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Three-Dimensional Variational Nodal Method with Finite Sub-element Treatment for Heterogeneous Nodes

Yongping Wang, Hongchun Wu and Yunzhao Li*
School of Nuclear Science and Technology
Xi'an Jiaotong University
28 West Xianning Road, Xi'an, Shaanxi 710049, China

*Corresponding author: Yunzhao Li
Email: yunzhao@mail.xjtu.edu.cn

1. Introduction

Nodal methods[1] typically utilize homogeneous cross section for assembly-size nodes. For this requirement, homogenization is needed for each node which may introduces errors or even decreases the computational efficiency. To eliminate the need of homogenization in a node, several methods for treating heterogeneous nodes have been developed. Fanning and Palmiotti[2] developed a heterogeneous nodal method based on Variational Nodal Method (VNM)[3]. It separates each of the integrals over the heterogeneous node into a set of homogeneous integrals according to the piece-wise flat distributed cross section to obtain the response matrices. However, it is difficult for this method to obtain satisfactory results in problems with large flux gradient. Smith[4] developed a heterogeneous nodal method which divides the nodes into sub-elements and expands the flux by finite element trial functions in space. This method obtains accurate results in the problems with large flux gradient. Another method for heterogeneous treatment was developed by Makoto Tsuiki[5]. 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. However, computing the numerical expansion functions becomes an additional burden of this method.

After our former work on heterogeneous nodal methods[6, 7], this paper derives a finite sub-element method based on VNM with diffusion approximation in three-dimensional Cartesian geometry. Tetrahedron sub-elements are used to describe explicitly the heterogeneous assembly with pin-by-pin cross sections. So the heterogeneity in a node is allowed in this method which is quite different from existing homogeneous VNM. In addition, Flux and source in the nodes as well as net current in the nodal surfaces are expanded with finite trial functions.

2. Theory

The three-dimension within-group diffusion equation is:

$$\begin{cases} \nabla \cdot \boldsymbol{J}(\boldsymbol{r}) + \Sigma_t(\boldsymbol{r})\Phi(\boldsymbol{r}) = \Sigma_s(\boldsymbol{r})\Phi(\boldsymbol{r}) + S(\boldsymbol{r}) \\ \frac{1}{3}\nabla\Phi(\boldsymbol{r}) + \Sigma_t(\boldsymbol{r})\boldsymbol{J}(\boldsymbol{r}) = 0 \end{cases} \tag{1}$$

where Φ is the scalar flux ($cm^{-2}\cdot s^{-1}$), $\boldsymbol{J}$ is net current ($cm^{-2}\cdot s^{-1}$), Σ_t is the total cross section (cm^{-1}), Σ_s is the within-group scattering cross section (cm^{-1}), and S is the source term ($cm^{-3}\cdot s^{-1}$) including scattering and fission.

Same as the homogeneous VNM, the entire problem domain is decomposed into subdomains V_v (nodes) and the functional can be written as a superposition of nodal contributions:

$$F[\Phi, J] = \sum_v F_v[\Phi, J] \tag{2}$$

However, to consider the nodal heterogeneity in this method, each node is further divided into a set of homogeneous sub-regions named sub-elements. That's the main difference between current VNM and this method. The nodal functional is then written as a superposition of sub-element functional:

$$F_v[\Phi, J] = \sum_e F_e[\Phi_e, J] \tag{3}$$

where the element functional is written as:

$$F_e[\Phi_e, J] = \int_e dV\{D_e(\nabla\Phi_e)^2 + (\Sigma_{t,e} - \Sigma_{s,e})\Phi_e^2 - 2\Phi_e S_e\} + 2\sum_\gamma \int_\gamma \Phi_{e,\gamma} J_{e,\gamma} d\Gamma \tag{4}$$

The surface term in Eq. (4) only appears in those sub-elements adjacent to nodal interfaces because continuous trial functions are used within each node.

We expand the flux and source within the sub-element and net current along the sub-element's surfaces as:

$$\begin{cases} \Phi_e(\boldsymbol{r}) = \sum_{m=1}^{M} \varphi_{e,m} f_{e,m}(\boldsymbol{r}) \\ S_e(\boldsymbol{r}) = \sum_{m=1}^{M} s_{e,m} f_{e,m}(\boldsymbol{r}) \quad , \boldsymbol{r} \in e \\ J_{e,\gamma}(\boldsymbol{r}) = \sum_{n=1}^{N} j_{e,\gamma,n} h_{e,\gamma,n}(\boldsymbol{r}) \end{cases} \tag{5}$$

Different from polynomial expansion in the current homogeneous VNM, $\boldsymbol{f}(\boldsymbol{r})$ and $\boldsymbol{h}(\boldsymbol{r})$ are the finite element trial functions defined in the volume and on the surfaces. $\boldsymbol{\varphi}$, $\boldsymbol{s}$ and $\boldsymbol{j}$ are the unknown coefficients. *M* and *N* respectively represent the number of nodes within the sub-element and on its surface. For the cross sections in each element are homogeneous, the relationship between flux and source moments is written as:

$$s_{e,m} = \left(\Sigma_e + \frac{1}{k} v\Sigma_{f,e} \right) \varphi_{e,m} \tag{6}$$

Substituting Eq. (6) into the element functional in Eq. (4) yields the reduced functional:

$$F_e[\boldsymbol{\varphi}, \boldsymbol{j}] = \boldsymbol{\varphi}_e^{\mathrm{T}} \boldsymbol{A}_e \boldsymbol{\varphi}_e - 2\boldsymbol{\varphi}_e^{\mathrm{T}} \boldsymbol{F}_e \boldsymbol{s}_e + 2\boldsymbol{\varphi}_e^{\mathrm{T}} \boldsymbol{M}_e \boldsymbol{j}_e \tag{7}$$

where

$$A_{e,mm'} = \int_e \left\{ D_e \cdot \nabla f(\boldsymbol{r})_{e,m} \cdot \nabla f_{e,m'}(\boldsymbol{r}) + \left(\Sigma_{t,e} - \Sigma_{s,e} \right) f_{e,m}(\boldsymbol{r}) f_{e,m'}(\boldsymbol{r}) \right\} dV \tag{8}$$

$$F_{e,mm'} = \int_e f_{e,m}(\boldsymbol{r}) f_{e,m'}(\boldsymbol{r}) dV \tag{9}$$

$$M_{e,mn'} = \int_\gamma f_{e,m}(\boldsymbol{r}) h_{e,\gamma,n'}(\boldsymbol{r}) d\Gamma \tag{10}$$

To obtain the nodal functional, we should use the Boolean transformation matrix Ξ_e to map the element trial function coefficients to the nodal expansion coefficients:

$$\boldsymbol{\varphi}_e = \Xi_e \boldsymbol{\varphi} \tag{11}$$

Substituting Eq. (11) into Eq. (7), and then substituting Eq. (7) into Eq. (2) leads to the nodal functional:

$$F_v[\boldsymbol{\varphi}, \boldsymbol{j}] = \boldsymbol{\varphi}^{\mathrm{T}} \boldsymbol{A} \boldsymbol{\varphi} - 2\boldsymbol{\varphi}^{\mathrm{T}} \boldsymbol{s} + 2\boldsymbol{\varphi}^{\mathrm{T}} \boldsymbol{M} \boldsymbol{j} \tag{12}$$

where

$$\boldsymbol{A} = \sum_e \Xi_e^T \boldsymbol{A}_e \Xi_e \tag{13}$$

$$\boldsymbol{s} = \sum_e \Xi_e^T \boldsymbol{F}_e \boldsymbol{s}_e \tag{14}$$

$$\boldsymbol{M} = \sum_e \Xi_e^T \boldsymbol{M}_e \tag{15}$$

As we obtain the nodal functional, the following derivation is same as that in homogeneous VNM. Taking the variation of the response matrix formulation, Eq. (12) with respect to $\boldsymbol{\varphi}$ and setting the variation to zero yields:

$$\boldsymbol{\varphi} = \boldsymbol{A}^{-1} \left(\boldsymbol{s} - \boldsymbol{M} \boldsymbol{j} \right) \tag{16}$$

The variation with respect to $\boldsymbol{j}$ yields the condition that

$$\psi_\gamma = \boldsymbol{M}_\gamma^{\mathrm{T}} \boldsymbol{\varphi} \tag{17}$$

be continuous across each nodal interface. Define the partial currents as:

$$j_\gamma^{\pm} = \frac{1}{4} \psi_\gamma \pm \frac{1}{2} j_\gamma \tag{18}$$

substituting Eq. (18) into Eq. (16) and Eq. (17) we can obtain the response matrix equation:

$$\boldsymbol{j}^+ = \boldsymbol{B}\boldsymbol{s} + \boldsymbol{R}\boldsymbol{j}^- \tag{19}$$

$$\boldsymbol{\varphi} = \boldsymbol{H}\boldsymbol{s} - \boldsymbol{C}\left(\boldsymbol{j}^+ - \boldsymbol{j}^- \right) \tag{20}$$

where

$$\boldsymbol{B} = \frac{1}{2}\left[\boldsymbol{G} + \boldsymbol{I} \right]^{-1} \boldsymbol{C}^{\mathrm{T}} \tag{21}$$

$$\boldsymbol{R} = \left[\boldsymbol{G} + \boldsymbol{I} \right]^{-1} \left[\boldsymbol{G} - \boldsymbol{I} \right] \tag{22}$$

$$G_{\gamma\gamma'} = \frac{1}{2} \boldsymbol{M}_\gamma^{\mathrm{T}} \boldsymbol{A}^{-1} \boldsymbol{M}_{\gamma'} \tag{23}$$

$$C_\gamma^{\mathrm{T}} = \boldsymbol{M}_\gamma^{\mathrm{T}} \boldsymbol{A}^{-1} \tag{24}$$

$$\boldsymbol{H} = \boldsymbol{A}^{-1} \tag{25}$$

Eq. (19) and Eq. (20) are used to update the moments of partial current and scalar flux. The moments of source are updated by Eq. (6).

3. Results

A code named Violet-Het3D has been developed to treat 3D problems in Cartesian geometry with heterogeneous nodes based on the theory aforementioned. To demonstrate the accuracy of the Violet-Het3D, a PWR pin-by-pin problem was formulated to test the treatment of heterogeneous nodes in the code.

The radial core configuration of the problem is shown in Fig. 1. Each pin is 1.26 cm in length and width, and the moderator region is 21.46 cm. In axial direction, the fuel region is 60 cm in height and there is a moderator region (9 cm thick) both at the top and the bottom of the core. The cross sections in each pin are homogenized. Ideally the neutron-transport equation should be solved in this problem. However in order to evaluate Violet-Het3D's ability of treating spatial heterogeneity, the neutron-diffusion equation was solved for demonstration purpose. The reference calculation takes each individual pin as a node in radial, while the Violet-Het3D treats an entire assembly as a single node with heterogeneous structure inside. Both calculations take 3 cm as the height of each node, so the entire problem is divided into 26 layers in total. In addition, it's a two-energy group problem.

The reference model treats each pin as a node (including reflector assembly), so the whole problem

consists of 67626 nodes. And the reference solution is obtained by the code named Violet-Hom3D which adopts the theory of homogeneous VNM. While the Violet-Het3D calculation only employs 234 nodes. As shown in Fig. 2, each assembly (including reflector assembly) in Violet-Het3D calculation is divided into tetrahedrons by the commercial program called Freefem[8] which is not needed in the reference calculation. Tetrahedron is chosen for its good geometrical adaptability. And it can be found in Fig. 2 that each pin consists of 6 tetrahedrons which is enough to describe explicitly the heterogeneous assembly. Further refining the tetrahedrons will greatly decrease the computing efficiency and obtain little improvement for the result. The results of k_{eff} are shown in table I and the power distribution is shown in Fig. 3. Table II shows the difference of the power distribution compared with the reference and Violet-Het3D obtains accurate results obviously.

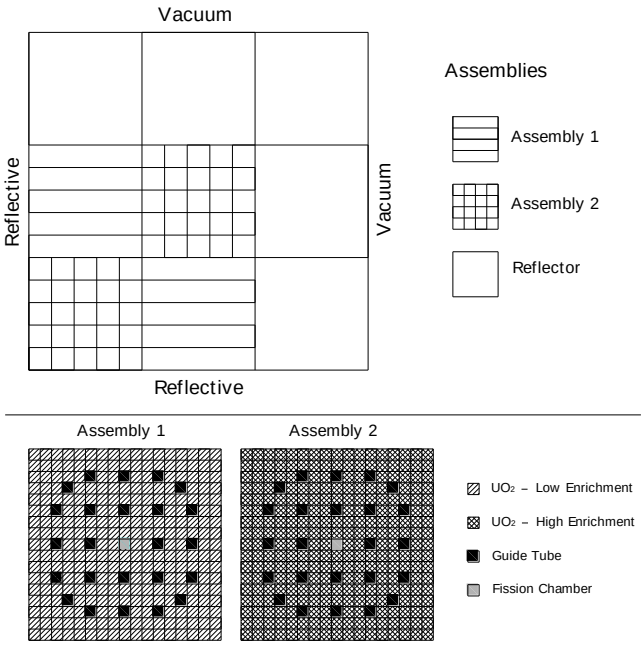

Fig. 1. Radial core and assembly configuration

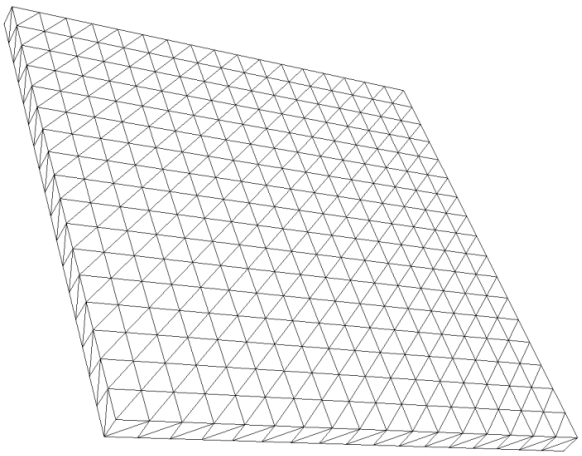

Fig. 2. Sub-elements configuration in each layer of the assembly

Table I. k_{eff} Comparison for the pin-by-pin problem

	Reference	Violet-Het3D	Error / pcm
k_{eff}	1.00438	1.00350	-88

Table II. Power Comparison of the pin-by-pin problem

Case	Reference	Violet-Het3D	Error/%
Maxpower	2.8410	2.8430	0.07
Minpower	0.0756	0.0748	-1.06
MaxError	-	-	1.5

The average error of power distribution is below 1.0% and the regions closed to moderator usually have low power and relatively high error. The positions of the maximum power, minimum power and maximum error are shown in Fig. 4.

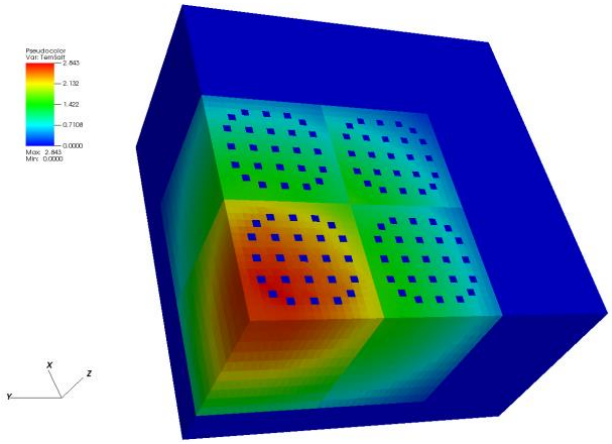

Fig. 3. Power distribution of the pin-by-pin problem

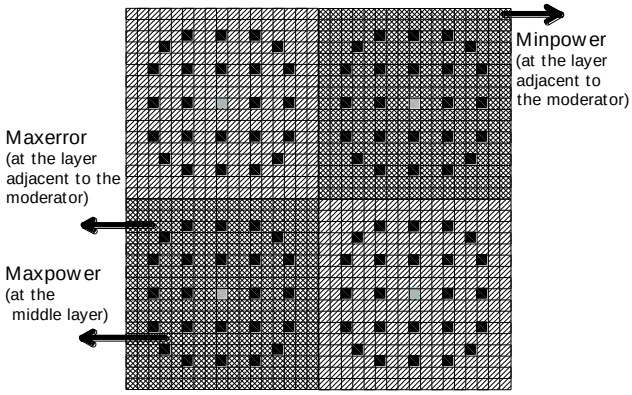

Fig. 4. Positions of the maximum power, minimum power and maximum error

4. Conclusions

This paper derives a finite sub-element method based on VNM with diffusion approximation in three-dimension Cartesian geometry. The Violet-Het3D has been developed and a pin-by-pin problem was calculated. The numerical results show that high accuracy can be obtained with the treatment for heterogeneity. The maximum relative error of the 3D pin power distribution is about 1.5% at the pin adjacent to the moderator region

at the bottom of the core. However, this method currently costs more time than what we expected for computing the pin-by-pin problem. The corresponding analysis and techniques to overcome this problem is on the way. Additionally, Violet-Het3D will be expanded to the neutron-transport equation in the future.

Acknowledgements

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