Automate Multigroup Cross Section Library Verification Using Eigenvalue Analysis

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Abstract – In deterministic reactor core analysis, verification of multigroup cross sections calculated from a problem-independent multigroup library often requires substantial efforts. When discrepancies between the results of the deterministic code and the reference solution occur, it is often lack of useful information (mostly only \(k_{\text{eff}}\) and power distribution) for a library developer to identify the potential issues of an existing cross section library and the associated resonance self-shielding methods. In the verification and validation of the CASL neutronics code MPACT, such difficulties occur when the cross section library or methods are updated or to be used for new applications. To reduce the verification efforts, it is crucial to develop an eigenvalue analysis tool that is able to quickly pinpoint the eigenvalue error in regard to an isotope, a reaction channel and an energy group. This paper discusses two candidate methods for eigenvalue analysis, i.e., perturbation method and neutron balance method. The two methods are implemented into MPACT V&V and the difference between the two methods is discussed. The applications of using eigenvalue analysis to improve the energy group structure and to compare the resonance methods are also presented.

I. INTRODUCTION

In deterministic reactor core analysis, the multigroup (MG) theory is usually applied to treat the energy complexity of cross sections. A number of physical and mathematical approximations have been used in this process [1], so the accuracy of a deterministic neutron transport code is largely depending on the quality of the MG cross section library and the associated resonance self-shielding method. In general, the MG cross section library and resonance method are verified against benchmark problems from Monte Carlo calculation. However, assessing a MG library by the commonly interested core parameters such as reactivity and power distribution is often insufficient. In order to locate the error source of a biased eigenvalue, the following question is often raised: which isotopes, reaction channels and energy groups contribute most to the eigenvalue bias? A quick and precise answer to this question will help developers to identify the deficiency of the cross section library for further improvement.

In the verification and validation (V&V) of the CASL neutronics code MPACT [2], the previously released 47-group cross section library shows a few issues in obtaining consistent results as compared to the continuous-energy (CE) Monte Carlo solution [3]. Recently, the procedure of generating MPACT MG library has been reviewed in Oak Ridge National Laboratory, and a few new versions of MPACT libraries are generated to improve the results of PWR and BWR problems [4,5]. To reduce the verification efforts for updates of the cross section library and method, it is crucial to develop an eigenvalue analysis tool to quickly answer the foregoing question, i.e., pinpointing the eigenvalue error in regard to an isotope, a reaction channel and an energy group. This paper describes the candidate methods for the analysis tool and its integration into the MPACT V&V. An initial set of problems has been developed to demonstrate the analysis tool. The applications of using the eigenvalue analysis to improve the energy group structure and compare the resonance methods are also presented.

II. THEORY

Eigenvalue analysis aims at converting the multigroup cross section error into the eigenvalue error between the results of a deterministic code and Monte Carlo reference. Two candidate methods are discussed in this section, perturbation method and neutron balance method [6].

1. Perturbation method

A common application of the perturbation theory is to predict the change in eigenvalue due to the small perturbation of a reactor. Previously, the perturbation theory has been widely used for cross section sensitivity analysis [7]. In this paper, a similar approach is taken to verify the generation of MG cross section. The neutron balance equation of a base problem and a perturbed problem are defined as,

\[
\begin{align*}
M\Phi &= \lambda F\Phi \\
(M + \Delta M)(\Phi + \Delta \Phi) &= (\lambda + \Delta \lambda)(F + \Delta F)(\Phi + \Delta \Phi)
\end{align*}
\] (1)

where \(F\) is the operator of fission and \(M\) includes the other non-fission terms. \(\lambda\) is the reverse of the reactor
multiplication factor $k_{eff}$. In our case, the small perturbation $\Delta M$ and $\Delta F$ can be viewed as the error of MG cross section from the deterministic calculation to the Monte Carlo calculation. Using the first-order perturbation theory [8], one can obtain the eigenvalue change due to the error of MG cross section without solving the perturbed neutron balance equation,

$$\Delta k = \frac{\Phi^* (k \Delta F - k^2 \Delta M) \Phi}{\Phi^* F \Phi}$$  \hspace{1cm} (2)

where $\langle \rangle$ denotes the integration over all phase spaces. In Eq. (2), $\Phi^*$ is the adjoint flux that obeys the equation,

$$M^* \Phi^* = \lambda F^* \Phi^*$$  \hspace{1cm} (3)

To obtain the eigenvalue error from a material region $j$, isotope $i$ and energy group $g$, one can write out the components of Eq. (2),

$$\langle \Phi^* F \Phi \rangle = \sum_{g, i, j} \sum_{g} \chi_{g, j, i} \phi_{g, i}^* \sum_{g} \nu_{f, g, j, i} \phi_{g, i} V_j$$  \hspace{1cm} (4-a)

$$\langle \Phi^* k \Delta F \Phi \rangle^{\text{test}}_{g, i, j} = kV \phi_{g, i}^* (\Sigma_{r, g, j, i}^{\text{test}} - \nu_{r, g, j, i}^{\text{ref}}) \phi_{g, i}$$  \hspace{1cm} (4-b)

$$\langle \Phi^* k^2 \Delta M \Phi \rangle^{\text{test}}_{g, i, j} = k^2 \phi_{g, i}^* \phi_{g, i} (\Sigma_{s, r, g, j, i}^{\text{test}} - \Sigma_{s, r, g, j, i}^{\text{ref}})$$

$$-2kV \phi_{g, i}^* \phi_{g, i} \sum_{g'} \Sigma_{r, s, g', g}^{\text{test}} - \Sigma_{r, s, g', g}^{\text{ref}}) \phi_{g', i}$$  \hspace{1cm} (4-c)

$$\langle \Phi^* k \Delta M \Phi \rangle^{\text{abs}}_{g, i, j} = k^2 \phi_{g, i}^* \phi_{g, i} (\Sigma_{r, g, j, i}^{\text{test}} - \Sigma_{r, g, j, i}^{\text{ref}})$$

$$-2kV \phi_{g, i}^* \phi_{g, i} \sum_{g'} \Sigma_{r, s, g', g}^{\text{test}} - \Sigma_{r, s, g', g}^{\text{ref}}) \phi_{g', i}$$  \hspace{1cm} (4-d)

In these equations, the superscripts $\text{test}$ and $\text{ref}$ denote the deterministic and Monte Carlo cross sections. The transport corrected P0 is used in Eq. (4-d) for brevity. Note the leakage term in operator $M$ is omitted since the eigenvalue analysis is usually performed for an infinite pin cell or lattice with reflective boundaries. By using Eq. (4), $\Delta k$ due to fission, absorption and scattering cross section errors can be evaluated as (4-b)/(4-a), (4-c)/(4-a) and (4-d)/(4-a), respectively.

Assuming the deterministic solver is consistent with the Monte Carlo solver if the consistent MG cross section ($M$ and $F$) are provided, three options are possible for obtaining the forward and adjoint flux in Eq. (4),

1. **Deterministic method with Monte Carlo tallied cross section.** Perform Monte Carlo calculation and tally MG 1-D cross sections and scattering matrices. Using these cross sections to set up $M$ and $F$ (and thus $M^*$ and $F^*$), solve the forward and adjoint equations with the deterministic solver.

2. **Deterministic method with deterministic cross section.** Compute MG cross sections using the MG library and resonance methods by the deterministic solver. Solve the forward and adjoint equations using deterministic solver.

3. **Monte Carlo method with deterministic cross section.** Compute MG cross section using MG library and resonance methods by the deterministic solver. Perform MG Monte Carlo forward and adjoint calculations using these MG cross sections.

The difference between Options 1 and 2 is the base case (either using the reference cross section from Monte Carlo, or the cross section from deterministic calculation). Option 2 is easier to achieve since generating the isotopic scattering matrices is not a common capability for most Monte Carlo codes. Instead of using the deterministic solver in Option 2, Option 3 uses the Monte Carlo solver with the multigroup cross sections. If the adjoint capability is available in the Monte Carlo code rather than the deterministic code, Option 3 can be considered.

In this paper, Option 2 is chosen by taking advantage of the MOC adjoint capability in MPACT [9,10]. The multigroup forward and adjoint transport equations are written as

$$\Omega \cdot \nabla \psi_g (r, \Omega) + \sum_{i, g} (r) \psi_g (r, \Omega) =$$

$$\sum_{g} \int_{\Omega} \Sigma_{r, g, i, g} (r, \Omega') \psi_g (r, \Omega') d\Omega'$$  \hspace{1cm} (5-a)

$$- \sum_{g} \int_{\Omega} \sum_{i, g, i, g} (r, \Omega') \psi_g (r, \Omega') d\Omega'$$

$$- \sum_{g} \int_{\Omega} \sum_{i, g, i, g} (r, \Omega') \psi_g (r, \Omega') d\Omega'$$

$$- \sum_{g} \int_{\Omega} \sum_{i, g, i, g} (r, \Omega') \psi_g (r, \Omega') d\Omega'$$

$$= \frac{\Sigma_{f, g} (r)}{4\pi k_{eff}} \sum_{g} \int_{\Omega} \Sigma_{f, g, g} (r, \Omega') \psi_g (r, \Omega') d\Omega'$$

$$= \frac{\Sigma_{f, g} (r)}{4\pi k_{eff}} \sum_{g} \int_{\Omega} \Sigma_{f, g, g} (r, \Omega') \psi_g (r, \Omega') d\Omega'$$

where $\psi_g$ and $\psi_g^*$ are the forward and adjoint angular flux, and all other symbols are standard in the neutron transport equation. By changing the variable $\psi_g^* (r, \Omega) = \psi_g (r, -\Omega)$ and setting $\Omega = -\Omega$ in Eq. (5-b), the only difference between (5-a) and (5-b) is the source term, where the scattering matrix is reversed and the nu-fission cross section is exchanged with the fission spectrum. Therefore, the same MOC solver can be used to solve both (5-a) and (5-b).
2. Neutron balance method

The neutron balance method for eigenvalue analysis was previously introduced to verify a cross section library [6]. Considering a case with reflective boundary, the eigenvalue can be written as the ratio of neutron production to the neutron absorption,

\[ k_{inf} = \frac{\sum_{j'} \sum_{i'} \sum_{g'} \Sigma_{f,j',g'} \phi_{j',g'} V_{j'} - \sum_{j} \sum_{i} \sum_{g} \Sigma_{a,g} \phi_{g} V_{j}}{\sum_{j'} \sum_{i'} \sum_{g'} \Sigma_{t,g'} \phi_{g'} V_{j'}} \]  

(6)

In Eq. (6), \( i, j, g \) are the indices of isotope, material region and energy group, respectively. Similar to the perturbation method, the leakage term is not needed because of the reflective boundary conditions in our applications. Estimation of the \( k_{inf} \) error due to an isotopic reaction rate error of group \( g \) is given as,

\[
\Delta k_{a,g,i,j} = \frac{\sum_{j'} \sum_{i'} \sum_{g'} \Sigma_{f,j',g'} \phi_{j',g'} V_{j'} + \Delta R_{a,g,i,j} - k_{inf}^{ref}}{\sum_{j'} \sum_{i'} \sum_{g'} \Sigma_{a,g'} \phi_{g'} V_{j'}} - k_{inf}^{ref} \\
\Delta k_{f,g,i,j} = \frac{\sum_{j'} \sum_{i'} \sum_{g'} \Sigma_{g'} \phi_{g'} V_{j'} + \Delta R_{f,g,i,j} - k_{inf}^{ref}}{\sum_{j'} \sum_{i'} \sum_{g'} \Sigma_{a,g'} \phi_{g'} V_{j'}} - k_{inf}^{ref} 
\]

(7)

All the quantities of Eqs. (6) and (7) except the \( \Delta R \) term are from the reference calculation. The \( \Delta R \) term can be defined as the reaction rate error between test and reference results,

\[
\left\{ \begin{array}{l}
\Delta R_{a,g,i,j} = V_{j'} (\Sigma_{a,g,i}^{ref} \phi_{a,i}^{ref} - \Sigma_{a,g,i} \phi_{a,i}^{Ref}) \\
\Delta R_{f,g,i,j} = V_{j'} (\Sigma_{f,g,i}^{ref} \phi_{f,i}^{ref} - \Sigma_{f,g,i} \phi_{f,i}^{Ref})
\end{array} \right. 
\]  

(8)

Ref. [6] also includes another definition of \( \Delta R \) to isolate the cross section error by using the reference flux,

\[
\left\{ \begin{array}{l}
\Delta R_{a,g,i,j} = V_{j'} \phi_{a,i}^{ref} (\Sigma_{a,g,i}^{ref} - \Sigma_{a,g,i}^{ref}) \\
\Delta R_{f,g,i,j} = V_{j'} \phi_{f,i}^{ref} (\Sigma_{f,g,i}^{ref} - \Sigma_{f,g,i}^{ref})
\end{array} \right. 
\]

(9)

Rigorously speaking, neither of the two definitions are the true error introduced by the discrepancy of 1-D cross section of group \( g \). Eq. (8) produces the \( k_{inf} \) error of group \( g \) due to both errors of cross section and flux, where the latter is also dependent on the scattering matrix. Unfortunately, scattering matrix cannot be assessed with the neutron balance method. Eq. (9) produces the \( k_{inf} \) error due only to the cross section error, but identical fluxes between Monte Carlo and deterministic results are assumed. This assumption is questionable, since the 1-D cross section error could more or less affect the flux. Comparison of the two definitions of the neutron balance method and the perturbation method is performed in Section III.1.

III. NUMERICAL RESULTS

The two eigenvalue analysis methods are implemented into the MPACT V&V suite. To minimize the manual efforts and assure the extendibility of the tool, HDF5 data [11] is used to facilitate the data transition and comparison. A uniform data structure is defined to store the effective cross section (absorption, nu-fission, scattering and fission spectrum), flux, adjoint flux, core geometry and material composition. This allows the analysis to be extended to any two codes by implementing an edit routine for each code with the uniform HDF5 data structure. Currently, we’ve implemented the edit routines for MPACT and MCNP [12]. Future plan is to include SHIFT [13] and KENO [14] as alternative reference solutions.

The analysis script takes two HDF5 files for comparison. All quantities (flux, cross section, etc.) are saved in a mesh defined by the material regions of a geometry configuration, but one can choose to perform the analysis either for the predefined mesh, or for an integrated coarse mesh (e.g., integrated over subdivided fuel rings). In the rest of this section, the tool is first demonstrated by comparing the analysis methods discussed in Section II. Then a few group structures and resonance methods are examined with the tool.

1. Demonstration of the tool

As shown in Table I, the tool is demonstrated by analyzing a set of 2-D pin cell problems that cover the issues found in the past versions of MPACT libraries [3]. A beta version of the MPACT 51-group library is used with the subgroup method to obtain the deterministic results. The MCNP calculations are performed with reaction rate tallies in the same group structure. 40 million neutron histories are used for each run to ensure that the statistic errors of \( k_{eff} \) for all group-wise reaction rates are well within 0.1%. These reaction rates are then converted to effective cross sections.

Three levels of results are generated with various details to help the developer identify the potential issues in a cross section library and associated resonance methods. The first level presents the overall information, as shown in Table II. The cases with large eigenvalue bias can be identified from the column of ‘dk’. The column of ‘dk-RR’ shows the total eigenvalue error from the neutron balance method by summing the reaction rate errors obtained from Eqs. (7) and (8) over all energy groups, isotopes and material regions. ‘dk-RR’ should be essentially equal to ‘dk’, since summation of the reaction rate errors approximately preserve the overall eigenvalue error.
The second level of analysis presents the eigenvalue bias contributed by each isotope in every cell (material region). Table III shows the results of Case 4, by which the 'problematic' isotopes can be quickly identified. We denote the neutron balance method as $M^{RR}$ and $M^{XS}$ by using Eqs. (7)+(8), and Eqs. (7)+(9), respectively. The perturbation method is denoted as $M^{PUR}$. The cross section errors computed by $M^{XS}$ and $M^{PUR}$ have large discrepancies from the reaction rate errors of $M^{RR}$, which are due to both 1-D cross section and flux (including the error of scattering matrix). Most values between $M^{XS}$ and $M^{PUR}$ are close, except for U-238 absorption, which will be explained by the results of the third level.

The cell index starts from moderator

Group-dependent eigenvalue errors can be viewed from the results of the third level, as shown in Figs. 1 and 2. In each figure, the upper plot shows the reference absorption and nu-fission cross section, and the lower plot shows the eigenvalue error per energy group (rather than per lethargy). To improve the cross section library, extra efforts should be made to the ‘hot spots’ where large eigenvalue errors occur, e.g., the U-238 resonance cross sections and U-235 thermal cross sections. From Fig. 1, the error of U-238 6.67eV absorption predicted by $M^{PUR}$ is much smaller than $M^{XS}$. In this group, the absorption cross section is underestimated by MPACT (positive eigenvalue error). Since $M^{XS}$ uses the reference flux from MCNP, the change of flux due to the biased cross section is not considered. $M^{PUR}$ is able to capture this effect by adjoint flux weighting. As shown in Fig. 3, the adjoint flux in the fuel region is much smaller around 6.67eV.

It is observed from Table III that $M^{XS}$ and $M^{PUR}$ do not preserve the true eigenvalue error from MPACT to MCNP. Currently, MCNP cannot generate isotopic scattering matrices. If this capability is available, $M^{PUR}$ can be improved to preserve the true eigenvalue error by assessing the scattering matrices, but $M^{XS}$ cannot. As the neutron balance equation is used in $M^{RR}$, the true eigenvalue error is automatically preserved, but the group-wise reaction rate errors obtained in $M^{RR}$ come from a mixed effect of both 1-D and 2-D cross sections (not an isolated error for absorption or nu-fission). In spite of the limitations for $M^{RR}$ and $M^{XS}$, they can be utilized to perform a ‘quick and rough’ judgement until the scattering matrix assessment is available in $M^{PUR}$. In the next two subsections, $M^{RR}$ and $M^{XS}$ will be used to evaluate a few group structures and resonance methods.
2. Comparison of group structures

An important application of the eigenvalue analysis tool is to verify the progress of cross section library development for MPACT. Previously, a 47-group MPACT library was developed for PWR applications [4]. However, substantial discrepancies were identified when the 47-group library is used for BWR calculations. Figs. 4a and 4b show the eigenvalue analysis of a 90% void BWR pin cell (Case 12 in Table II). The cross section and reaction rate errors in the plot correspond to $M^{XS}$ and $M^{RR}$ previously discussed. As neutron spectrum becomes harder for a high void BWR pin cell, significant errors are observed in the intermediate and high energy groups.
To improve the library for BWR applications, the recently released 51-group MPACT library refined a few resonance groups including the broad group (130eV-2035eV), and extended the upper energy boundary of self-shielding calculation from 9118eV to 50keV [5]. Fig. 5 shows the eigenvalue analysis for the same case with the 51-group library. The cross section errors are significantly reduced as compared to the 47-group library. In some groups, the sign of cross section error and reaction rate error is different, indicating large biases of neutron flux. These biases may result from the inaccuracy of scattering matrices, which is an ongoing task of the library development.

Another application of eigenvalue analysis is to verify the resonance self-shielding methods. Three self-shielding methods are available in MPACT, the physical subgroup method (referred to as subgroup method in the rest of the paper) [15], the embedded self-shielding method (ESSM) [16,17], and ESSM-X [18]. Among a few important physics phenomena that a self-shielding model needs to account for [19], the long-standing problem, resonance interference, can be verified against resonance methods using the eigenvalue analysis tool.

In Fig. 6, eigenvalue analysis is performed for a PWR pin cell with 4.1 wt% U-235 enrichment (Case 3 in Table II). By comparing the ‘pcm’ error of U-235 in the resonance energy range (between the two blue lines), one can easily pinpoint the groups that are interfered due to the presence of U-238. Since the subgroup method and ESSM approximately handle the resonance interference using Bondarenko iteration [20], larger errors are observed as compare to ESSM-X, in which the slowing-down calculation is performed to correct the interference effect. It would be straightforward to obtain the percentage errors of cross sections and reaction rates, but the percentage errors sometimes disguise the groups that may have larger contribution to the eigenvalue. For example, Fig. 7 shows the percentage error of the same case for subgroup method. It looks like the two groups near U-238 6.67eV resonance have ~30% errors for U-235, but as converted to eigenvalue, the errors are less important than the groups near U-238 21eV resonance as seen from Fig. 6.

In addition to the resonance groups, substantial discrepancies are found in many thermal groups, where the eigenvalue errors are somewhat cancelled out between absorption and fission. This is not related to resonance interference. Further efforts should be made to improve the thermal cross sections, since the biased fission sources may affect the power distribution for an assembly or full core calculation.

IV. CONCLUSION

The eigenvalue analysis methods have been investigated and implemented into the MPACT V&V. The neutron balance method could provide useful information for a developer to quickly pinpoint the large eigenvalue errors in regard to isotope, reaction channel and energy group. However, the results of the neutron balance method are either a mixture of effects, or less accurate compared to the perturbation method. Given the neutron balance method is free from adjoint calculation, it can perform a ‘quick and rough’ judgement in the quality of a cross section library. To obtain the accurate and isolated error information, the perturbation method could be used. Further study is needed to include the scattering matrix verification, which will involve the generation of isotopic scattering matrices from Monte Carlo codes.

3. Comparison of resonance methods
Applications of the eigenvalue analysis include verifying the group structure and the resonance self-shielding methods. Moreover, the analysis can be used for mesh convergence study to visualize the trend in reaction rate when refining the mesh. This could be a helpful addition to optimize the calculation mesh by providing more detailed information, rather than a single $k_{\text{eff}}$ value that could bear error cancellations.

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