



# An improved variational nodal method for the solution of the three-dimensional steady-state multi-group neutron transport equation



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## ABSTRACT

An improved variational nodal method is presented for the solution of the three-dimensional (3D) steady-state multi-group neutron transport equation. The variational functional is constructed that reproduces the even parity neutron transport equation with isotropic scattering. 3D orthogonal polynomials are used to approximate the spatial flux distribution within the nodes and across the nodal interfaces. The angular discretization utilizes a 3D even-parity integral method within the nodes, and standard spherical harmonics ( $P_N$ ) on the interfaces. The generalized partitioned matrix (GPM) acceleration is derived and performed to speed up outer iterations of the transport formulation. Examined against three sets of TAKEDA benchmark cases, the integral method exhibits superior accuracy and efficiency than the standard VNM approach. In addition, the GPM method presents remarkable acceleration to outer iterations when tested on the 3D PWR problem. The joint employment of the GPM method and the PM method yields a gain of over 20 in the response matrix solution time.

## 1. Introduction

The Boltzmann transport equation (BTE) is the essential governing equation in the reactor physics field. It is routinely used to describe the statistical behavior of neutrons interacting within the mediums inside a three-dimensional (3D) nuclear reactor core (Lewis and Miller, 2010). The equation is expressed with seven-dimensional phase space of independent variables (Welch et al., 2017). Among the seven variables, the evolution with time is neglected for the steady-state condition; meanwhile the complex continuous energy dependency and the heterogeneous geometry are generally accounted by group-collapse and spatial homogenization schemes to obtain homogenized few-group cross-sections (XSs) over coarse nodes (Buchan et al., 2015). By doing so, the resulting steady-state multi-group neutron transport equation (SMNTE) requires way less effort to describe the space-energy domain than the exact BTE, thus can be solved fairly cheaply. Even so, when accounting for large and geometrically complex nuclear reactor core designs, solution of the SMNTE remains a significant challenge even for contemporary state-of-the-art numerical algorithms (Welch et al., 2017; Schunert et al., 2017).

One of the widespread approaches employed for the solution of the SMNTE is the variational nodal method (VNM). The method aims for the weak form solution of SMNTE and has marched its long journey through the beginning of 1990's (when it was initially implemented in

the VARIANT (Smith et al., 2014) code) to date. In theory, the technique was derived basing on the functional for the second-order neutron transport equation, to which odd-parity Lagrange multipliers are appended to enforce nodal balance. Viewed as one typical response matrix method, the VNM is performed in sequence by a) constructing the response matrices, and b) solving the resulting response matrix equations in iterative manners. For diversified application purposes, it proves to be compatible with a variety of discretization methods, such as orthogonal polynomials in space with spherical harmonics (SHs) in angle (Lewis et al., 1996), finite sub-elements in space with SHs in angle (Smith et al., 2003; Zhang et al., 2017a,b), or finite elements in space and discrete ordinates ( $S_N$ ) in angle (Schunert et al., 2017), etc. Besides, the VNM can achieve straightforward  $p$  refinements in both space and angle with ease, making it a powerful tool for comprehensive uses. Over the years the VNM has witnessed success in abundant neutronics codes such as ERANOS (Allen et al., 2011; Talamo et al., 2011), RATTLESNAKE (Schunert et al., 2015; Wang et al., 2017), NECP-Bamboo (Liang et al., 2018), VIOLET (Wang et al., 2017), PANX (Zhang et al., 2017a,b), etc.

Recently, advancements in computing resources have motivated attempts of high order  $P_N$  simulations in place of the classical diffusion approximations (Baudron et al., 2014; Jamelot and Ciarlet, 2013; Anistratov et al., 2017). However, high angular orders come at prices of excessive computational costs (Yang et al., 2001). For the VNM, a

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higher  $P_N$  order increases not only the total number of DOFs but also the size of response matrices, inducing prohibitive storage occupations and computational time. As a result, acceleration methods tailored to the VNM have been studied extensively over the course of last decades: the nonlinear diffusion acceleration method (NDA) (Wang et al., 2017), the block-diagonalization approaches (BD) (Yang et al., 2001; Li et al., 2017), the partitioned matrix algorithm (PM) (Carrico et al., 1992), the integral method (Smith et al., 2004), etc. The NDA was designed mainly for the first order transport formulation with unstructured meshes and is beyond the scope of this work. The BD approaches delicately utilized techniques such as the variable-transformation algorithm (Yang et al., 2001) or the symmetry group theory (Li et al., 2017) to convert response matrices into block-diagonal ones which require less computational efforts. Even though the methods proved well suitable, the theories are difficult for replication. The legacy PM algorithm yields favorable acceleration to inner iterations, but is hardly effective to outer iterations. For this reason, Li extended the PM method to outer iterations in diffusion calculations (Li et al., 2015). In addition, it appeared that considerable savings in forming response matrices can be achieved by employing the integral method (Smith et al., 2004), in which the within node angular dependency are treated with a  $S_N$ -like manner. The formulation of this approach, unfortunately, was confined merely to two-dimensional (2D) problems with finite element spatial trial functions.

In this work, we propose an improved VNM for the solution of 3D SMNTE, that provides more accurate and efficient solutions to practical nuclear reactor problems. The integral method is derived within a 3D framework to construct response matrices cheaply. Orthogonal polynomials in space and spherical harmonics in angle are employed for the Ritz procedure. In addition, a generalized partitioned matrix (GPM) is formulated upon the transport solution process, resulting in remarkable acceleration to the outer iterations. The work is verified using a series of benchmark cases, and the cost-accuracy trade-offs are compared.

The following contexts are organized as follows. In Section 2 the variational functional of the 3D integral method is derived, and the Ritz discretization is performed to formulate the response matrix equations. At the end of Section 2, the GPM method is elaborated. In Section 3, the VITAS code (Variational-Integral-Transport-Analysis-Solver) is employed to examine the accuracy and the efficiency of the proposed methods, using the TAKEDA benchmark cases (Takeda and Tamitani, 1988) and the 3D PWR problem. Section 4 briefly summarizes the work and points to possible directions for further researches.

## 2. Theory

The three-dimensional variational nodal method is based upon the within-group transport equation with isotropic scattering (Smith et al., 2014):

$$\Omega \cdot \nabla \psi(\mathbf{r}, \Omega) + \Sigma_t(\mathbf{r})\psi(\mathbf{r}, \Omega) = \Sigma_s(\mathbf{r})\phi(\mathbf{r}) + q(\mathbf{r}), \quad (1)$$

where  $\psi(\mathbf{r}, \Omega)$  is the angular flux at position  $\mathbf{r}$  in direction  $\Omega$ ;  $\Sigma_t(\mathbf{r})$  and  $\Sigma_s(\mathbf{r})$  are the macroscopic total and scattering cross sections, respectively. The group source  $q(\mathbf{r})$  is represented as the contributions from scattering and fission:

$$q(\mathbf{r}) = \sum_{g' \neq g} \Sigma_{\text{sgg}'}(\mathbf{r})\phi_{g'}(\mathbf{r}) + k_{\text{eff}}^{-1} \chi_g \sum_{g'} \nu \Sigma_{\text{fg}'}(\mathbf{r})\phi_{g'}(\mathbf{r}), \quad (2)$$

in which the scalar flux is given by

$$\phi(\mathbf{r}) = \int d\Omega \psi(\mathbf{r}, \Omega). \quad (3)$$

Note that to remove factors of  $\pi$  from these equations,  $\psi$  has been normalized as  $4\pi$  times the standard definition, and  $d\Omega$  such that

$$\int d\Omega = 1 \quad (4)$$

### 2.1. The variational nodal formulation

As is routinely used as the basis of the variational nodal method (Lewis and Miller, 2010), the even-parity form of Eq. (1) is derived first. The even- and odd-parity components  $\psi^+(\mathbf{r}, \Omega)$ ,  $\psi^-(\mathbf{r}, \Omega)$  are defined by

$$\psi^\pm(\mathbf{r}, \Omega) = \frac{1}{2} \left[ \psi(\mathbf{r}, \Omega) \pm \psi(\mathbf{r}, -\Omega) \right]. \quad (5)$$

Subtraction of Eq. (1) evaluated at  $\Omega$  and  $-\Omega$  yields:

$$\Omega \cdot \nabla \psi^-(\mathbf{r}, \Omega) + \Sigma_t \psi^+(\mathbf{r}, \Omega) = \Sigma_s \phi(\mathbf{r}) + q(\mathbf{r}), \quad (6)$$

and

$$\Omega \cdot \nabla \psi^+(\mathbf{r}, \Omega) + \Sigma_t \psi^-(\mathbf{r}, \Omega) = 0. \quad (7)$$

Eliminating  $\psi^-(\mathbf{r}, \Omega)$  between Eqs. (6) and (7) yields the desired even-parity equation:

$$-\Omega \cdot \nabla \Sigma_t^{-1} \Omega \cdot \nabla \psi^+(\mathbf{r}, \Omega) + \Sigma_t \psi^+(\mathbf{r}, \Omega) = \Sigma_s \phi(\mathbf{r}) + q(\mathbf{r}). \quad (8)$$

For brevity we suppress  $\mathbf{r}$  and  $\Omega$  in the unknowns in the following derivations. The functional form following a procedure detailed in earlier work is represented as

$$F[\psi^+, \psi^-] = \sum_v F_v[\psi^+, \psi^-], \quad (9)$$

where the problem domain is the superposition of the nodal volumes  $V_v$ . Specifically, the functional can be written as (Smith et al., 2014):

$$F_v \left[ \psi^+, \psi^- \right] = \int_{V_v} dV \left\{ \int d\Omega \left[ \Sigma_t^{-1} (\Omega \cdot \nabla \psi^+)^2 + \Sigma_t \psi^{+2} \right] - \Sigma_s \phi^2 - 2\phi q \right\} + 2 \sum_{u,v,w=x,y,z} \int dv \int dw \int d\Omega \mathbf{n}_u \cdot \Omega \psi^+ \psi^-|_{u+}. \quad (10)$$

In local coordinates, the nodal volume is defined within  $-\Delta x/2 \leq x \leq \Delta x/2$ ,  $-\Delta y/2 \leq y \leq \Delta y/2$ ,  $-\Delta z/2 \leq z \leq \Delta z/2$ ;  $\mathbf{n}_u$  are the outward normal to lateral interfaces. Requiring this functional to be stationary with respect to variations in  $\psi^+$  within  $V_v$  yields Eq. (8) as the Euler-Lagrange equation. Across the interfaces,  $\psi^-$  is defined to be continuous; requiring Eq. (10) to be stationary with respect to variations in  $\psi^-$  yields the conditions that  $\mathbf{n}_u \cdot \Omega \psi^+$  be continuous across the interfaces.

### 2.2. The discretized functional

The following section elaborates the discretization of the nodal functional given by Eq. (10). Within the node, the spatial distribution of the even-parity flux is approximated by

$$\psi^+(\mathbf{r}, \Omega) \approx \mathbf{f}^T(x, y, z) \boldsymbol{\psi}(\Omega). \quad (11)$$

indicating the scalar flux expanded as

$$\phi(\mathbf{r}) = \mathbf{f}^T(x, y, z) \boldsymbol{\phi}, \quad (12)$$

where the scalar flux moments are defined by  $\boldsymbol{\phi} = \int d\Omega \psi(\Omega)$ . Denote  $\mathbf{f}(x, y, z)$  as the vector of orthogonal polynomials, with the length of  $Nv$ , and

$$\int \mathbf{f}(x, y, z) \mathbf{f}^T(x, y, z) dV = \mathbf{I}_v. \quad (13)$$

in which  $\mathbf{I}_v$  is a diagonal matrix of dimension  $Nv$  and the diagonal terms equal the volume of the node. Within a node, the cross sections are homogeneous in all three directions. Compared with the standard VNM (Lewis et al., 1996), the distinctive feature of this method lies in Eq. (11), where angular dependencies are included in the expansion moments in an implicit way, rather than in the trial functions. As will be shown in the results section, it eases the computational burden caused by inverting large coefficient matrices. The odd-parity flux is approximated on interfaces by

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