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Investigation on generalized Variational Nodal Methods for heterogeneous nodes

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ABSTRACT

The Variational Nodal Method (VNM) is generalized for heterogeneous nodes and applied to four kinds of problems including Molten Salt Reactor (MSR) core problem with continuous cross section profile, Pressurized Water Reactor (PWR) control rod cusping effect problem, PWR whole-core pin-by-pin problem, and heterogeneous PWR core problem without fuel-coolant homogenization in each pin cell. Two approaches have been investigated for the treatment of the nodal heterogeneity in this paper. To concentrate on spatial heterogeneity, diffusion approximation was adopted for the angular variable in neutron transport equation. To provide demonstrative numerical results, the codes in this paper were developed in slab geometry. The first method, named as function expansion (FE) method, expands nodal flux by orthogonal polynomials and the nodal cross sections are also expressed as spatial depended functions. The second path, named as finite sub-element (FS) method, takes advantage of the finite-element method by dividing each node into numbers of homogeneous sub-elements and expanding nodal flux into the combination of linear sub-element trial functions. Numerical tests have been carried out to evaluate the ability of the two nodal (coarse-mesh) heterogeneous VNMs by comparing with the fine-mesh homogeneous VNM. It has been demonstrated that both heterogeneous approaches can handle heterogeneous nodes. The FE method is good at continuous-changing heterogeneity as in the MSR core problem, while the FS method is good at discontinuous-changing heterogeneity such as the PWR pin-by-pin problem and heterogeneous PWR core problem. For problems with only one or two discontinuity points such as the PWR control rod cusping effect problem, both of the two methods can catch the effect with high efficiency.

1. Introduction

Modern nodal methods play an important role in reactor core neutronics calculation due to its high computation efficiency and accuracy (Wagner and Koebke, 1983). However, traditional nodal methods usually require cross-section homogenization within each node which unavoidably introduces errors or reduces the computational efficiency in the following scenarios.

Firstly, in new reactor design such as Molten Salt Reactor (MSR), the fluid fuel is continuously flowing. Continuous temperature and nuclide density distributions result in continuous cross section distribution in space especially in axial direction. Volume- or approximate flux-volume-weighted homogenization scheme within each node is needed if traditional nodal methods are employed. However, if we adopt volume-weighted homogenization scheme for the nodes, it will introduce obvious error to the flux distribution. In addition, accurate flux distribution cannot be obtained even the approximate flux-volume-weighted homogenization scheme is employed. Some tests have been done in the 'Results' part of this paper and we can find the most effective way for traditional nodal methods to reduce the error caused by homogenization is adopting fine nodal mesh, which will reduce the computational efficiency unfortunately.

Secondly, in the Pressurized Water Reactor (PWR) core, control rods keep moving along the axial direction with a step size of about 2 cm, while the nodal size of neutronics simulation is usually about 20 cm. It is common to have one or more control rods partially inserted into the corresponding nodes. In this case, a single node would consist of different materials with different macroscopic cross sections within the framework of the traditional two-step simulation method. The numerically simulated curve of control rod worth is not even a smooth curve but with a lot of wiggles. It is the so-called control rod cusping effect. Since 1980s, many

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methods have been investigated to eliminate it, such as flux-volume-weighted method (Yamamoto, 2004; Dall'Osso, 2002) and adaptive mesh method (Zhang, 2014). The former has to obtain an approximated flux distribution, while the later has to regenerate the spatial mesh after each control rod movement to avoid the appearance of heterogeneous nodes.

Thirdly, traditional PWR core computation employs two-step scheme: lattice calculation to provide assembly-homogenized cross sections, then core diffusion calculation and pin-power reconstruction to provide pin-power profile within the core. To reduce the error introduced by assembly homogenization and pin-power reconstruction, the following pin-by-pin scheme has caught the concentration: assembly calculation with pin-cell homogenization and then whole-core pin-by-pin calculation. Several pin-by-pin calculation codes have been developed, such as SCOPE2 (Tatsumi and Yamamoto, 2003) and EFEN (Li et al., 2014). However, the whole-core pin-by-pin problem consists of millions of meshes. Computational efficiency becomes one of main problems in whole-core pin-by-pin calculation. For example, a PWR can be divided into 10 million spatial meshes. Together with the SP_3 approximation and 4 energy groups, the calculation time is about 24 h for a single CPU (Yang et al., 2014) if there is no acceleration.

Fourthly, in recent years, High-Fidelity computing aims to carry out whole-core heterogeneous simulations with homogenization fully eliminated. In High-Fidelity computing of PWR, the heterogeneity within each pin-cell requires an extremely refined mesh which leads to the total number of spatial meshes becoming billions. The increase of spatial meshes does not only increase the number of unknowns, but also slows down the convergence. In this case, the convergence can be significantly improved if a heterogeneous coarse-mesh nodal method can be employed to replace the fine mesh methods.

To overcome difficulties from the above four scenarios, traditional homogeneous nodal methods are expected to be generalized into heterogeneous nodal methods to maintain the computing efficiency with high accuracy. Among those homogeneous nodal methods, Variational Nodal Method (Palmiotti et al., 1995) (VNM) is chosen due to its advantages (Lawrence, 1986; Wagner, 1989; Li et al., 2015) compared with the others. VNM is based on a functional for even-parity transport equation and the nodes are coupled together by odd-parity Lagrange multipliers. Response matrices are obtained by using a Ritz procedure and the flux, current and source are expanded by orthogonal polynomials. The exclusion of the transverse integration technique in VNM guarantees its advantages in accuracy.

Fanning and Palmiotti (Fanning and Palmiotti, 1997) developed a heterogeneous nodal method based on VNM for piece-wise constant heterogeneous nodes. The even- and odd-parity fluxes are expanded by polynomials. Throughout the derivation, the functional for the heterogeneous node is obtained which has the same form as that in homogeneous VNM. To calculate the response matrices, the heterogeneous node is divided into a number of homogeneous elements and then the integrals over the node are divided into a set of homogeneous integrals. This method has high efficiency with low expansion order. However, when the configuration and material is complicated within the heterogeneous node, the flux will change sharply in space. As the flux is expanded by polynomials over the entire node in this method, it's difficult for it to describe the flux distribution with sharp gradient accurately over the node. Smith (Smith et al., 2003) developed another heterogeneous Variational Nodal Method also for piece-wise constant heterogeneous nodes. It divides each node into sub-elements in which the cross sections are constants, and expands the flux by finite trial functions in space and spherical or simplified spherical harmonics in angle. In this method, high-order angular approximation is required to obtain accurate results in the problems with sharp flux gradient throughout the geometry, while the results are less sensitive to the refinement of the sub-elements. The main disadvantage of this method is the low computational efficiency when high spherical harmonics expansion order is adopted. Another heterogeneous nodal method for solving diffusion equation was developed by Makoto Tsuiki (Tsuiki and Hval, 2002). The most distinctive feature of this method is that the flux in a node is expanded into a set of functions which are numerically obtained by single-assembly calculations without assembly homogenization. Highly accurate results can be obtained because the assembly heterogeneous effect is taken into account in the single-assembly calculation. Besides, the accuracy of this method can be improved simply by increasing the order of expansion. However, computing the numerical expansion functions becomes an additional burden of the method.

This paper mainly concentrates on the spatial distribution of the flux and power affected by the heterogeneous node with diffusion approximation adopted. To assess the performances of different methods for different problems, we choose the one-dimensional (1D) slab geometry. In this paper, two approaches are investigated for the treatment of the nodal heterogeneity. In function expansion (FE) method, the flux is expanded into the sum of polynomials and the cross section is also expressed as a function of space. Additionally, unlike the method developed by Fanning and Palmiotti, the heterogeneous nodes needn't to be divided into homogeneous elements which means this method can treat both continuous and piecewise continuous cross section distribution. The finite sub-element (FS) method employs finite-element basis functions to expand flux in each node. In this method, the heterogeneous node should be divided into homogeneous sub-elements.

The rest of this paper is organized as following. In Section 2, the theories of two heterogeneous VNMs including the FE method and the FS method are introduced in 1D slab geometry for neutron-diffusion equation. In Section 3, the two methods are applied to the four kinds of problems: MSR core problem, PWR control rod cusping effect problem, PWR pin-by-pin problem and heterogeneous PWR core problem. The capabilities and limitations of these two methods are then discussed.

2. Theory

This basic theory of homogeneous VNM is presented in Palmiotti et al. (1995) and Li et al. (2015) clearly. Based on this, Sections 2.1 and 2.2 introduce the treatments for heterogeneous nodes in FE method and FS method respectively. The following theory is derived in 1D slab geometry with diffusion approximation.

2.1. The function expansion heterogeneous Variational Nodal Method

To treat the heterogeneous nodes in FE method, the cross sections are assumed to be functions of space. Then the diffusion functional for each node can be written as

$$F_v[\Phi,J]=\int_v dV\left\{D(x)\left(\frac{d}{dx}\Phi(x)\right)^2+(\Sigma_t(x)-\Sigma_s(x))\Phi(x)^2-2\Phi(x)S(x)\right\}+2\sum_{\gamma=1}^{2}\Phi(x)J(x). \tag{1}$$

where Φ is the scalar flux ($cm^{-2}\cdot s^{-1}$); D is the diffusion coefficient (cm); Σ_t is the total cross section (cm^{-1}); Σ_s is the within-group scattering cross section (cm^{-1}); S is the source term ($cm^{-3}\cdot s^{-1}$) including isotropic scattering and fission; γ represents the surfaces