

Monte Carlo Sensitivity and Uncertainty Analysis with Continuous-Energy Covariance Data

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Abstract – The conventional continuous-energy Monte Carlo (MC) sensitivity and uncertainty (S/U) analysis using multi-group covariance matrices has a theoretical pitfall that it is inconsistent with the principle of continuous-energy MC neutronics calculations in that it regards covariance data as multi-group variables rather than continuous-energy ones. As a way to get around this deficiency and perform the MC S/U analysis with theoretical consistency, a new continuous-energy MC S/U analysis formulation which directly utilizes the continuous-energy covariance data in the evaluated nuclear data libraries was proposed by previous studies. As an extension of the preceding researches, this paper deals with the Doppler broadening effect on the new MC S/U analysis along with the recently modified formulation. The validity of the new MC S/U formulation is examined in terms of the input-nuclear-data-induced k uncertainty of the TMI-1 pin cell problem by a Seoul National University MC code, McCARD.

I. INTRODUCTION

The nuclear design parameters are bound to have uncertainties because of uncertainties of input data used to compute them, regardless of deterministic or Monte Carlo (MC) design calculations. For the economic and safety evaluation of nuclear design, it is indispensable to make quantitative estimation of their uncertainties. This paper is intended to introduce a recent advancement on the formulation for the continuous-energy MC sensitivity and uncertainty (S/U) analysis method designed to quantify nuclear design parameter uncertainties caused by input data uncertainties-particularly nuclear cross section input data uncertainties.

The MC estimates on nuclear design parameters generally carry two types of uncertainties; one statistical and the other input-data-uncertainty-induced uncertainties. Earlier we presented a continuous-energy MC S/U formulation which is capable of computing the two types of uncertainties separately, and demonstrated its applications for computing uncertainties induced by those of nuclear cross section input data independently from the statistical uncertainty in terms of criticality benchmark problem calculations [1]. Recently, however, we recognized a theoretical pitfall of the early formulation that it is not consistent with the spirit of the continuous-energy MC analysis because it treats the nuclear cross sections as discrete parameters instead of continuous parameters. We presented a new continuous-energy MC SU formulation that treats uncertain nuclear cross section inputs as continuous parameters in consistent with the continuous MC design analysis.[2] Also, we showed performance of the new formulation in comparison with the early one in the continuous-energy MC S/U analysis for a thermal and a fast spectrum criticality benchmark problem calculations.

In our continuous efforts to examine how the new formulation plays out in the continuous-energy MC S/U analysis, this paper presents how the new MC S/U

formulation can deal with the Doppler broadening effect on quantification of nuclear design parameter uncertainties arising from uncertain resonance parameters, which have been left out in our previous study [2]. As a numerical example of illustrating the Doppler broadening effect in the uncertainty quantification, k -uncertainty of the TMI pin cell criticality problem [3] is analyzed by the new MC S/U analysis, and its results are compared with those by the early MC S/U analysis [1] based on multi-group covariances.

The new continuous-energy MC S/U formulation is not well publicized, simply because it is formulated very recently. Despite the risk of repletion, therefore, we outline the formulation in the following section.

II. DERIVATION OF CONTINUOUS-ENERGY SANDWICH EQUATION

A nuclear design parameter or tally denoted by Q here can be expressed as an integral of its tally response over all the neutron collision sites [4]:

$$Q = \int_V \int_0^\infty \int_{4\pi} g(\mathbf{r}, E, \boldsymbol{\Omega}) \Psi(\mathbf{r}, E, \boldsymbol{\Omega}) d\mathbf{r} dE d\boldsymbol{\Omega}, \quad (1)$$

where \mathbf{r} , E , and $\boldsymbol{\Omega}$ are the location, energy, and direction of neutron, respectively, and V is the spatial volume of the tally Q . g is the tally response function to Q . Ψ is the neutron collision density that may be obtained from the neutron transport equation.

Suppose that one is conducting a continuous-energy MC neutron transport calculation to compute the nuclear design parameter Q . Assume that the continuous-energy nuclear data inputted for the MC calculation have uncertainties. Then, there can be an infinite number of different input nuclear data sets, which is denoted by

$$\mathbf{x}^\kappa(E) = \{x_r^{i,\kappa}(E) \mid i \in I, r \in R\}; E \in (0, \infty) (\kappa = 1, 2, \dots) \quad (2)$$

where $x_r^{i,\kappa}(E)$ is the r -type nuclear datum of nuclide i for neutron of energy E of set κ , and I and R are the total number of nuclides and reaction types involved, respectively.

Viewing Q from κ -th data set or Q_κ as a functional of input data set, $\mathbf{x}^\kappa(E)$, one may express it as,

$$Q_\kappa \equiv Q(\mathbf{x}^\kappa(E)), \quad (3)$$

It is shown in Ref. 1 that the uncertainty of Q due to those of input data, $\sigma_i^2[Q]$, can be calculated separately from statistical one by

$$\sigma_i^2[Q] = \lim_{K \rightarrow \infty} \frac{1}{K-1} \sum_{\kappa=1}^K (\langle Q_\kappa \rangle - \bar{Q})^2; \quad (4)$$

$$\bar{Q} = \lim_{K \rightarrow \infty} \frac{1}{K} \sum_{\kappa=1}^K Q_\kappa, \quad (5)$$

where the angular bracket above, $\langle \rangle$, is used to denote the expected value of the quantity in it.

To describe Eq. (4) in terms of uncertainties of cross section input data, let us take the first-order Taylor expansion approximation of $\langle Q_\kappa \rangle$ in the fluctuation of $x_r^{i,\kappa}(E)$ about its average values, namely $\overline{x_r^{i,\kappa}(E)} = \overline{x_r^i(E)}$, as follows,

$$\langle Q_\kappa \rangle - \bar{Q} \cong \sum_i \sum_r \int \frac{\partial \langle Q \rangle}{\partial x_r^i(E)} \bigg|_0 (x_r^{i,\kappa}(E) - \overline{x_r^i(E)}) dE, \quad (6)$$

$$\overline{x_r^i(E)} = \lim_{K \rightarrow \infty} \frac{1}{K} \sum_{\kappa=1}^K x_r^{i,\kappa}(E), \quad (7)$$

where \bar{Q} is assumed to be

$$\bar{Q} \cong \langle Q(\bar{\mathbf{x}}(E)) \rangle. \quad (8)$$

The notation “ $\big|_0$ ” in Eq. (6) implies calculating the sensitivity $\partial \langle Q \rangle / \partial x_r^i(E)$ by putting $x_r^{i,\kappa}(E) = \overline{x_r^i(E)}$. The integration over energy E in the right hand side of Eq. (6) is a result of the Taylor expansion of the functional Q_κ in energy-dependent cross sections, $x_r^{i,\kappa}(E)$ [5].

Substituting Eq. (6) into Eq. (4) results in continuous-energy (CE) sandwich equation,

$$\sigma_i^2[Q] = \sum_{i,r} \sum_{i',r'} \sigma^2[Q; x_r^i, x_{r'}^{i'}], \quad (9)$$

$$\sigma^2[Q; x_r^i, x_{r'}^{i'}] = \iint \text{cov}[x_r^i(E), x_{r'}^{i'}(E')] \times \frac{\partial \langle Q \rangle}{\partial x_r^i(E)} \bigg|_0 \cdot \frac{\partial \langle Q \rangle}{\partial x_{r'}^{i'}(E')} \bigg|_0 dE dE', \quad (10)$$

$$\text{cov}[x_r^i(E), x_{r'}^{i'}(E')] = \lim_{K \rightarrow \infty} \frac{1}{K-1} \sum_{\kappa=1}^K (x_r^{i,\kappa}(E) - \overline{x_r^i(E)}) (x_{r'}^{i',\kappa}(E') - \overline{x_{r'}^{i'}(E')}). \quad (11)$$

III. MC S/U ANALYSIS FOR CONTINUOUS-ENERGY SANDWICH EQUATION

Eq (9), Eq. (10) and Eq. (11) can serve as a theoretical basis to quantify $\sigma_i^2[Q]$. The double integrals of multiplication of the sensitivities at two different energy points, however, are difficult to directly utilize in the course of the MC particle tracking. Thus the double integrals are needed to be degraded into single ones for practical purpose, and it can be achieved by extracting energy-independent parameters from ENDF covariance data.

The ENDF represents covariance data in two formats [6], File32 and File33. The File32 covers the short-range covariance components of partial resonance cross sections by containing covariance of resonance parameters, while File 33 does the long-range ones by storing energy-group-wise matrix form. By the definition of covariance in ENDF, $\text{cov}[x_r^i(E), x_{r'}^{i'}(E')]$, in CE sandwich Eq. (10), can be denoted by

$$\text{cov}[x_r^i(E), x_{r'}^{i'}(E')] = \text{cov}_{\text{MF32}}[x_r^i(E | \Gamma^i), x_{r'}^{i'}(E' | \Gamma^{i'})] + \text{cov}_{\text{MF33}}[x_r^i(E), x_{r'}^{i'}(E')], \quad (12)$$

where Γ^i is a vector whose elements are the uncertain resonance parameters that affect the uncertainty of the partial resonance cross sections of nuclide i .

Use of Eq. (12) for Eq. (9) divides $\sigma_i^2[Q]$ into two uncertainty components as,

$$\sigma^2[Q; x_r^i, x_{r'}^{i'}] = \sigma_{\text{MF32}}^2[Q; x_r^i, x_{r'}^{i'}] + \sigma_{\text{MF33}}^2[Q; x_r^i, x_{r'}^{i'}]; \quad (13)$$

$$\sigma_{\text{MF32}}^2[Q; x_r^i, x_{r'}^{i'}] = \iint \text{cov}_{\text{MF32}}[x_r^i(E | \Gamma^i), x_{r'}^{i'}(E' | \Gamma^{i'})] \times \frac{\partial \langle Q \rangle}{\partial x_r^i(E)} \bigg|_0 \cdot \frac{\partial \langle Q \rangle}{\partial x_{r'}^{i'}(E')} \bigg|_0 dE dE', \quad (14)$$

$$\sigma_{\text{MF33}}^2 [Q; x_r^i, x_{r'}^{i'}] = \iint \text{cov}_{\text{MF33}} [x_r^i(E), x_{r'}^{i'}(E')] \times \left. \frac{\partial \langle Q \rangle}{\partial x_r^i(E)} \right|_0 \cdot \left. \frac{\partial \langle Q \rangle}{\partial x_{r'}^{i'}(E')} \right|_0 dE dE' \quad (15)$$

By the uncertainty propagation rule [7], the uncertainty component from File32, $\text{cov}_{\text{MF32}} [x_r^i(E | \Gamma^i), x_{r'}^{i'}(E' | \Gamma^{i'})]$, can be expanded as,

$$\text{cov}_{\text{MF32}} [x_r^i(E | \Gamma^i), x_{r'}^{i'}(E' | \Gamma^{i'})] = \sum_m \sum_{m'} \frac{\partial x_r^i(E | \Gamma^i)}{\partial \Gamma_m^i} \cdot \frac{\partial x_{r'}^{i'}(E' | \Gamma^{i'})}{\partial \Gamma_{m'}^{i'}} \cdot \text{cov}[\Gamma_m^i, \Gamma_{m'}^{i'}] \quad (16)$$

where Γ_m^i is the m -th element of vector Γ^i .

By substituting Eq. (16) for Eq. (14), Eq. (14) can then be rewritten as,

$$\sigma_{\text{MF32}}^2 [Q; x_r^i, x_{r'}^{i'}] = \sum_m \sum_{m'} \text{cov}[\Gamma_m^i, \Gamma_{m'}^{i'}] \cdot S^Q [x_r^i, \Gamma_m^i] \cdot S^Q [x_{r'}^{i'}, \Gamma_{m'}^{i'}]; \quad (17)$$

$$S^Q [x_r^i, \Gamma_m^i] = \int \frac{\partial x_r^i(E | \Gamma^i)}{\partial \Gamma_m^i} \cdot \left. \frac{\partial \langle Q \rangle}{\partial x_r^i(E)} \right|_0 dE \quad (18)$$

The cross section sensitivity to a resonance parameter, $\partial x_r^i(E | \Gamma^i) / \partial \Gamma_m^i$ in Eq. (18), can be computed by a second order finite difference scheme as applied in ERRORJ [8];

$$\frac{\partial x_r^i(E | \Gamma^i)}{\partial \Gamma_m^i} = \frac{x_r^i(E | \dots, \Gamma_m^i + \Delta \Gamma_m^i, \dots) - x_r^i(E | \dots, \Gamma_m^i - \Delta \Gamma_m^i, \dots)}{2 \Delta \Gamma_m^i} \quad (19)$$

$\Delta \Gamma_m^i$ is set to $0.01 \cdot \Gamma_m^i$ for this paper.

For uncertainty components from File33, it also has finite parameters for discrete energy. Instead of providing the point-energy covariance directly, File 33 does in the following matrix form [6];

$$\text{rcov}_{\text{MF33}} [x_r^i(E), x_{r'}^{i'}(E')] = \left(\text{rcov}_{\text{MF33}} [x_r^i, x_{r'}^{i'}] \right)_{gg'} \quad (20)$$

$$(E_g \leq E < E_{g-1}, E_{g'} \leq E' < E_{g'-1}),$$

where $\text{rcov}[X, Y]$ indicates the relative covariance between X and Y , $\text{rcov}[X, Y] = \text{cov}[X, Y] / (E[X] \cdot E[Y])$. Note that $\left(\text{rcov}_{\text{MF33}} [x_r^i, x_{r'}^{i'}] \right)_{gg'}$ is constant within each energy group.

By introducing Eq. (20) into Eq. (15), double-integral equation for File 33 can also be rewritten as follows,

$$\sigma_{\text{MF33}}^2 [Q; x_r^i, x_{r'}^{i'}] = \sum_g \sum_{g'} \left(\text{rcov}_{\text{MF33}} [x_r^i, x_{r'}^{i'}] \right)_{gg'} \cdot S_g^Q [x_r^i] \cdot S_{g'}^Q [x_{r'}^{i'}] \quad (21)$$

$$S_g^Q [x_r^i] = \int_{E_g}^{E_{g-1}} x_r^i(E) \frac{\partial \langle Q \rangle}{\partial x_r^i(E)} dE \quad (22)$$

Before applying this result for computation, it is important to note that File 33 provides the covariance data in two types of format, NI-type and NC-type [6], depending on the reaction type. In case of the NI-type covariance data, values of are explicitly given and therefore Eq. (21) can be straightforwardly applicable. On the other hand, in case of the NC-type covariance data, the corresponding cross section is provided by a linear combination of those cross sections whose covariance data are given in the NI-type as follows;

$$x_r^i(E) = \sum_{\hat{r}} C_{r, \hat{r}}^i x_{\hat{r}}^i(E), \quad (23)$$

where $C_{r, \hat{r}}^i$ is a correlation constant of the two reaction types r and \hat{r} of nuclide i .

Then the relative covariance of the NC-type reaction cross sections in this case becomes

$$\text{rcov}_{\text{MF33}}^{\text{NC}} [x_r^i(E), x_{r'}^{i'}(E')] = \sum_{\hat{r}} \sum_{\hat{r}'} C_{r, \hat{r}}^i C_{r', \hat{r}'}^{i'} \frac{x_{\hat{r}}^i(E) x_{\hat{r}'}^{i'}(E')}{x_r^i(E) x_{r'}^{i'}(E')} \text{rcov}_{\text{MF33}} [x_{\hat{r}}^i(E), x_{\hat{r}'}^{i'}(E')] \quad (24)$$

By using Eq. (24), $\sigma_{\text{MF33}}^2 [Q; x_r^i, x_{r'}^{i'}]$ of Eq. (21) for the NC-type reaction, $\sigma_{\text{MF33-NC}}^2 [Q; x_r^i, x_{r'}^{i'}]$ can be written as

$$\sigma_{\text{MF33-NC}}^2 [Q; x_r^i, x_{r'}^{i'}] = \sum_{\hat{r}, g} \sum_{\hat{r}', g'} C_{r, \hat{r}}^i C_{r', \hat{r}'}^{i'} \left(\text{rcov}_{\text{MF33}} [x_{\hat{r}}^i, x_{\hat{r}'}^{i'}] \right)_{gg'} \times S_g^Q [x_{\hat{r}}^i, x_{\hat{r}'}^{i'}] \cdot S_{g'}^Q [x_{\hat{r}'}^{i'}, x_{\hat{r}}^i]; \quad (25)$$

Equations (14), (18), (21), and (25) imply that $\sigma_i^2[Q]$ can be determined directly using the covariance data given in File 32 and 33 of ENDF. What is needed to do so is calculate sensitivities to the resonance parameters, $S^Q [x_r^i, \Gamma_m^i]$ of Eq. (18) and those to cross sections, $S_g^Q [x_r^i]$ of Eq. (22). They can readily be obtained by taking advantage of the conventional MC AWP [9], which has been used to estimate $\int_{E_g}^{E_{g-1}} \partial \langle Q \rangle / \partial x_r^i(E) dE$. All one has to do to get the required sensitivities is to modify MC AWP

calculation by introducing weighting factors, $\partial x_r^i(E|\Gamma^i)/\partial \Gamma_m^i$ or $x_r^i(E)$.

IV. DOPPLER BROADENING EFFECT ON S/U ANALYSIS

In the conventional nuclear data processing codes, the calculation of sensitivities to resonance parameter, $\partial x_r^i(E|\Gamma^i)/\partial \Gamma_m^i$, is conducted for 0 K cross sections. Because of this, Doppler broadening effect is not properly handled [10]. In the previous study by our new continuous energy MC S/U analysis [2], this scheme was also used since it is consistent with the nuclear data processing codes.

As a way to properly deal with Doppler broadening effect in this study by the new MC S/U analysis, we modified Eq. (19) as follows.

$$\frac{\partial x_r^{i,T}(E|\Gamma^i)}{\partial \Gamma_m^i} = \frac{x_r^{i,T}(E|\dots, \Gamma_m^i + \Delta \Gamma_m^i, \dots) - x_r^{i,T}(E|\dots, \Gamma_m^i, \dots)}{\Delta \Gamma_m^i}, \quad (26)$$

where T denotes the temperature.

Instead of an on-the-fly calculation strategy of our previous study [2], this study utilizes pre-generated Doppler broadened cross sections for every perturbed resonance parameters for Eq. (19), because calculation of sensitivity to resonance parameter with Doppler broadening is too time-consuming for applying it for the on-the-fly simulation currently. In addition, the first-order finite difference approximation is chosen to reduce the required number of pre-generated cross section sets. Note that this is just a preliminary strategy at this point and more improved one will be introduced in the future.

V. NUMERICAL RESULTS

The proposed method, with and without Doppler broadening, have been implemented in McCARD [11], a Seoul National University MC code. Then it is applied to estimate the k -uncertainty induced by the uncertainty of ^{238}U capture cross section in JENDL-3.3 File 32 for the TMI-1 pin-cell problem [3]. The cross section sensitivities to the resonance parameter in Eq. (26), $\partial x_r^i(E|\Gamma^i)/\partial \Gamma_m^i$, is calculated at 0 K and 900 K for each case. The results are compared with those from the early MC S/U analysis [1,9] using SCALE-44 group [12] covariance data and more fine groups, 334g, 634g and 934g, generated by the ERRORR module in NJOY along with reaction-type-wise comparison between with and without Doppler broadening cases. The MC calculations are performed on 100 active cycles with 1,000,000 histories per cycle. For MC Wielandt Method [13], which is employed here to save computer memory space required for the adjoint angular flux estimations [14],

the k_e and convergence interval of the adjoint angular flux is set to 1.5 and 10, respectively.

Table I. k -Uncertainties [pcm] induced by the those of ^{238}U capture cross section in JENDL-3.3 File 32 for TMI-1 pin-cell problem

# of Groups	Doppler Broadening	$\Delta k/k$	SD
44G	w/o (0 K)	230.95	0.17
334G	w/o (0 K)	216.22	0.16
634G	w/o (0 K)	206.77	0.16
934G	w/o (0 K)	203.15	0.16
CE	w/o (0 K)	214.11	0.21
CE	w/ (900 K)	221.42	0.21

Table II. k -Uncertainties [pcm] induced by the those of ^{238}U cross sections in JENDL-3.3 File 32 for TMI-1 pin-cell problem with cross section sensitivities to resonance parameters at 0 K and 900 K

Covariance Type	Doppler Broadening of Resonance Uncertainty			
	w/o (0 K)		w/ (900 K)	
	$\Delta k/k$	SD	$\Delta k/k$	SD
(n, γ), (n, γ)	214.0	0.1	221.9	0.1
(n, γ), (n, fis)	-0.2	0.0	-0.3	0.0
(n, γ), (n, n)	17.7	0.9	-19.6	0.8
(n, fis), (n, fis)	0.0	0.0	0.0	0.0
(n, fis), (n, n)	0.0	0.0	0.0	0.0
(n, n), (n, n)	15.3	0.3	27.0	0.2

VI. CONCLUSION

The new continuous energy MC S/U formulation has been implemented in McCARD and applied for the k -uncertainty quantification for TMI-1 pin-cell problem. From the results, it is found that the k -uncertainties due to the covariance of the resonance parameters notably differ from those from the early MC S/U counterpart. The way proposed in this paper aimed at taking into account Doppler broadening effect by the new continuous-energy MC S/U analysis is a preliminary but a useful one. More improved strategies for applying Doppler broadening on MC S/U analysis and further finding from those will be discussed in the conference.

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