Implicit Resonance Self-Shielding Effect of Multi-Group Covariance in RXSP code

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1. Introduction

RXSP is a nuclear cross section processing code being originally developed by REAL group from Department of Engineering Physics at Tsinghua University in China, which is mainly intended to reactor analysis. The Beta3.0 version is being developed jointly by UNIST and Tsinghua University [1]. Recently, RXSP has extended its capability of multi-group covariance matrices processing from correlation matrix data stored in Evaluated Nuclear Data Files for averaged number of neutrons per fission (MF31), resonance parameters (MF32), and neutron cross sections (MF33), and fission spectrum (MF35). MF31, MF33 and MF35 data blocks can be processed by multi-group neutron flux based weighting integral to compute self-shielded group-wise cross sections covariance matrices [2].

However, MF32 only stores evaluated experimental measurements caused uncertainty for resonance parameters in resolved resonance range (RRR), for instance, the standard deviation of resonance level, elastic scattering, capture, fission reaction widths. In order to calculate uncertainties of cross sections in RRR from above resonance parameters uncertainty, the MF32 stored R-Matrix approximated resonance formulae should be used. ERRORR module in NJOY [3] code introduces covariance data processing method used initiated from ERRORJ code, which can handled all common used R-Matrix approximate resonance formulae, including Single-level Breit-Wigner, Multi-level Breit-Wigner and Reich-Moore.

However, ERRORR module simply applies the smooth weighting function to generate the multi-group averaged covariance, which cannot consider the self-shielding effect in resonance range. This paper borrowed the method used in GROUPR module of NJOY code, together with point-wise cross sections to treat with the self-shielding effect during the multi-group covariance data processing for resonance parameters. This uncertainty caused by the self-shielding effect from resonance parameters uncertainty is the implicit uncertainty, which will be taken into account in this paper.

2. Methodologies

The implicit uncertainty lying in the resonance parameters should be computed by these steps in the following.

2.1 Covariance from Resonance Parameters

In general, the covariance of cross section in resonance range can be computed according to the propagation-of-error formula again in the following,

$$\mathrm{cov}\left(\sigma_I,\sigma_J\right)=\sum_{i,j}\left(\frac{\partial\sigma_I}{\partial p_i}\right)\left(\frac{\partial\sigma_J}{\partial p_j}\right)\mathrm{cov}\left(p_i,p_j\right), \quad (1)$$

where $\mathrm{cov}\left(p_i,p_j\right)$ represents the covariance matrix of resonance parameters, which then will be re-constructed to generate the point-wise (actually multi-group) cross section in resonance range. Moreover, the $\left(\frac{\partial\sigma_I}{\partial p_i}\right)$ and $\left(\frac{\partial\sigma_J}{\partial p_j}\right)$ are the sensitivity of multi-group cross sections to the resonance parameters, which will be described in detailed in the following chapter.

The resonance covariance expression in Eq. (1) can be written in form of sensitivity as follow,

$$\mathrm{cov}\left(\sigma_m,\sigma_n\right)=\sum_{i,j}S_i^m S_j^n\,\mathrm{cov}\left(p_i,p_j\right), \quad (2)$$

where

$$S_i^m=\frac{d\sigma_m}{dp_i}, \quad (3)$$

and

$$\sigma_m=\frac{\sum_{i\in m}\sigma_i\phi_i}{\sum_{i\in m}\phi_i}. \quad (4)$$

If R-Matrix Limited formula is given in MF2 and MF32, there is analytical formulation to calculate the sensitivity of point-wise cross sections to resonance parameters, borrowed from SAMMY code [4]. If not, the one-percent method will be used to compute it by numerical difference like this,

$$S_i^m = \frac{\sigma_m(1.01\times p_i) - \sigma_m(0.99\times p_i)}{1.01\times p_i - 0.99\times p_i}. \quad (5)$$

Furthermore, the weighting flux currently adopts Bondarenko narrow resonance method,

$$\phi_i = \frac{W_i}{\sigma_{t,i} + \sigma_0}. \quad (6)$$

2.2 Implicit Effect

The Bondarenko marrow resonance method can be applied for practical fast reactor problems. However, for nuclear systems sensitive to energies from 1 to 500 eV, there are many broad and intermediated width resonance. And these self-shielding can be insufficiently accurate using this method. Therefore, NJOY provides the flux calculator to solve it. That is to say, the weighting flux can be computed from the slowing-down equation for a heavy absorber in a light moderator. And then all the self-shielded cross sections are averaged in a unified way [4]. By this mean, the weighting flux is computed as followings,

$$\begin{aligned}[\sigma_0 + \sigma_t(E)]\phi_f(E) = (1-\beta)C(E)\sigma_0 \\ + \int_E^{E/\alpha_m} \frac{\beta\sigma_e}{(1-\alpha_m)E'}\phi_f(E')dE', \\ + \int_E^{E/\alpha_f} \frac{\sigma_{sf}(E')}{(1-\alpha_f)E'}\phi_f(E')dE'\end{aligned} \quad (7)$$

where σ_0 is the value of σ_e divided by fuel density, α_m and α_f are the maximal fractional energy change in scattering for the two isotopes, σ_{sf} is the microscopic scattering cross sections of fuel material. Besides, the subscript m and f stand for moderator and fuel materials respectively. And β is a heterogeneity parameter given by this,

$$\beta = \frac{V_f\sigma_e}{V_m\sigma_m}. \quad (8)$$

Once again, to further improve the accuracy of implicit uncertainty, the temperature dependent point-wise cross sections for fuel (uranium-238) and moderator (hydrogen-1) materials are provided by the interpolation from ACE-formatted cross sections files. By default, the energy grid of the point-wise cross sections is constructed by 10,000 equal-lethargy bins from 10^{-5} eV to 20 MeV.

2.3 Code Development

The general procedure for processing covariance of multi-group cross sections, nu-bar, fission spectrum and resonance parameters is shown in Fig. 1. The procedure starts from input parameter to get control information for this covariance data processing. And then the union grid corresponding to user defined group structure and intrinsic energy grid from ENDF data blocks will be constructed. Based on this union energy grid, the weighing flux or spectrum should be calculated and compute the group-averaged multi-group cross sections and their covariance matrixes. It is followed that the group collapse for covariance matrixes from union energy grid to user defined group structure. Finally, the COVFIL format of output covariance data should be converted into COVERX format to meet the demands of sensitivity and uncertainty analysis code.

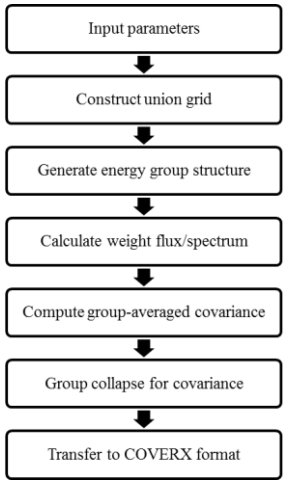

Fig. 1. General procedure of ERRORC module of RXSP code.

Noted that in the last procedure for converting COVFIL data into COVERX format, the "MAT" identifier determining the material (isotope) should be transferred to "ZA" identifier. For instance, the MAT of ^{235}U is 9228, while its ZA is 92235.

In other word, the MTs identifier if fission spectrum ("chi" for short) in ENDF-6 format is different from that in COVERX format. That is to say, MF=35 and MT=18 in ENDF represents covariance of fission spectrum, while it should be converted into MT=1018 in COVERX format.

3. Numerical Results

In order to verify the developed ERRORC module of RXSP code, all the nuclides in ENDF/B-VII.1 [4] having point-wise covariance data block (MF31 or MF32 or MF33) has been processed by ERRORC

module of RXSP code. As a reference, the same processing are conducted by ERRORR module of NJOY code.

The 44-group energy boundary is used, which can be referred in SCALE user manual. And the weighting function option "IWT=6" is used to assume the weighting flux is the combination of "thermal-1/E-fission and fusion spectrum".

The following figures show in detail the multi-group covariance matrices generated by RXSP and NJOY code, including the group-wise uncertainty at the top, the group-wise cross sections values at the right, and the normalized correlation matrix itself at the centre.

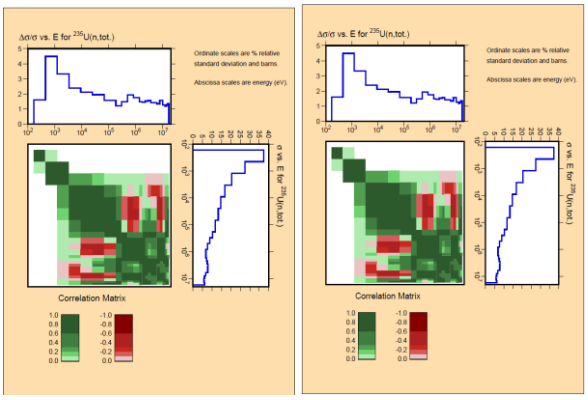

Fig. 2. Covariances of ^{235}U for total to total cross sections (left: RXSP, right: NJOY).

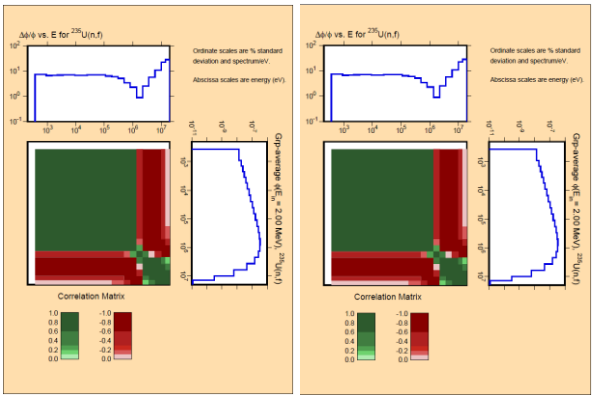

Fig. 3. Covariance of ^{235}U for fission spectrum (left: RXSP, right: NJOY).

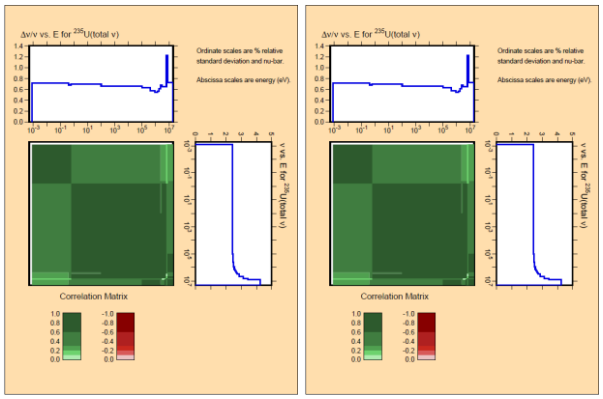

Fig. 4. Covariance of ^{235}U for total Nu-bar(left: RXSP, rgiht:NJOY).

Looking at the Figure 2 through 4, there are multi-group covariance data of ^{235}U for the total to total cross sections presented to show the performance of ERRORC module of RXSP code, which has visually the same accurate capability to produce multi-group covariance data based on ENDF-6 type point-wise covariance matrices in MF33. Moreover, Figure 3 and 4 show the comparison of covariance for fission spectrum and total nu-bar data, which also verify the performance of ERRORC module to process the data in MF31 and MF35.

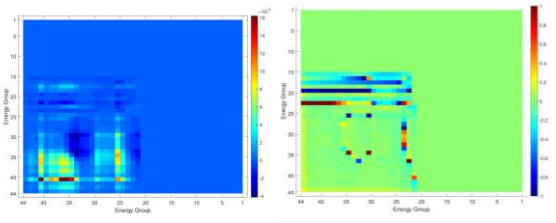

Fig. 5. Covariance contribution from resonance parameters in resolve resonance range for ^{235}U processed by RXSP code (left) and the relative error due to the self-shielding effect.

Likely, the covariance contrition from resonance parameters for ^{235}U in resolved resonance range is also illustrated in Figure 5, which can be used to demonstrate the capability of ERRORC module to handle the covariance along with implicit uncertainty from resonance parameters stored in MF32 data block.

4. Conclusions

The ERRORC module has been developed into RXSP code to extend its capability of multi-group covariance matrices processing from point-wise covariance matrix data stored in Evaluated Nuclear Data Files for averaged number of neutrons per fission, resonance parameters with implicit uncertainty caused

by self-shielding effect, and neutron cross sections, and fission spectrum. Posterior to the code development, the comparison of microscopic multi-group cross sections covariance matrices of nu-bar, fission spectrum, reaction cross sections for ^{235}U nuclide has been conducted between RXSP and NJOY code to verify its accuracy. Besides, the covariance contribution from resonance parameters in resolve resonance range for ^{235}U has been presented and perform the treatment capability for implicit effect from the uncertainty of resonance parameters.

5. Acknowledgement

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT). (No.NRF-2017M2B2A9A02049916)

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