[Annals of Nuclear Energy 117 \(2018\) 114–130](https://doi.org/10.1016/j.anucene.2018.03.019)

Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

Adaptive expansion order for diffusion Variational Nodal Method

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article info

Article history: Received 13 October 2017 Received in revised form 23 January 2018 Accepted 14 March 2018 Available online 21 March 2018

Keywords: PWR core neutron-diffusion calculation Variational Nodal Method Adaptive technique CMFD NECP-Bamboo

ABSTRACT

The Variational Nodal Method (VNM) has been employed as the diffusion module in our PWR core analysis code Bamboo-Core within our PWR fuel management code system NECP-Bamboo. It expands the nodal volumetric flux and surface partial currents into the sums of orthogonal basis functions without using the transverse integration technique. To reduce the extra computing cost by the uniform expansion order setting, an adaptive expansion order technique has been developed in this paper. After estimating the net currents between each pair of neighboring nodes by using the Coarse-Mesh Finite-Difference (CMFD) technique, it estimates the required expansion orders in each node analytically. This technique increases the complexity of the code, but reduces the computational efforts both in computing time and memory storage by a factor of about 5 and 4, respectively. In addition, the CMFD acceleration is also employed to further improve the performance of the code. It is demonstrated by the numerical results that the CMFD acceleration technique can provide a speedup ratio of about 17.

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1. Introduction

As the key component of the Pressurized Water Reactor (PWR) software for nuclear power plants, core analysis code indicates the nuclear power development. Hence, Nuclear Engineering Computational Physics Lab. (NECP) in Xi'an Jiaotong University, China developed a PWR core analysis code Bamboo-Core within our PWR fuel management code system NECP-Bamboo ([Li et al.,](#page--1-0) [2015\)](#page--1-0). Currently, it contains several modules including a generalized cross section module, diffusion module using the Variational Nodal Method (VNM) [\(Li, 2017; Lewis and Miller, 1984; Carrico](#page--1-0) [et al., 1992\)](#page--1-0), depletion calculation using the traditional macroscopic and microscopic models, thermal-hydraulics module solving the parallel multi-channel heat transfer equation and 1D heat conduction equation.

The VNM was first developed by Northwestern University and Argonne National Laboratory (ANL) to solve the multi-group (MG) steady-state neutron-diffusion and -transport equations mainly for fast reactor core calculations. It uses a variational principle for the even-parity form of the Boltzmann neutron-transport equation. In this variational principle, the odd-parity Lagrange multipliers defined along the nodal interfaces guarantee neutron conservation for each node. The classical Ritz variation method is employed with orthogonal polynomials in space and spherical harThe VARIANT code ([Palmiotti et al., 1995\)](#page--1-0), developed at ANL in mid 90 s, is the first production code based on the Varitational Nodal Method. It has been employed by both the REBUS code [\(Toppel](#page--1-0) [and Capability, 1983\)](#page--1-0) in ANL and the ERANOS code [\(Doriath](#page--1-0) [et al., 1001](#page--1-0)) in Europe for routinely fast reactor core design. In 2007, a new version of the VARIANT code named NODAL was developed in ANL as one of the solvers in the UNIC package ([Palmiotti et al., 2007; Li, 2013\)](#page--1-0). In 2011, it has also been implemented into the INSTANT code [\(Wang et al., 2011](#page--1-0)) in Idaho National Laboratory (INL) as a solver of RattleSnake ([DeHart](#page--1-0) [et al., 2016](#page--1-0)). In 2014; the VNM code NECP-Violet [\(Wang et al.,](#page--1-0) [2014; Wang et al., 2016; Li et al., 2015](#page--1-0)) was developed as the neutron diffusion module of the Bamboo-Core code for PWR core calculation due to its advantages in control rod cusping effect elimination, pin power reconstruction, consistency of the mathematical and physical adjoint fluxes. Additionally, the NECP-Violet code was then extended to solve the neutron transport equation in hexagonal-z geometry [\(Li et al., 2017](#page--1-0)), to be employed as the solver of our fast reactor core calculation code system NECP-SARAX ([Du et al., 2017](#page--1-0)).

monics in angle. Nodal response matrices then can be formed for the volumetric flux moments and surface partial current moments.

Different from fast reactor core neutron transport applications, PWR core neutron diffusion calculation has to provide not only the assembly- or node-averaged power distribution, but also the pinwise power or flux distribution within each node or assembly. Especially for VNM, the detailed flux distribution within each node is expected to be provided directly by constructing the expansion

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moments and the basis functions together, which is different from other nodal diffusion methods with transverse integration. However, high-accuracy especially for the pin-wise distribution requires high-order polynomial expansion in space, which further increases the spatial polynomial expansion order compared with the traditional PWR core nodal methods. Of course, it costs more computing time and memory storage.

In fact, however, high-order expansion is unnecessary for each node to obtain the same level of accuracy. The key issue is how to identify the nodes that require high-order. Generally speaking, the more rugged the nodal flux distribution is, the higher expansion order would be required.

To reduce the extra computing cost by the uniform expansion order setting, Dr. Zhang developed an adaptive technique for the within-group (WG) iteration [\(Zhang et al., 2001; Zhang and](#page--1-0) [Lewis, 2002\)](#page--1-0) in 2001 and 2002. It adjusts the expansion order on nodal surface with the volumetric expansion order fixed. A posteriori error estimator ([Zamonsky et al., 2000; Zienkiewicz and Zhu,](#page--1-0) [1992; Zienkiewicz and Zhu, 1997](#page--1-0)) after each WG iteration was employed to estimate the best active surface expansion order. This method does reduce the time of iteration, but still has to construct the response matrixes with full expansion orders, leaving the nodal response matrix construction computing time and storage requirement unreduced. Considering the facts that the code spends more than 90% storage memory on response matrixes and that the calculation of response matrixes costs much more time than the iteration process in the application cases of NECP-Violet especially for a depleted core analysis, the effectiveness of the adaptive technique was limited.

Consequently, we developed a new polynomial expansion order adaptive technique before nodal response matrixes calculation by pre-estimating the effective multiplication factor and the surface net currents. The Coarse-Mesh Finite-Difference (CMFD) is employed to estimate those quantities. As a byproduct, the CMFD ([Zimin et al., 1998; Smith, 1986; Zimin and Ninokata, 1997;](#page--1-0) [Engrand and Maldonado, 1992; Smith, 1983; Joo, 1998; Hotta](#page--1-0) [et al., Nov. 1999; Moon et al., 1999\)](#page--1-0) acceleration for VNM was also investigated to further improve the performance of the code.

The rest of this paper is organized as following. Section 2 describes the theory of the adaptive technique together with the CMFD acceleration. Section [3](#page--1-0) assesses the adaptive technique and CMFD acceleration numerically by using two typical PWR core calculation problems. Section [4](#page--1-0) makes the summary.

2. Theoretical formulation

Before the adaptive technique is described in detail, we will introduce the Variational Nodal Method (VNM) in Sections 2.1 and 2.2, and the Coarse-Mesh Finite-Difference (CMFD) acceleration in Section [2.3](#page--1-0) as the foundation of the adaptive technique in Sections [2.4 and 2.5.](#page--1-0)

2.1. The VNM Method

The VNM theory starts with the three-dimensional (3D) multigroup neutron-diffusion equation with its albedo boundary condition:

$$
-\nabla\cdot D_g\nabla\Phi_g(\boldsymbol{r})+\Sigma_{r,g}\Phi_g(\boldsymbol{r})=\Sigma_{s,g}\Phi_g(\boldsymbol{r})+S_g(\boldsymbol{r}), g=1,\sim,G\qquad \quad (1)
$$

$$
S_{g}(\mathbf{r}) = \sum_{g' \neq g}^{G} \sum_{g'' \sim g} \Phi_{g'}(\mathbf{r}) + \frac{\chi_{g}}{k_{eff}} \sum_{g'=1}^{G} \nu \Sigma_{f,g'} \Phi_{g'}(\mathbf{r})
$$
(2)

$$
\Phi_{g} - 2\mathbf{J}_{g}^{\mathrm{T}} \mathbf{n}_{\gamma} = \beta_{\gamma g} \cdot (\Phi_{g} + 2\mathbf{J}_{g}^{\mathrm{T}} \mathbf{n}_{\gamma})
$$
\n(3)

where g and g' is the energy group index, G is the total number of energy groups, D_g is the diffusion coefficient (cm⁻¹), $\Sigma_{r,g}$ is the transport corrected removal cross section (cm^{-1}) , $\Sigma_{g'\to g}$ is the scatting cross section (cm⁻¹) from group g' to group g, χ_{g} is the fission neutron spectrum, k_{eff} is effective multiplication factor, v is the average number of fission neutrons per fission, Σ_{fg} is the fission cross section (cm⁻¹), **r** is the spatial coordinate (cm), $\Phi_{g}(\mathbf{r})$ is volu-
metric flux (cm⁻² s⁻¹), S (**r**) is volumetric source (cm⁻² s⁻¹), vis the metric flux $(\text{cm}^{-2} \cdot \text{s}^{-1})$, $S_g(\mathbf{r})$ is volumetric source $(\text{cm}^{-2} \cdot \text{s}^{-1})$, γ is the surface index β is the albedo, and **r** is the unit pormal vector of surface index, $\beta_{\gamma g}$ is the albedo, and \mathbf{n}_{γ} is the unit normal vector of surface γ .

On the basis of Galerkin variational principle, the neutrondiffusion equation (coordinate index omitted) turns out to be:

$$
F[\Phi_{g}, \mathbf{J}_{g}] = \sum_{v} F_{v}[\Phi_{g}, \mathbf{J}_{g}] \tag{4}
$$

And the node ν contribution

$$
F_{\nu}[\Phi_{g}J_{g}] = \int_{\nu} dV \{ D \nabla \Phi_{g} \nabla \Phi_{g} + \Sigma_{r,g} \Phi_{g}^{2} - 2 \Phi_{g} S_{g} \} + 2 \sum_{\gamma=1}^{6} \int_{\gamma} \Phi_{g} J_{g}^{T} \mathbf{n}_{\gamma} d\Gamma
$$
\n(5)

where $J_g = -D_g \nabla \Phi$ is a vector containing the surface net outgoing current.

For each energy group and each node, the flux and source are expanded as:

$$
\Phi_{\mathbf{g}}(\mathbf{r}) = \sum_{i=1}^{I} \varphi_{i\mathbf{g}} f_i(\mathbf{r}) = \mathbf{f}^{\mathrm{T}} \boldsymbol{\varphi}_{\mathbf{g}}
$$
\n(6)

$$
S_{g}(\mathbf{r}) = \sum_{i=1}^{I} s_{i,g} f_{i}(\mathbf{r}) = \mathbf{f}^{\mathrm{T}} \mathbf{s}_{g}
$$
\n(7)

And the surface net current is expanded as

$$
\boldsymbol{J}_{g}^{\mathrm{T}}(\boldsymbol{r})\boldsymbol{n}_{\gamma} = \sum_{l=1}^{L} j_{\gamma,l,g} h_{\gamma,l}(\boldsymbol{r}) = \boldsymbol{h}_{\gamma}^{\mathrm{T}} \boldsymbol{j}_{\gamma,g}
$$
(8)

where $f_i(\mathbf{r})$ and $h_{\gamma,l}(\mathbf{r})$ are orthogonal polynomial basis functions defined on nodal volume and surface respectively, I and L are the number of corresponding expansion terms, $\varphi_{\rm g}$, $\bm{s}_{\rm g}$, $\bm{j}_{\gamma,\rm g}$, \bm{f} and \bm{h}_{γ} are column vectors containing the corresponding moments and functions.

Substituting the above expansions in Eqs. $(6)-(8)$ into the functional in Eq. (1) , the source in Eq. (2) and the boundary conditions in Eq. (3) , and then requiring the functional to be stable in terms of φ_{g} and $\pmb{j}_{\gamma,g}$ respectively, yield:

$$
\mathbf{s}_{g} = \sum_{g' \neq g}^{G} \sum_{g' \to g} \boldsymbol{\varphi}_{g'} + \frac{\chi_{g}}{k_{eff}} \sum_{g'=1}^{G} \nu \Sigma_{f,g'} \boldsymbol{\varphi}_{g'} \tag{9}
$$

$$
\boldsymbol{j}_{g}^{+} = \boldsymbol{B}_{g}\boldsymbol{S}_{g} + \boldsymbol{R}_{g}\boldsymbol{j}_{g}^{-} \tag{10}
$$

$$
\boldsymbol{\varphi}_{g} = \boldsymbol{H}_{g}\boldsymbol{s}_{g} - \boldsymbol{C}_{g}(\boldsymbol{j}_{g}^{+} - \boldsymbol{j}_{g}^{-})
$$
\n(11)

$$
\boldsymbol{j}_{g}^{\pm} = \frac{1}{4} \boldsymbol{M}^{\mathrm{T}} \boldsymbol{\varphi}_{g} \pm \frac{1}{2} \boldsymbol{j}_{g}
$$
 (12)

$$
\boldsymbol{j}_{g} = \begin{bmatrix} \boldsymbol{j}_{1g}^{\mathrm{T}} & \cdots & \boldsymbol{j}_{\gamma g}^{\mathrm{T}} & \cdots \end{bmatrix}^{\mathrm{T}} \tag{13}
$$

where the response matrices are block diagonal over spatial nodes with their diagonal blocks

$$
\boldsymbol{B}_{g} = \frac{1}{2} [\boldsymbol{G}_{g} + \boldsymbol{I}]^{-1} \boldsymbol{C}_{g}^{T}
$$
 (14)

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