2D Neutron Diffusion Calculation Based on Local/Global Iterations Using Proper Orthogonal Decomposition

M. Ito^{a*}, T. Endo^a, A. Yamamoto^a, T. Takeishi^b, Y. Kodama^b, H. Nagano^b

^aNagoya University, Furo-cho, Chikusa-ku, Nagoya-shi, Aichi, 464-8603, Japan ^bNuclear Fuel Industries, Ltd., 1-950 AsashiroNishi, Kumatori-cho, Sennan-gun, Osaka, 590-0481, Japan ^{*}Corresponding author: ma-ito@fermi.energy.nagoya-u.ac.jp

1. Introduction

Proper orthogonal decomposition (POD) is а numerical analysis method to reduce the core calculation cost [1,2]. In the POD technique, to extract the main components in the neutron flux distribution, POD bases can be obtained by a data-driven method. By expanding the neutron flux with a few POD bases, the dimension of the target equation (e.g., discretized neutron diffusion equation) can be reduced. However, if the POD method is directly applied to the heterogeneous whole core calculation, a larger number of POD bases is required for sufficient accuracy, *i.e.*, the effectiveness of POD may be degraded. In this study, we proposed a new core calculation method by combining POD and local/global iteration [3,4] (hereafter referred to as the POD-LG). In the POD-LG, POD is applied to each single assembly calculation. Because a single assembly is smaller in size and has less heterogeneity than those of the whole core, a more effective application of POD to the assembly calculation is expected. In the present study, POD-LG is tested on the two-dimensional(2-D) colorset problem.

2. Numerical methods

2.1 Overview of POD-LG scheme

In the POD-LG, the single assembly fine mesh calculation using POD (local calculation) and the whole core coarse mesh calculation (global calculation) are alternately iterated. From the local and global calculation results, the local albedo boundary condition is updated on the surface of each of the assemblies.

2.2 Local calculation using POD

In the POD approach, the neutron flux distribution ϕ_g of the *g* th energy group in each of the assemblies is expanded by POD bases as follows:

$$\vec{\phi}_g = \sum_{i=1}^{NB} \vec{u}_{i,g} h_{i,g},\tag{1}$$

where NB is the total number of POD bases; $\vec{u}_{i,g}$ and $h_{i,g}$ represent the spatial distribution and the expansion coefficient for the *i* th POD base, respectively; the subscript g and *i* represent the energy group index and the order of the POD base, respectively.

In the local calculation using POD, the k_{eff} eigenvalue equation of the expansion coefficient $h_{i,g}$ is numerically solved under an albedo boundary condition, which is updated as explained in Sec. 2.4. The equation of the expansion coefficient $h_{i,g}$ is derived from the discretized

neutron diffusion equation [1,2]. Note that thanks to the POD, the dimension of the target equation can be reduced from the total number of spatial meshes *NR* to the total number of POD bases *NB*. Finally, the neutron flux distribution $\vec{\phi}_g$ in each of the assemblies can be reconstructed based on Eq. (1) with the obtained $h_{i,g}$.

2.3 Global calculation

The reconstructed $\vec{\phi}_g$ by the local calculation is used to obtain both the spatially homogenized cross section and the discontinuity factor (DF) for each of the assemblies. In the global calculation, the conventional CMFD calculation with the updated DF [5] is used in this study. The k_{eff} and the coarse mesh neutron flux on the whole core are obtained by the global calculation.

2.4 Update of albedo boundary condition

To obtain the albedo value, the surface neutron flux ϕ_s and the net neutron current J are necessary. First, as a result of the global calculation, $\overline{\phi}_s$ and \overline{J} are calculated at each of the assembly boundaries, where the bar represents the surface-averaged value. Note that the fine mesh distribution of ϕ_s and J cannot be calculated directly from the global calculation result. Thus, the spatial distribution of ϕ_s and J are estimated using the reconstructed $\overline{\phi}_g$ by the local calculation. However, the surface-averaged $\overline{\phi}_s$ and \overline{J} of the local calculation are not equal to those of the global calculation. Therefore, the following two different DFs for the surface neutron flux and the net neutron current are introduced.

$$FS = \bar{\phi}_s^G / \bar{\phi}_s^L, \qquad FJ = \bar{J}^G / \bar{J}^L, \qquad (2)$$

where the superscript L and G represent the results of the local and the global calculations, respectively.

Utilizing the two DFs (*FS*, *FJ*) and the reconstructed $\vec{\phi}_g$ by the local calculation, the fine mesh distributions of $\phi_{s,i}$ and J_i at the *i*-th spatial mesh on the assembly boundary are updated. The updated surface-averaged values for $\phi_{s,i}$ and J_i are equal to $\bar{\phi}_s^G$ and \bar{J}^G of the global calculation. Using these updated $\phi_{s,i}$ and J_i , incoming and outgoing neutron currents J_i^{in} and J_i^{out} are calculated. Finally, the albedo distribution of α_i can be estimated by $\alpha_i = J_i^{in}/J_i^{out}$. In this paper, this updating method for the albedo distribution is referred to as Non-linear iterative Updating fine Mesh Albedo (NUMA) method.

3. Numerical analysis

3.1 Calculation conditions

The 2-D colorset without control rods of the C5G7 benchmark problem [6]shown in Fig. 1 was used for the verification. The symbols (A) and (B) represent the UO₂ assembly and the MOX assembly, respectively. The GENESIS code [7,8] was used to prepare the pin-by-pin homogenized two-group cross section in advance. The total number of fine meshes in the single assembly was $17 \times 17 = 289$. The reference value was obtained by the fine mesh diffusion calculation for the heterogeneous colorset geometry. The numerical result was compared to the POD-LG which updates only surface-averaged albedo value obtained by the global calculation (hereafter referred to as the "POD-LG without NUMA method").



Fig. 1. Geometry of 2-D colorset

3.2 Pre-calculations to construct POD bases

The POD bases for each of the two assemblies were calculated independently. The snapshot data were prepared from the neutron fluxes in the assemblies by these single assembly calculations under various albedo boundary conditions, which were spatially uniform using random numbers for each assembly boundary. The total number of the POD bases was determined using Wilks' method [9] so that the absolute error of k_{eff} (k_{eff} error) and the relative root-mean-square error of the neutron flux (flux-RMSE) in the test single assembly calculations were less than or equal to 0.1% and 10pcm, respectively. In this verification, the total number of the POD bases for the UO₂ and MOX assemblies are 42 and 41, respectively. Thus, thanks to the POD, the dimension of the target equation can be reduced from 289 to around ~40.

3.3 Numerical results

The relative errors of the fast and thermal neutron flux distribution are shown in Fig. 2. The k_{eff} error and the flux-RMSE are summarized in Table I. Figure 2 and Table I indicate that the POD-LG using NUMA method can accurately reproduce the reference value. Namely, the spatial distribution of albedo value can be appropriately estimated by the NUMA method.

4. Conclusions

In this study, we proposed a new 2-D core calculation method by combining POD and local/global iteration. The POD-LG using the NUMA method was investigated for the 2-D colorset problem. As a result, we confirmed that our proposed method can accurately reproduce the reference value obtained by fine mesh calculation.



Table I: Calculation error

Method	POD-LG	POD-LG
	without NUMA	using NUMA
k _{eff} error [pcm]	50.68	0.07
flux-RMSE [%]	2.98	0.03

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