameters propagated from the statistical uncertainty in multi-group cross sections. To achieve this goal, new formulations for uncertainty propagations were developed. By applying the developed formulations, the propagated uncertainty of eigenvalue was quantified. The accuracy of the calculated uncertainty was validated by using the direct sampling method. Through this study, it is possible to accurately evaluate the uncertainty propagated from the statistical uncertainty in multi-group cross sections. This study can support the reliability of multi-group cross sections created by Monte Carlo method. In addition, the individual contribution of the statistical uncertainty of multi-group cross sections to the uncertainty of the eigenvalue can be calculated. It can provide the helpful information to produce accurate multi-group cross sections by Monte Carlo method.

1. Introduction

The multi-group cross section (MGXS) is required in the deterministic method to solve the transport equation. As the neutron spectrum is unknown before solving the transport equation, the approximated spectrum is used when MGXS are generated by the deterministic codes. In the deterministic method, the space of a system, energy of the neutron, and direction of the neutron are grouped approximately. These approximations and the assumed spectrum cause uncertainties in MGXSs. The MGXS is well known as the main cause of the uncertainty of the calculated reactor physics results (Alpan and Haghighat, 2005). To obtain the accurate MGXS, properly approximated parameters are required. However, when generating the MGXS of new types of reactors, it is difficult to set appropriate approximations and spectrums. To overcome these shortcomings of the deterministic method, Redmond (1997) proposed the use of the Monte Carlo (MC) method to generate MGXSs. In the MC method, there are almost no approximations of the space, energy, and direction. In addition, as continuous-energy cross sections and exact descriptions of the geometry of a system are used, it is possible to simulate the exact behavior of neutrons in the given reactor system. There are many studies related to generating MGXSs by the MC method (Pounders, 2006; Pirouzmand and Mohammadhasani, 2015; Park et al., 2015). The main idea of these studies is to use the MC method to create MGXSs and to adopt the created MGXSs in the deterministic method for the calculation of the reactor physics parameters.

The results of the MC calculation are obtained by sampling the behavior of neutrons. The statistical uncertainties occur in this process. The statistical uncertainties of MGXSs are propagated when MGXSs are employed in the deterministic calculation. The uncertainty propagation analysis should be completed for the reliability of the results. However, few studies about propagation of the statistical uncertainty of MGXSs have been carried out. Park et al. (2013) performed a study to quantify the uncertainty of few-group constants generated by the MC method. However, some assumptions were made in the study: pre-processed covariance data files were used for the propagation calculation. These covariance data files include the covariance error of evaluated nuclear data files (ENDF). To calculate the propagation of the statistical uncertainty caused by the MC calculation, using the covariance that is created in the MC calculation is more appropriate instead of using the covariance of the evaluated data.

The aim of this study is to calculate the propagation of statistical uncertainties in the MGXS generated by the MC method. For the propagation analysis of the statistical uncertainty in MGXSs, the

* Corresponding author.
E-mail address: jkkim1@hanyang.ac.kr (J.K. Kim).

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linear uncertainty propagation formula (Bevington and Robinson, 2003) was used. New formulations were derived to quantify the covariance of generated MGXSs. By applying the developed formulations, the uncertainty of the eigenvalue propagated from the statistical error of MGXS was evaluated in two simple problems. The quantified uncertainties were validated by the direct sampling method (Bostelmann et al., 2015).

2. Background for the MC-based MGXS generation

The definition of the MGXS (Redmond, 1997) is as follows:

$$\sum_{\alpha,g} = \frac{\int_{E_g}^{E_{g-1}} \sum_{j=1}^{J} n_j \sigma_{\alpha,j}(E) \rho\, \Phi(E) dE}{\int_{E_g}^{E_{g-1}} \Phi(E) dE}, \tag{1}$$

where $\sum_{\alpha,g}$ denotes the α-type g group cross section, $\sigma_{\alpha,j}(E)$ denotes the α-type microscopic cross section of the j-th isotope of a material as a function of energy E, n_j denotes the associated atom fraction of the j-th isotope of a material, ρ denotes the atomic density of the material, and $\Phi(E)$ denotes the neutron flux as a function of energy E. The numerator of Eq. (1) is the group reaction rate and the denominator is the group flux. To calculate the group reaction rate and group flux in the MC calculation, the track-length tally estimator can be used (Redmond, 1997). The group reaction rate is calculated by the track length estimator as

$$\sum_{\alpha,g} \phi_g = \frac{\int_{E_g}^{E_{g-1}} dE \int_V dV \sum_{i=1}^{N} w_i l_i \Sigma_\alpha(E)}{V \sum_{i=1}^{N} w_i^0}, \tag{2}$$

where w_i is the weight of the i-th particle and l_i is the track length of the i-th particle in volume V, $\Sigma_\alpha(E)$ is a macroscopic cross section as a function of energy, w_i^0 is the original weight of the i-th particle, and N is the number of sampled particles. The track length estimator to calculate the group flux is written as

$$\phi_g = \frac{\int_{E_g}^{E_{g-1}} dE \int_V dV \sum_{i=1}^{N} w_i l_i}{V \sum_{i=1}^{N} w_i^0}. \tag{3}$$

In the MC calculation, results are obtained after the transportation of sampled particles. In this process, every single transportation has each calculated value. The final results are obtained by averaging the values of each transportation. The variance of the mean is used to describe the statistical uncertainty of the MC calculation. The variance of the MGXS generated by the MC method was derived by Redmond. The derivation will be simply introduced. Equation (1) can be rewritten as

$$\bar{x} = \frac{\bar{u}}{\bar{v}}, \tag{4}$$

where $\bar{x}$ is the mean MGXS, $\bar{u}$ is the mean group reaction rate, and $\bar{v}$ is the mean group neutron flux. As the MGXS is a function of two variables, using the uncertainty propagation formula (Bevington and Robinson, 2003), the variance of the MGXS is expressed as

$$S_x^2 = S_u^2 \left(\frac{\partial \overline{x}}{\partial \overline{u}}\right)^2 + S_v^2 \left(\frac{\partial \overline{x}}{\partial \overline{v}}\right)^2 + 2Cov(u, v) \left(\frac{\partial \overline{x}}{\partial \overline{u}}\right) \left(\frac{\partial \overline{x}}{\partial \overline{v}}\right), \tag{5}$$

where S_x^2 is the variance of x and $Cov(u, v)$ is the covariance between u and v. The covariance is defined as

$$Cov(u, v) \equiv \frac{1}{N-1} \sum_{i=1}^{N} (u_i - \overline{u})(v_i - \overline{v}), \tag{6}$$

where u_i is the macroscopic cross section times the track length on i-th particle and v_i is the calculated track length on i-th particle. According to Redmond, the variance of MGXS is calculated as

$$\begin{aligned} S_x^2 &= \frac{1}{N-1} \left[\begin{array}{c} \left(\sum_{i=1}^{N} (u_i - \overline{u})^2\right) \left(\frac{1}{\overline{v}}\right)^2 + \left(\sum_{i=1}^{N} (v_i - \overline{v})^2\right) \left(-\frac{\overline{u}}{\overline{v}^2}\right)^2 \\ +2\left(\sum_{i=1}^{N} [(u_i - u)(v_i - v)]\right) \left(\frac{1}{\overline{v}}\right) \left(-\frac{\overline{u}}{\overline{v}^2}\right) \end{array} \right], \\ &= \frac{N}{N-1} \left[(\overline{u^2} - \bar{u}^2) \left(\frac{1}{\bar{v}^2}\right) + (\overline{v^2} - \bar{v}^2) \left(\frac{\bar{u}^2}{\bar{v}^4}\right) - 2(\overline{u v} - \bar{u} \times \bar{v}) \left(\frac{\bar{u}}{\bar{v}^3}\right) \right]. \end{aligned} \tag{7}$$

The variance of the sample mean of the MGXS is expressed as

$$\begin{aligned} S_{\bar{x}}^2 &= \frac{1}{N} S_x, \\ &= \frac{1}{N-1} \left[(\overline{u^2} - \bar{u}^2) \left(\frac{1}{\bar{v}^2}\right) + (\overline{v^2} - \bar{v}^2) \left(\frac{\bar{u}^2}{\bar{v}^4}\right) - 2(\overline{u v} - \bar{u} \times \bar{v}) \left(\frac{\bar{u}}{\bar{v}^3}\right) \right]. \end{aligned} \tag{8}$$

3. Proposed uncertainty propagation method of statistical uncertainties

Let the reactor physics parameter X be calculated with the MGXS created by the MC method. The parameter X is a function of the MGXSs. If there are l numbers of MGXSs, X can be expressed as

$$X = X(\overline{C_1}, \overline{C_2}, \cdots, \overline{C_l}), \tag{9}$$

where $\overline{C_l}$ denotes the l-th MGXS generated by the MC method. To calculate the uncertainty of X propagated from statistical uncertainties in MGXSs, the linear uncertainty propagation formula (Bevington and Robinson, 2003) can be used:

$$S_X^2 = \mathbf{G}^{\mathbf{T}} \mathbf{V} \mathbf{G}, \tag{10}$$

where $\mathbf{V}$ is the covariance matrix and the i-th element of the vector $\mathbf{G}$ is $\partial X / \partial \overline{C_i}$. To calculate the covariance of MGXSs, the sum of two MGXSs $\overline{C_t}$ can be defined as

$$\overline{C_t} \equiv \overline{C_k} + \overline{C_l}. \tag{11}$$

Applying the uncertainty propagation formula, the variance of C_t is given as

$$S_{C_t}^2 = S_{C_k}^2 + S_{C_l}^2 + 2Cov(C_k, C_l). \tag{12}$$

As $\overline{C_t}$ is a function of the k-th group reaction rate, k-th group flux, l-th group reaction rate, and l-th group flux, Eq. (11) can be rewritten as

$$\overline{C_t} = \frac{\overline{u_k}}{\overline{v_k}} + \frac{\overline{u_l}}{\overline{v_l}}, \tag{13}$$

where $\overline{u_k}$ denotes the reaction rate of the k-th group calculated by the MC method and $\overline{v_k}$ denotes the group flux of the k-th group calculated by the MC method. By the uncertainty propagation formula, the variance of C_t can be calculated as

$$\begin{aligned} S_{C_t}^2 = {} & S_{u_k}^2 \left(\frac{\partial \overline{C_t}}{\partial \overline{u_k}}\right)^2 + S_{v_k}^2 \left(\frac{\partial \overline{C_t}}{\partial \overline{v_k}}\right)^2 + S_{u_l}^2 \left(\frac{\partial \overline{C_t}}{\partial \overline{u_l}}\right)^2 + S_{v_l}^2 \left(\frac{\partial \overline{C_t}}{\partial \overline{v_l}}\right)^2 \\ & + 2Cov(u_k, v_k) \left(\frac{\partial \overline{C_t}}{\partial \overline{u_k}}\right) \left(\frac{\partial \overline{C_t}}{\partial \overline{v_k}}\right) + 2Cov(u_k, u_l) \left(\frac{\partial \overline{C_t}}{\partial \overline{u_k}}\right) \left(\frac{\partial \overline{C_t}}{\partial \overline{u_l}}\right) \\ & + 2Cov(u_k, v_l) \left(\frac{\partial \overline{C_t}}{\partial \overline{u_k}}\right) \left(\frac{\partial \overline{C_t}}{\partial \overline{v_l}}\right) + 2Cov(u_l, v_k) \left(\frac{\partial \overline{C_t}}{\partial \overline{v_k}}\right) \left(\frac{\partial \overline{C_t}}{\partial \overline{u_l}}\right) \\ & + 2Cov(v_k, v_l) \left(\frac{\partial \overline{C_t}}{\partial \overline{v_k}}\right) \left(\frac{\partial \overline{C_t}}{\partial \overline{v_l}}\right) + 2Cov(u_l, v_l) \left(\frac{\partial \overline{C_t}}{\partial \overline{u_l}}\right) \left(\frac{\partial \overline{C_t}}{\partial \overline{v_l}}\right). \end{aligned} \tag{14}$$