Heterogeneous Variational Nodal Method with Continuous Cross Section Distribution in Space

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INTRODUCTION

According to the optical thickness of the mesh, numerical methods for solving neutron diffusion equation can be simply classified into fine mesh methods and coarse mesh methods. Fine mesh methods employ linear or other lower order approximations for the detailed neutron flux within each mesh. It is this approximation that makes these algorithms insufficiently accurate for large meshes. Hence, the number of grids in fine mesh methods is usually tremendously large for reactor core problems. In contrast, coarse mesh methods employ high order approximations within each mesh (named a node), which provides high computing efficiency. Consequently, coarse mesh methods such as nodal methods play an important role in reactor core neutronics simulation.

Both fine and coarse mesh methods assume a homogeneous distribution of cross section within each mesh, which requires the spatial homogenization. It works well for traditional PWR with the legacy neutronics simulation schemes [1]. However, new reactor concepts such as Molten Salt Reactor (MSR) [2] and the improved computing schemes such as pin-by-pin calculations [3] are demanding the improvement of coarse mesh methods to treat heterogeneous distribution of cross section within each mesh. For instance, heterogeneous [4] and sub-element [5, 6] variational nodal methods were developed to carry out whole assembly heterogeneous calculation. Heterogeneous Nodal Expansion Method [7] was designed to capture the differential worth of control rods without control rod cusping effect [8, 9].

Instead of homogeneous cross section distribution, these heterogeneous methods can handle piece wise cross section distribution within each node. However, simulation with continuous cross section distribution still remains unresolved. Unfortunately, this occurs in the Molten Salt Reactor [2] core. Due to the continuous change of fuel temperature and density, neutron cross section varies continuously in space. It is this application that motivates our investigation of heterogeneous variational nodal method with continuous distribution of cross section in one dimensional Cartesian space.

THEORETIC MODEL

In one dimensional slab geometry, one group steady state neutron diffusion equation with isotropic scattering and fission is:

$$\begin{cases} \dfrac{d}{dx}J(x)+\Sigma_t(x)\Phi(x)=\Sigma_s(x)+S(x) \\ \dfrac{1}{3}\dfrac{d}{dx}\Phi(x)+\Sigma_t(x)J(x)=0 \end{cases} \tag{1}$$

where the source

$$S(x)=\frac{1}{k}\Sigma_f(x)\Phi(x), \tag{2}$$

$J(x)$ and $\Phi(x)$ respectively refer to net current and flux profile (cm^{-2}·s^{-1}), $\Sigma_s(x)$ and $\Sigma_f(x)$ stands for macroscopic absorption and fission cross section (cm^{-1}), and k is the effective multiplication factor.

The functional similar with the one for homogeneous node is as following:

$$F[\Phi,J]=\sum_v F_v[\Phi,J] \tag{3}$$

And the contribution from node v is

$$F_v[\Phi,J] = \int_v dV\left[\frac{1}{3\Sigma_t}\left(\frac{d\Phi}{dx}\right)^2+\Sigma_a\Phi^2-2\Phi S\right]+2(\Phi J)_{x=x_l}^{x=x_r} \tag{4}$$

where $\Sigma_a(x)= \Sigma_t(x) - \Sigma_s(x)$. Similar with the homogeneous variational nodal method [10], it can be proved that the Euler-Lagrange equation of the functional in Eq. (4) is the diffusion equation in Eq. (1).

Apply Ritz procedure by approximating the volume flux and source as expansions of orthogonal spatial trial functions with unknown coefficients:

$$\begin{cases} \Phi(x)=\sum_i \varphi_i f_i(x) \\ s(x)=\sum_i s_i f_i(x) \end{cases}. \tag{5}$$

Substituting Eq. (5) into Eq. (2) leads to the relationship between the flux and source moments:

$$s_i=\frac{1}{k}\sum_{i'}\varphi_{i'}\Sigma_{f,ii'} \tag{6}$$

where

$$\Sigma_{f,ii'}=\int_v \Sigma_f(x)f_i(x)f_{i'}(x)dx\,. \tag{7}$$

Substituting Eq. (5) into Eq. (4) yields:

$$F_v[\boldsymbol{\varphi},\boldsymbol{j}]=\boldsymbol{\varphi}^{\mathrm{T}}\boldsymbol{A}\boldsymbol{\varphi}-2\boldsymbol{\varphi}^{\mathrm{T}}\boldsymbol{s}+2\boldsymbol{\varphi}^{\mathrm{T}}\boldsymbol{M}\boldsymbol{j}\,. \tag{8}$$

where $\boldsymbol{\varphi}$, $\boldsymbol{j}$ and $\boldsymbol{s}$ are vectors over the entire node constructed by the respective expansion moments, the matrix

$$A_{ii'} = \int_v dx \left[\frac{1}{3\Sigma_t(x)} \frac{df_i(x)}{dx} \frac{df_{i'}(x)}{dx} + \Sigma_a(x) f_i(x) f_j(x) \right] \quad (9)$$

$$M_{i\gamma} = f_i(x)\big|_{x=x_\gamma} \quad (10)$$

Requiring the function to be stationary with respect to variations in $\boldsymbol{\varphi}^{\mathrm{T}}$ yields:

$$\boldsymbol{\varphi} = \boldsymbol{A}^{-1}(\boldsymbol{s} - \boldsymbol{M}\boldsymbol{j}) \quad (11)$$

The variation with respect to j_γ yields the requirement that:

$$\psi_\gamma = \boldsymbol{M}_\gamma^{\mathrm{T}} \boldsymbol{\varphi} \quad (12)$$

be continuous. Define the partial currents as:

$$j_\gamma^{\pm} = \frac{1}{4}\psi_\gamma \pm \frac{1}{2} j_\gamma \quad (13)$$

and substituting Eq. (11) into Eq. (12) leads to the nodal response matrix equations:

$$\boldsymbol{j}^{+} = \boldsymbol{B}\boldsymbol{s} + \boldsymbol{R}\boldsymbol{j}^{-} \quad (14)$$

$$\boldsymbol{\varphi} = \boldsymbol{H}\boldsymbol{s} - \boldsymbol{C}\left(\boldsymbol{j}^{+} - \boldsymbol{j}^{-}\right) \quad (15)$$

where

$$\boldsymbol{B} = \frac{1}{2}[\boldsymbol{G} + \boldsymbol{I}]^{-1} \boldsymbol{C}^{\mathrm{T}} \quad (16)$$

$$\boldsymbol{R} = [\boldsymbol{G} + \boldsymbol{I}]^{-1}[\boldsymbol{G} - \boldsymbol{I}] \quad (17)$$

$$G_{\gamma\gamma'} = \frac{1}{2} \boldsymbol{M}_\gamma^{\mathrm{T}} \boldsymbol{A}^{-1} \boldsymbol{M}_{\gamma'} \quad (18)$$

$$\boldsymbol{C}_\gamma^{T} = \boldsymbol{M}_\gamma^{\mathrm{T}} \boldsymbol{A}^{-1} \quad (19)$$

$$\boldsymbol{H} = \boldsymbol{A}^{-1}. \quad (20)$$

The heterogeneous variational nodal method can be implemented using Eqs. (6), (14) and (15). The treatment of boundary conditions are the same as in literature [10]. The difference between homogeneous and heterogeneous variational nodal methods lies in Eqs. (7), (9) and (10).

Numerical Results

Based on the above theory and formulas, a code named Violet has been developed in FORTRAN. According to the design of Molten Salt Reactor [2], a one dimensional MSR core problem is designed and used to test the heterogeneous variational nodal method.

The one dimensional MSR core problems is 400 cm long with local coordinate origin located as the bottom. Vacuum boundary condition is applied to both top and bottom. One group macroscopic cross sections are:

$$\Sigma_\gamma(x) = 0.2 \times (1 + 0.0001x),\ x \in [0,400] \text{ cm} \quad (21)$$

$$\Sigma_f(x) = 0.1 \times (1 + 0.0001x),\ x \in [0,400] \text{ cm} \quad (22)$$

$$\Sigma_s(x) = 0.5 \times (1 + 0.0001x),\ x \in [0,400] \text{ cm}. \quad (23)$$

A reference solution is obtained from homogeneous variational nodal method. It divides the entire domain into 80 regions and assumes a flat cross section distribution within each 5 cm node. The multiplication factor is 0.666603. The detailed flux profile is shown in Fig. 1.

The heterogeneous variational nodal method divides the entire domain into 8 nodes with each node 50 cm wide. Within each node, a cubic flux expansion was employed. The multiplication factor is 0.666602, which is only 0.1 pcm different from the reference solution. The flux profile in Fig. 1 demonstrates the agreement of it with the reference solution.

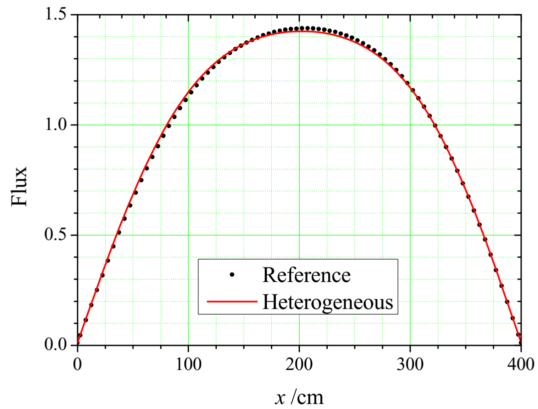

Fig. 1 Flux profiles of Vacuum-Vacuum B.C..

In addition, another case was also used to test the code. The only difference between the second and the first cases is the boundary condition on the top. Instead of vacuum, reflective boundary condition is set. A cubic detailed flux expansion was also employed in the heterogeneous calculation. Both the reference k_{eff} and the one from heterogeneous nodal method are 0.666644. The agreement of their flux profiles can be found in Fig. 2.

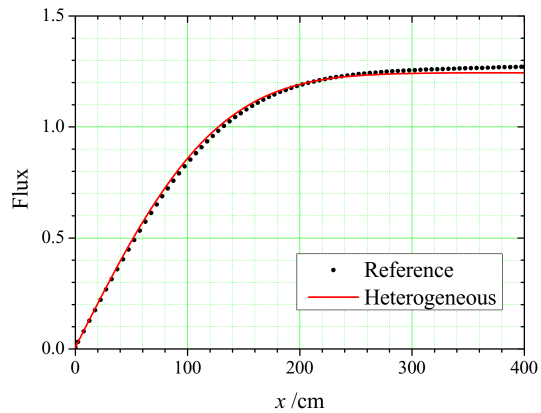

Fig. 2 Flux profile with Vacuum-Reflective B.C..

CONCLUSION

To handle continuous cross section distribution, heterogeneous variational nodal method is investigated in one dimensional Cartesian space. A one dimensional test problem has been used to verify the theory and code developments. Promising results demonstrate their reliability.

However, this investigation is still pretty initial. More analysis in one dimensional case and further development in multi-dimensional cases are required in the future.

ACKNOWLEDGMENT

This work was financially supported by the National Natural Science Foundation of China (11305123).

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