Transactions of the Korean Nuclear Society Spring Meeting
Jeju, Korea, May 18-19, 2023

Development of a Resonance Calculation Scheme Involving Exact Scattering Kernels

Han Gyu Lee, Han Gyu Joo*
Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 08826, Korea
**Corresponding author: joohan@snu.ac.kr*

1. Introduction

Resonance calculation is a requisite for the accurate evaluation of effective cross sections (XSs) in multi-group (MG) neutronics simulations. There have been developed many resonance calculation methods [1][2][3], and the objectives of them are to achieve high accuracy by rigorous consideration of many factors such as spatial heterogeneity [4] or resonance scatterings [5]. Among the several approximations for practicality, the slowing-down scattering approximation is adopted by all the methods.

However, up-scattering events of ^{238}U in the epi-thermal energy range affect the reactivity and the fuel temperature coefficients (FTCs) [6]. In particular, about 10% of differences occur from the exact scattering kernel with Doppler broadened rejection correction (DBRC) method. Although a few correction techniques were devised [7][8], the validity of the correlation between the exact XSs of ^{238}U and background XSs in heterogeneous geometry is not guaranteed.

The most direct resolution is to put the up-scattering sources into the equation of the fixed source problem (FSP) solved during resonance calculations. However, it is not feasible for any of the traditional methods. Only the ultra-fine-group (UFG) methods can handle it, but the extreme burden of treating the exact scattering kernels is an obstacle for the methods [9]. To make it feasible, the Resonance calculation using energy Spectral Expansion (RSE) method [10], which is the recently proposed method, was selected.

The RSE method reduces the degree of freedom (DOF) based on the reduced order model. In the RSE method, UFG spectra can be reproduced with the basis functions while keeping the number of variables way smaller than those in UFG methods. It has great potential when dealing with the exact scattering kernel because of the small size of the scattering matrix.

Despite the potential, the conventional RSE method also adopts the slowing-down scattering approximation. Thus, this paper presents a new pathway to eliminate the slowing-down scattering approximation in the resonance calculation with the generalized RSE method. The process of generating XS moments including exact scattering kernels via a continuous-energy (CE) Monte Carlo (MC) code, PRAGMA [11], is also illustrated. The verification results of the new resonance calculation method are shown with the nonuniform temperature profile benchmark problem developed by Seoul national university (SNU) [12].

2. Background about the Conventional RSE Method

This section introduces a brief sequence of the conventional RSE method. The key of the RSE method is to extract a UFG basis function set. Here, the functions are different from the traditional basis functions such as those in Legendre or Fourier series. The set is driven from the POD to a matrix of snapshots, and each snapshot is a UFG flux spectrum as the reference solution of a representative problem. Provided that n UFG spectra, ϕ, with t UFGs are given, the snapshot matrix, $\mathbf{A}$, is composed as follows:

$$\mathbf{A}=\begin{pmatrix}\phi_1(E_1) & \cdots & \phi_1(E_t)\\ \vdots & \ddots & \vdots\\ \phi_n(E_1) & \cdots & \phi_n(E_t)\end{pmatrix}\in\mathbb{R}^{n\times t}. \quad (1)$$

To extract the basis functions in the POD, the singular value decomposition (SVD) can be employed. With the notations where $\mathbf{U}$ and $\mathbf{V}$ are the left and right singular vector spaces, and $\mathbf{\Sigma}$ is the diagonal matrix with singular values of $\mathbf{A}$, the following relations are derived:

$$\mathbf{A}=\mathbf{U\Sigma V}^T,\ \mathbf{U}\in\mathbb{R}^{n\times m}\ \&\ \mathbf{\Sigma}\in\mathbb{R}^{m\times m}\ \&\ \mathbf{V}\in\mathbb{R}^{t\times m}, \quad (2)$$

$$\mathbf{U}^T\mathbf{U}=\mathbf{V}^T\mathbf{V}=\mathbf{I}_m, \quad (3)$$

where m is the rank of $\mathbf{A}$. A subset of the right singular vector space can be a set of POD modes, which are the basis functions [13]. Due to the semi-unitarity of singular vector matrices, the orthogonality holds for the subset.

The reference UFG spectra in the conventional RSE method were obtained via UFG calculations for several slowing-down problems. The basic approach solves homogeneous problems for typical fuel compositions with the variations of temperatures or background XSs, while another approach takes the solutions of a set of single pin cell problems too [14].

To derive the FSP equation solved in the RSE method, the regular FSP transport equation is presented with the basis expansion on energy-dependent angular flux, ψ :

$$\begin{aligned}&\mathbf{\Omega}\cdot\nabla\psi(E,\mathbf{\Omega},\mathbf{r})+\Sigma_t(E,\mathbf{r})\psi(E,\mathbf{\Omega},\mathbf{r})\\ &=\frac{1}{4\pi}\int\Sigma_s(E'\to E)\phi(E',\mathbf{r})dE'+Q_{fix}(E,\mathbf{\Omega},\mathbf{r}),\end{aligned} \quad (4)$$

$$\psi(E,\mathbf{\Omega},\mathbf{r})\simeq\sum_k\psi_k(\mathbf{\Omega},\mathbf{r})f_k(E), \quad (5)$$

where

$\mathbf{r}$: position vector
$\mathbf{\Omega}$: direction vector

E : energy
$\psi(E,\mathbf{\Omega},\mathbf{r})$: angular flux
$\phi(E,\mathbf{r})$: scalar flux
$\Sigma_t(E,\mathbf{r})$: total XS
$\Sigma_s(E'\to E,\mathbf{r})$: scattering XS
$Q_{fix}(E,\mathbf{\Omega},\mathbf{r})$: fixed source
$\psi_k(\mathbf{\Omega},\mathbf{r})$: k-th angular flux moment
$f_k(E)$: k-th basis function.

A weak form of Eq. (4) can be derived after obtaining the inner product over energy, $\int f_k(E)dE\times$, weighted by each basis function as the test function:

$$\begin{aligned}&\mathbf{\Omega}\cdot\nabla\psi_k(\mathbf{\Omega},\mathbf{r})+\sum_{k'}\Sigma_{t,kk'}(\mathbf{r})\psi_k(\mathbf{\Omega},\mathbf{r})\\&=\frac{1}{4\pi}\sum_{k'}\Sigma_{s,kk'}(\mathbf{r})\phi_{k'}(\mathbf{r})+q_{fix,k}(\mathbf{\Omega},\mathbf{r})\ ,\end{aligned}\tag{6}$$

and the several moments are defined as,

$$\Sigma_{t,kk'}(\mathbf{r})=\int f_k(E)\Sigma_t(E,\mathbf{r})f_{k'}(E)dE\ ,\tag{7}$$

$$\Sigma_{s,kk'}(\mathbf{r})=\iint f_k(E)\Sigma_s(E'\to E,\mathbf{r})f_{k'}(E')dE'dE\ ,\tag{8}$$

$$q_{fix,k}(\mathbf{\Omega},\mathbf{r})=\int f_k(E)Q_{fix}(E,\mathbf{\Omega},\mathbf{r})dE\ ,\tag{9}$$

where
$\Sigma_{t,kk'}(\mathbf{r})$: total XS moment
$\Sigma_{s,kk'}(\mathbf{r})$: scattering XS moment
$q_{fix,k}(\mathbf{\Omega},\mathbf{r})$: fixed source moment.

Note that the scattering sources and scattering XS moments in the conventional RSE method are computed with slowing-down scattering kernels. The FSP in Eq. (6) is solved through the method of characteristics (MOC) solver while it includes matrix exponential solution due to the dense total XS matrix in the collision term.

3. Generation of Exact Cross Section Moments via Monte Carlo Method

The definition of scattering XS moments in Eq. (8) shows the possibility of using exact scattering kernels. It is easily applicable by just giving the exact scattering XSs for $\Sigma_s(E'\to E)$. However, considering the size of a matrix for the kernel in a UFG structure, it becomes extremely inefficient to compute the moments with the large kernel data. In addition, the computational burden is another concern because every moment for each pair of basis functions should be computed. To overcome the overheads, another form of the definition for XS moment is introduced.

To derive the alternative definitions, two rates are defined omitting spatial dependence of the quantities:

$$R_{t,k'}(E)=\Sigma_t(E)f_{k'}(E)\ ,\tag{10}$$

$$S_{k'}(E)=\int\Sigma_s(E'\to E)f_{k'}(E')dE'\ .\tag{11}$$

Here, the quantity, $R_{t,k'}(E)$, can be interpreted as the UFG total reaction rate for a unit level of flux when the shape is given the basis function, $f_{k'}(E)$. In the same, the source rate, $S_{k'}(E)$, can be seen as the UFG source when the incident energy distribution follows $f_{k'}(E')$.

With the new definitions of rates for a basis function, the XS moments in Eq. (7) and Eq. (8) are expressed as follows:

$$\Sigma_{t,kk'}=\int f_k(E)R_{t,k'}(E)dE\ ,\tag{12}$$

$$\Sigma_{s,kk'}=\int f_k(E)S_{k'}(E)dE\ .\tag{13}$$

The definitions in Eq. (12) and Eq. (13) provide a way to compute the moments efficiently by eliminating the overheads for memory requirements and excessive operations needed. Once the rates for all the orders are obtained, simple numerical integrations are only needed to get the inner production of every pair of a rate and a basis function.

What remains for the generation of XS moments is to find out an efficient way of evaluating the rates. It can be realized by utilizing a CE MC code when calculating the exact rates. By employing the tally functionalities for reaction rates and scattering sources, the UFG rates can be easily estimated. However, there is a tricky issue due to the negative values in basis functions when giving the energy distribution of samples for each basis of an order.

Basis functions usually include negative values, and this feature makes it hard to directly define the functions as probability density functions (PDFs). Therefore, the absolute of a basis function is selected as the PDF, and the weight of a sample is given as the sign of the basis function value at its energy. This way is illustrated in Fig. 1.

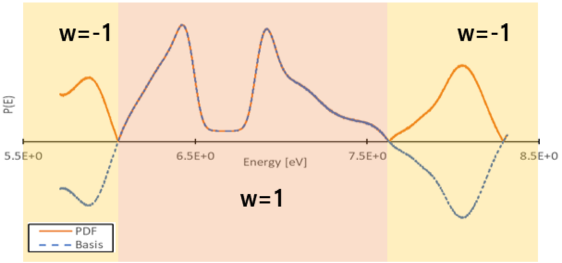

Fig. 1. Probability density function and the weights for a basis function including negative values.

A special mode named the integrator mode had to be developed in PRAGMA to realize these procedures. This capability is only for calculating the designated rates for a given energy spectrum. The integrator mode enables an efficient numerical integration via the stochastic method employing the same physics algorithms in PRAGMA.

5. Verifications

For the verification of the generalized RSE method, the nonuniform temperature benchmark from SNU [12][15] is solved. Ahead of the result of FTC estimation, the UFG spectrum reproduced from the RSE method is compared to two spectra from PRAGMA differing in the scattering kernels for ^{238}U and hydrogen, which are illustrated in Fig. 3 and Fig. 2. The solution spectra in the innermost fuel ring under the highest power condition, which is 200% of the normal condition, are compared.

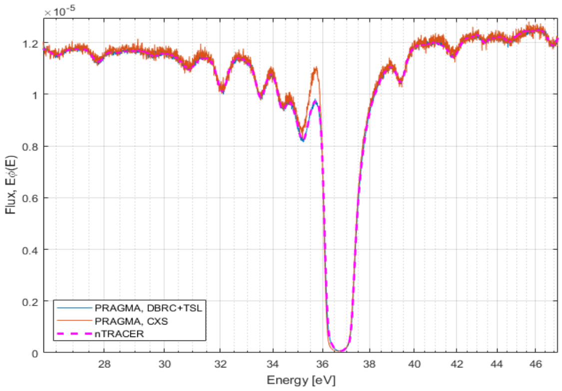

Fig. 2. UFG spectra in the epi-thermal range.

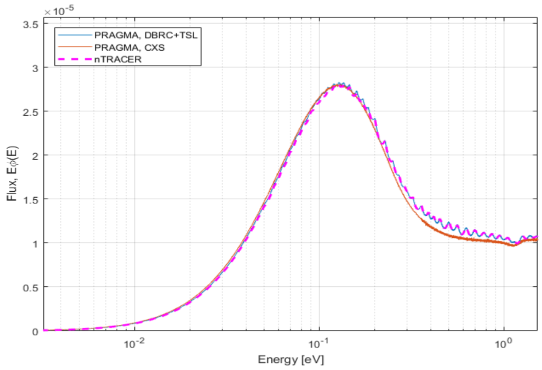

Fig. 3. UFG spectra in the thermal range.

The spectra of PRAGMA are plotted as solid lines when the blue one is the result of using the exact scattering kernels and the orange one is that of using asymptotic kernels. The spectrum from the RSE method is plotted as the pink dashed line. In the epi-thermal range, the effect of resonance up-scattering is well depicted by the RSE method. Although the thermal range is out of the scope of this work, Fig. 3 shows that the UFG spectrum represents the wavy shape which is the result of the thermal scattering law (TSL) of the hydrogen in a water molecule (hh2o).

The accuracy in reactivity estimation is examined by comparing the two methods that are the subgroup (SG) method and the RSE method. The previous research showed the effectiveness of the SG method in the FTC estimation [15], but the compared results are for when the constant cross section (CXS) kernel was employed. In Fig. 4 and Table 1, the results for two different kernels, which are the CXS and the DBRC, are all shown while only the DBRC is considered for the RSE method.

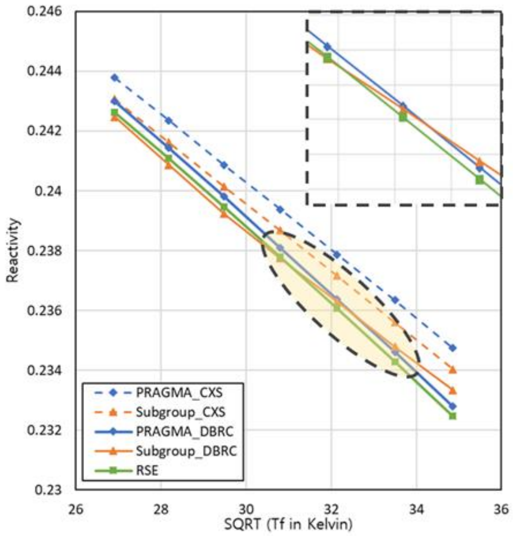

Fig. 4. Reactivities from different solutions for various fuel temperatures.

Table 1. Estimated FTCs from different solutions.

Scat. Kernel	Method	FTC [pcm/K]
CXS	MC	-1.834
	SG	-1.833 (-0.001)
DBRC	MC	-2.078
	SG	-1.847 (+0.231)
	RSE	-2.068 (-0.010)

In the figure, the reactivities with the CXS kernel are plotted with the dashed lines whereas those with the DBRC kernel are plotted with the solid lines. And, the blue line is for the PRAGMA results while the orange one is for the SG method and the green one is for the RSE method.

The reactivity changes with the CXS kernel were well evaluated by the SG method, which can be observed by the nearly parallel dashed lines in Fig. 4. However, when it comes to the DBRC cases, the SG method showed inaccurate results. The gradient of the SG results was more gradual than that of the PRAGMA results. On the other hand, the reactivity changes from the RSE method were quite similar to those from PRAGMA.

The results of the comparison of the estimated FTC values also show a similar tendency. The estimation of the SG method was good with the CXS kernel. However, when the DBRC was applied, there was about 10% difference in the values from PRAGMA while the FTC from the RSE method has little difference.

6. Conclusions

A new way of resonance calculation that implicitly considers the exact scattering kernels is realized through the generalized RSE method by incorporating a CE MC code into the calculation of XS moments for the exact FSP equations. The RSE method was selected due to the small size of the scattering matrix and the low computational burden to handle it. The key was to calculate the exact rates for each of the basis functions via the MC Code. Through the alternative definitions of XS moments, it was shown that the XS moments for exact physics can easily be computed only if the UFG rates are prepared. The stochastic integration with PRAGMA enables efficient calculations of the scattering source rates including the effect of exact scattering kernels.

The results showed good agreement with the PRAGMA results when considering the exact scattering effects. The reproduced UFG spectrum was able to depict the effects of the exact resonance up-scattering in the epi-thermal range and those of the TSL in the thermal range. The accuracy in FTC estimation was also superior compared to the SG method when the exact kernel was applied.

This paper suggests a way of resonance calculation that does not need any approximations or corrections. In fact, most of the resonance calculation methods should take correction techniques. to overcome the side effects from the approximations they apply. For example, the UFG methods assume the slowing-down approximation for their feasibility in terms of the performance in dealing with scattering sources. On the other hand, if the XS moments are well generated, the new way can naturally handle the exact scattering sources.

ACKNOWLEDGEMENTS

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (MSIT) (No. 2021M2D6A1048220).

REFERENCES

[1] R. J. J. Stamm'ler, M. J. Abbate, "Methods of Steady-State Reactor Physics in Nuclear Design," Academic Press, London (1983).

[2] M. N. Nikolaev et al., "The Method of Subgroups for Considering the Resonance Structure of the Cross Sections in Nuclear Calculations (Part 1)," Sov. At. Energy, vol. 29(1), p. 689 (1970).

[3] N. Sugimura, A. Yamamoto, "Resonance Treatment Based on Ultra-fine-group Spectrum Calculation in the AEGIS Code," Journal of Nuclear Science and Technology, vol. 44(7), p.958 (2007).

[4] Y. Liu, W. R. Martin, "Assessment of homogeneous and heterogeneous resonance integral tables and their applications to the embedded self-shielding method," Annals of Nuclear Energy, vol. 92, p. 186 (2016).

[5] S. Choi, D. Lee, "Resonance treatment using pin-based pointwise energy slowing-down method," Journal of Computational Physics, vol. 330, p. 134 (2017).

[6] D. Lee, K. Smith, J. Rhodes, "The impact of ^{238}U resonance elastic scattering approximation on thermal reactor Doppler reactivity," Annals of Nuclear Energy, vol. 36(3), p. 274 (2009).

[7] C. H. Lim, Y. S. Jung, H. G. Joo, "Incorporation of Resonance Upscattering and Intra-Pellet Power Profile in Direct Whole Core Calculation," Transactions of Korean Nuclear Society Spring Meeting, Jeju, Korea, May 17-18, 2012.

[8] K. S. Kim, et. al., "Development of the multigroup cross section library for the CASL neutronics simulator MPACT: Method and procedure," Annals of Nuclear Energy, vol. 133, p. 46 (2019).

[9] A. Gibson, "Novel Resonance Self-Shielding Methods for Nuclear Reactor Analysis (Doctoral Dissertation), MIT: Cambridge, 2016.

[10] R. Kondo, et. al., "A New Resonance Calculation Method Using Energy Expansion Based on a Reduced Order Model," Nuclear Science and Engineering, vol. 195, p. 694, 2021.

[11] N. Choi, K. M. Kim and H. G. Joo, "Initial Development of PRAGMA – A GPU-Based Continuous Energy Monte Carlo Code for Practical Applications," Transactions of Korean Nuclear Society Autumn Meeting, Goyang, Korea, Oct. 24-25, 2019.

[12] Y. S. Jung, C. H. Lim, H. G. Joo, "Temperature dependent subgroup formulation with number density adjustment for direct whole core power reactor calculation," Annals of Nuclear Energy, Vol. 96, p. 249, 2016.

[13] E. Shlizerman, et. al., "The Proper Orthogonal Decomposition for Dimensionality Reduction in Mode-Locked Lasers and Optical Systems," International Journal of Optics, vol. 2012, 831604 (2012).

[14] K. Yamaji, et. al., "Implementation of a Resonance Calculation Using Energy Spectral Expansion Method Into Heterogeneous Transport Calculation Code GALAXY-Z," International Conference on Mathematics and Computation Applied to Nuclear Science and Engineering (M&C 2021), virtual meeting, Oct. 3-7, 2021.

[15] S. Jae, H. G. Joo, "Analyses of on-the-fly generation of spectral superhomogenization factors for multigroup whole core calculation employing pin-wise slowing-down solutions," Nuclear Engineering and Technology, Vol. 55, no. 3, p. 1084, 2023.