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Partitioned-Matrix acceleration to the Fission-Source iteration of the Variational Nodal Method

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ABSTRACT

The Variational Nodal Method (VNM) expands the nodal volumetric flux and surface partial current into the sums of orthogonal basis functions without using the transverse integration technique. The exclusion of the transverse integration provides a number of advantages for employing the VNM in Pressurized Water Reactor (PWR) core simulation. The orthogonality of those basis functions guarantees the conservation of neutron balance regardless of the expansion orders, providing an opportunity to accelerate the computationally expensive full-order iteration by using cheap low-order sweeping with high-order moments fixed. This was named as the Partitioned-Matrix (PM) technique in the legacy VNM code VARIANT, and was applied to the within-group (WG) iteration. It is very effective for neutron-transport calculation, but less effective for neutron-diffusion mainly due to the reduced number of high-order partial current moments. In this paper, we extend the PM technique to the Fission-Source (FS) iteration to accelerate the flux convergence by using low-order flux moments also. From the macroscopic acceleration point of view, it converges the fission- and scattering-source distributions by using computationally cheap low-order iteration faster than the original full-order sweeping. Based on our new VNM code VIOLET, considering the fact that the discontinuity factor used for preserving neutron leakage rates during spatial homogenization slows down the nodal iteration convergence, numerical tests were carried out for two typical PWR problems respectively without and with discontinuity factors. By analyzing both the computational effort in terms of FLOP (FLoating-point OPeration) and computing time, the following conclusions have been demonstrated. The legacy PM technique for WG iteration can provide an acceleration ratio of about 2 for the PWR core neutron-diffusion calculation with or without using discontinuity factors, while the one for FS iteration itself can accelerate by a factor of about 3 which is higher. By accelerating both the WG and FS iteration simultaneously, the acceleration ratio is about 4 for both the two PWR problems. In addition, by extending the PM technique from the WG iteration to the FS iteration, the neutron-diffusion calculation of the VNM can be accelerated very effectively with almost no extra storage or implementation cost to the existing computer code.

1. Introduction

The Variational Nodal Method (VNM) (Lewis and Miller, 1984; Carrico et al., 1992) was first developed by Northwestern University and Argonne National Laboratory (ANL) to solve the multi-group steady-state neutron-diffusion and -transport equations for reactor core calculations. It uses a variational principle for the even-parity form of the Boltzmann transport equation. In this variational principle, the odd-parity Lagrange multipliers along the nodal interfaces guarantee neutron conservation for each node. The classical Ritz procedure is employed by using orthogonal polynomials in space and spherical harmonics in angle. Nodal response matrices are then formed for the volumetric flux moments and surface partial current moments. The VARIANT code (Palmiotti et al., 1995), developed at ANL in mid 90s was the first production code based on VNM. It has been employed for fast reactor routinely designing both in ANL such as the REBUS code (Toppel, March 1983) and in Europe such as the ERANOS code (Doriath et al., 1994). In 2007, a new version of the VARIANT code named NODAL was developed in ANL

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as one of the solvers in the UNìC package (Palmiotti et al., 2007; Li et al., 2015). In 2011, it has also been implemented into the INSTANT code in Idaho National Laboratory (INL) (Wang et al., 2011).

The exclusion of the transverse integration in the VNM provides several advantages (Lawrence, 1986; Wagner, 1989). Firstly, the VNM expands the volume flux by using basis functions which usually are orthogonal polynomials. Once obtained those flux moments, continuous flux profile within each node can be obtained, leaving no need for pin power reconstruction which usually introduces more approximations. Secondly, for adjoint flux calculation usually employed in transient simulation, the VNM can guarantee that the corresponding mathematical adjoint flux is exactly the same with the physical one. Thirdly, it is possible to extend the homogeneous VNM to heterogeneous VNM which can treat heterogeneous cross section distribution within each node (Smith et al., 2003; Li et al., 2014; Wang et al.). Fourthly, the VNM employs the Pn method for angular variable within which neutron-diffusion equation is equivalent to the P_1 approximation, enabling this method can to be consistently extended to neutron-transport calculation. Thus, recently a new VNM code named VIOLET has been developed at Xi'an Jiaotong University (XJTU) for thermal reactor such as Pressurized Water Reactor (PWR) neutron-diffusion simulation.

The numerical process of the VNM contains three levels of iteration. The outermost is the Fission-Source (FS) iteration (also termed as the outer iteration in literatures) based upon the Power Method (Lewis and Miller, 1984). At each FS iteration, just in case if up-scattering shows up, the multi-group (MG) flux system is solved by using the legacy Gauss-Seidel (GS) algorithm. Only one sweep over the energy groups is required if there is no up-scattering. For each group, the within-group (WG) response matrix system is solved by using the Red-Black Gauss-Seidel (RBGS) algorithm (Palmiotti et al., 1995). It is the so-called WG iteration (typically termed as the inner iteration in literatures).

Traditionally, the VARIANT code employs the Partitioned-Matrix (PM) technique to accelerate the WG iteration. Before each full-order partial current moments iteration, a number of low-order partial current moments iterations are carried out with the high-order ones fixed. Usually, only one full-order sweep is carried out for each energy group within each MG iteration. The PM technique performs very well in transport cases due to the large number of high-order moments. However, the effect is less effective in diffusion because there are fewer high-order moments to eliminate. Though other techniques or algorithms such as the Krylov (Saad, 2003; Saad and Schultz, 1986) ones including CG (Conjugate Gradient) (Wang et al., 2011) and GMRES (Generalized Minimal Residual Method) (Wang et al., 2011; Lewis et al., 2013; Li et al., 2012) have also been proposed and tested, they usually require more memory due to the storage of orthogonal vectors. In addition, these algorithms usually require preconditioners to be compatible with the PM accelerated WG RBGS iteration, making the code system much more complicated.

The rest of this paper is organized as following. Section 2 describes the theory of the VNM including its iteration process, the PM technique and its implementations to the both the WG and FS iterations of the VNM, Section 3 assesses the PM technique numerically by using two typical PWR problems respectively with and without discontinuity factors. Section 4 summarizes the conclusions and discussions.

2. Theoretical formulation

After introducing the VNM response matrices and the iteration process, the PM techniques for both the WG and FS iterations are described in detail. The computing efforts of applying these response matrices are evaluated and summarized based on these formulas.

2.1. The Variational Nodal Method

After the multi-group approximation for the energy variable and the P_1 approximation for the angular variable, isotropic scattering with transport correction and isotropic fission, the neutron-transport equation becomes the Multi-Group neutron-diffusion equation together with its albedo boundary condition:

$$\begin{cases} \nabla \boldsymbol{J}_g + \sum_{\mathrm{r},g} \Phi_g = S_g \\ \frac{1}{3}\nabla \Phi_g + \sum_{\mathrm{tr},g} \boldsymbol{J}_g = 0 \end{cases}, \quad g = 1 \sim G \tag{1}$$

$$S_g = \sum_{g' \neq g} \sum_{\mathrm{s},gg'} \Phi_{g'} + \frac{1}{k} \sum_{g'} F_{gg'} \Phi_{g'} \tag{2}$$

$$\Phi_g - 2\boldsymbol{J}_g^{\mathrm{T}} \boldsymbol{n}_\gamma = \beta_{\gamma,g} \cdot \left(\Phi_g + 2\boldsymbol{J}_g^{\mathrm{T}} \boldsymbol{n}_\gamma \right), \quad \mathbf{r} \in \Gamma_\gamma \tag{3}$$

where common symbols are used as in literature (Lewis and Miller, 1984), $\boldsymbol{J}_g$ and $\boldsymbol{n}_\gamma$ are column vectors. The variational principle (Lewis and Miller, 1984) turns out to be:

$$F\left[\Phi_g, \boldsymbol{J}_g\right] = \sum_v F_v\left[\Phi_g, \boldsymbol{J}_g\right] \tag{4}$$

$$F_v\left[\Phi_g, \boldsymbol{J}_g\right] = \int_v dV \left\{ \left(3\Sigma_{\mathrm{tr},g}\right)^{-1} \nabla \Phi_g \nabla \Phi_g + \Sigma_{\mathrm{r},g} \Phi_g^2 - 2\Phi_g S_g \right\} + 2 \times \sum_\gamma \int_\gamma \Phi_g \cdot \boldsymbol{J}_g^{\mathrm{T}} \boldsymbol{n}_\gamma d\Gamma \tag{5}$$

For each energy group and each node, the volumetric flux and source are expanded by using basis functions:

$$\Phi_g(\boldsymbol{r}) = \sum_{i=1}^{I} \phi_{i,g} f_i(\boldsymbol{r}) = \boldsymbol{f}^{\mathrm{T}} \boldsymbol{\varphi}_g, \quad \boldsymbol{r} \in v \tag{6}$$

$$S_g(\boldsymbol{r}) = \sum_{i=1}^{I} s_{i,g} f_i(\boldsymbol{r}) = \boldsymbol{f}^{\mathrm{T}} \boldsymbol{s}_g, \quad \boldsymbol{r} \in v \tag{7}$$

And the surface net outgoing current is expanded as

$$\boldsymbol{J}_g^{\mathrm{T}}(\boldsymbol{r}) \boldsymbol{n}_\gamma = \sum_{k=1}^{K} j_{\gamma,k,g} h_{\gamma,k}(\boldsymbol{r}) = \boldsymbol{h}_\gamma^{\mathrm{T}} \boldsymbol{j}_{\gamma,g} \quad \boldsymbol{r} \in \Gamma_\gamma \tag{8}$$

where $f_i(\boldsymbol{r})$ and $h_{\gamma,k}(\boldsymbol{r})$ are orthogonal polynomial basis functions respectively on nodal volume v and surface Γ_γ, I and K are the number of expansion terms, $\boldsymbol{\varphi}_g$, $\boldsymbol{s}_g$, $\boldsymbol{j}_{\gamma,g}$, $\boldsymbol{f}$ and $\boldsymbol{h}_\gamma$ are column vectors containing the corresponding moments and functions.

Nodal response matrices can be formed (Lewis and Miller, 1984; Carrico et al., 1992; Palmiotti et al., 1995; Wang et al., 2011) by firstly substituting the expansions in Eqs. (6)–(8) into the functional in Eq. (5), the boundary conditions in Eq. (3) and the source in Eq. (2) and then requiring the functional to be stable in terms of $\boldsymbol{\varphi}_g$ and $\boldsymbol{j}_g$ respectively: