A First-Order Integral Method Developed for the VARIANT Code

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A first order nodal integral method using spherical harmonic interface conditions is formulated and implemented into VARIANT [1-3], a variational nodal transport code developed at Argonne National Laboratory. The spatial domain is split into hybrid finite elements, called nodes, where orthogonal polynomial spatial trial functions are used within each node and spatial Lagrange multipliers are used along the node boundaries. The internal angular approximation is weighted with a complete odd-order spherical harmonics set and numerically integrated using a standard angular quadrature. Along the nodal boundaries, even-order Rumyantsev interface conditions are combined with the spatial Lagrange multipliers to couple the nodes together. The new method is implemented in Cartesian geometry and used to solve a fixed source two-dimensional benchmark problem.

KEYWORDS: neutron transport, nodal method, spherical harmonics, first-order form, VARIANT, void region problems

1. Introduction

In previous work, a spherical harmonics method applicable to low density or "void" regions was investigated [1]. This method was incorporated into a prototypical version of the VARIANT code [2,3] and used to solve a simple benchmark problem containing void regions. The variational nodal method currently implemented in the VARIANT code cannot itself be directly applied to voided nodes because the total cross section appears in the denominator of the second-order even-parity transport equation. Similar problems exist for low-density media which typically translate to convergence problems related to the ill conditioning of the matrix to be inverted rather than the direct singularity present with void regions. A straightforward solution to obviate these problems is to make use of the first order transport equation when forming the nodal response matrices.

In the previous work, a standard spherical harmonics approximation to the first order transport equation was carried out which led to the desired response matrix equations. This set of equations was found to display non-convergence when applied to void nodes indicating that the outer iteration matrix was ill-posed or singular. After some study, it was determined that the nodal boundary conditions imposed in the spherical harmonics approximation amounted to an over constraint of the spherical harmonics equations. These nodal boundary conditions are needed for compatibility with the second order form and thus it was undesirable to eliminate them. However, as a compromise, a reduced order spherical harmonics interface approximation was developed which eliminated the problems with the boundary condition constraints and thus the convergence problems. The results shown in the previous work [1], displayed the accuracy of the reduced order interface conditions when applied to problems with void regions in them.

The foremost issue that remains to be solved, is focused upon the expense of a high order angular approximation necessary to solve problems with low density and void regions. In this work, the integral method implemented in previous work [4] for problems that required high order angular approximations is revisited and applied to the first order transport equation. A modified version of the VARIANT code was created and the same benchmark problem used to display the accuracy of the first order spherical harmonics work is used for the first order integral form. A second issue not discussed in the previous work is the justification for an even-order spherical harmonics approximation along the interface. The current work will in part, try to explain the justifications for these interface conditions which allow both the first order integral method and the first order spherical harmonics method to obtain solutions to problems with void regions.

2. Theory

The starting point for the new method is the first-order form of the transport equation with total and isotropic scattering cross sections σ and σ_s given by Eq. (1).

$$\hat{\Omega}\cdot\vec{\nabla}\psi(\vec{r},\hat{\Omega})+\sigma_t\psi(\vec{r},\hat{\Omega})-\sigma_s\phi(\vec{r})-s(\vec{r})=0 \qquad \vec{r}\in V \qquad (1)$$

Using nodal decomposition of the spatial domain, we obtain the general boundary condition for each node where $\hat{n}$ is the outward normal.

$$\psi(\vec{r},\hat{\Omega})-\psi_\lambda(\vec{r},\hat{\Omega})=0 \qquad \vec{r}\in\Gamma,\ \hat{n}\cdot\hat{\Omega}<0 \quad (2)$$

These equations are multiplied by the weight vector $\mathbf{f}(\vec{r})$ and integrated over the nodal spatial domain to obtain the weighted residuals.

$$\int dV\,\mathbf{f}\left[\hat{\Omega}\cdot\vec{\nabla}\psi+\sigma_t\psi-\sigma_s\phi-s\right]-\int_{\hat{\Omega}\cdot\hat{n}<0} d\Gamma\,\hat{\Omega}\cdot\hat{n}\mathbf{f}\left[\psi-\psi_\lambda\right]=0 \qquad (3)$$

Applying the divergence theorem to the streaming term yields

$$-\int dV\ \hat{\Omega}\cdot\vec{\nabla}\mathbf{f}\,\psi+\int dV\,\mathbf{f}\left[\sigma_t\psi-\sigma_s\phi-s\right]+\int_{\hat{\Omega}\cdot n>0} d\Gamma\,\hat{\Omega}\cdot\hat{n}\,\mathbf{f}\,\psi+\int_{\hat{\Omega}\cdot n<0} d\Gamma\,\hat{\Omega}\cdot\hat{n}\,\mathbf{f}\,\psi_\lambda=0\,. \qquad (4)$$

The general convex surface Γ is replaced by a sum of flat surfaces Γ_γ each with an outward normal $\hat{n}_\gamma$ such that each node is consistent with that defined in the VARIANT code [2].

2.1 Spatial Discretization

The spatial component of the angular flux is approximated within the node by

$$\psi(\vec{r},\hat{\Omega})=\mathbf{f}^T(\vec{r})\boldsymbol{\psi}(\hat{\Omega}), \qquad \vec{r}\in V \qquad (5)$$

$$\phi(\vec{r})=\mathbf{f}^T(\vec{r})\int d\Omega\,\boldsymbol{\psi}(\hat{\Omega})=\mathbf{f}^T(\vec{r})\boldsymbol{\psi}_o, \qquad \vec{r}\in V \qquad (6)$$

and the boundary condition by

$$\psi_\lambda(\vec{r},\hat{\Omega})=\mathbf{h}_\gamma^T(\vec{r})\boldsymbol{\psi}_{\lambda\gamma}(\hat{\Omega}), \qquad \vec{r}\in\Gamma_\gamma,\ \hat{n}_\gamma\cdot\hat{\Omega}<0 \qquad (7)$$

Inserting these approximations into Eq. (4) yields

$$\begin{aligned}&\left[-\hat{\Omega}\cdot\int dV(\vec{\nabla}\mathbf{f})\mathbf{f}^T+\int dV\sigma_t\mathbf{f}\mathbf{f}^T+\sum_{\hat{\Omega}\cdot\hat{n}_\gamma>0}\hat{\Omega}\cdot\hat{n}_\gamma\int_\gamma d\Gamma\,\mathbf{f}\mathbf{f}^T\right]\boldsymbol{\psi}(\hat{\Omega})\\&=\int dV\sigma_s\mathbf{f}\mathbf{f}^T\int d\Omega'\,\boldsymbol{\psi}(\hat{\Omega}')+\mathbf{s}-\sum_{\hat{\Omega}\cdot\hat{n}_\gamma<0}\hat{\Omega}\cdot\hat{n}_\gamma\int_\gamma d\Gamma\,\mathbf{f}\,\mathbf{h}_\gamma^T\boldsymbol{\psi}_{\lambda\gamma}(\hat{\Omega})\end{aligned}, \qquad (8)$$

where

$$\mathbf{s} = \int dV\, \mathbf{f}\, s\,. \tag{9}$$

These equations can be compacted to obtain Eq. (10), by defining the integrals of the spatial trial functions as matrices and writing $\hat{\Omega}\cdot\int dV(\vec{\nabla}\mathbf{f})\mathbf{f}^T$ in terms of the direction cosines of $\hat{\Omega}$.

$$\left[-\sum_k \Omega_k \mathbf{U}_k + \mathbf{F}_t + \sum_{\hat{\Omega}\cdot\hat{n}_\gamma>0} \hat{\Omega}\cdot\hat{n}_\gamma \mathbf{W}_\gamma\right]\boldsymbol{\psi}(\hat{\Omega}) = \mathbf{F}_s\int d\Omega'\,\boldsymbol{\psi}(\hat{\Omega}') + \mathbf{s} - \sum_{\hat{\Omega}\cdot\hat{n}_\gamma<0} \hat{\Omega}\cdot\hat{n}_\gamma \mathbf{D}_\gamma \boldsymbol{\psi}_{\lambda\gamma}(\hat{\Omega}) \tag{10}$$

2.2 Spherical Harmonics Approximation

The goal is to obtain the angular flux expressed as a vector of orthonormal spherical harmonics of order *N,* $\mathbf{y}(\hat{\Omega})$, which has the form

$$\boldsymbol{\psi}(\hat{\Omega}) = \mathbf{y}^T(\hat{\Omega})\otimes\mathbf{I}_s\boldsymbol{\Psi}\,. \tag{11}$$

The identity matrix $\mathbf{I}_s$ has the dimensions of $\mathbf{f}$. $\boldsymbol{\Psi}$ is the vector of unknown coefficients for the angular flux expansion which can be written as

$$\boldsymbol{\Psi} = \int d\Omega\left(\mathbf{y}(\hat{\Omega})\otimes\mathbf{I}_s\right)\boldsymbol{\psi}(\hat{\Omega})\,. \tag{12}$$

Once $\boldsymbol{\Psi}$ has been determined, the angular flux may be constructed within the node by combining Eqs. (5) and (11) to obtain

$$\psi(\vec{r},\hat{\Omega}) = \mathbf{y}^T(\hat{\Omega})\otimes\mathbf{f}^T(\vec{r})\boldsymbol{\Psi}\,. \tag{13}$$

Up to this point, the derivation of the first order spherical harmonics approach and the first order integral form is the same. In the spherical harmonics form, Eq. (11) is substituted into Eq. (10) and the result is weighted with $\mathbf{y}(\hat{\Omega})\otimes\mathbf{I}_s$ and integrated over angle. This yields an expression of the form

$$\mathbf{A}\boldsymbol{\Psi} = \mathbf{J}\otimes\mathbf{s} - \sum_\gamma \int_{\hat{\Omega}\cdot\hat{n}_\gamma<0} d\Omega\;\hat{\Omega}\cdot\hat{n}_\gamma \mathbf{y}(\hat{\Omega})\otimes\mathbf{D}_\gamma\boldsymbol{\psi}_{\lambda\gamma}(\hat{\Omega})\,. \tag{15}$$

which is similar to the equation obtained in the first order integral form.

In the integral form, we define the following intermediate equation to simplify the subsequent integral process where the within group scattering term is temporarily combined with the group source.

$$\mathbf{A}(\hat{\Omega})\boldsymbol{\psi}(\hat{\Omega}) = \mathbf{s} - \sum_{\hat{\Omega}\cdot\hat{\mathrm{n}}_\gamma<0} \hat{\Omega}\cdot\hat{\mathrm{n}}_\gamma \mathbf{D}_\gamma\boldsymbol{\psi}_{\lambda\gamma}(\hat{\Omega}) \tag{16}$$

The new matrix with angular dependencies, $\mathbf{A}(\hat{\Omega})$, is notably similar to the form obtained in a standard discrete ordinates method. This matrix is inverted to obtain an expression for the internal angular flux given by

$$\boldsymbol{\psi}(\hat{\Omega}) = \mathbf{A}^{-1}(\hat{\Omega})\left[\mathbf{s} - \sum_{\hat{\Omega}\cdot\hat{\mathrm{n}}_\gamma<0} \hat{\Omega}\cdot\hat{\mathrm{n}}_\gamma \mathbf{D}_\gamma\boldsymbol{\psi}_{\lambda\gamma}(\hat{\Omega})\right]. \tag{17}$$

Equation 11 can now be inserted into Eq. (17) and weighted with $\mathbf{y}(\hat{\Omega})\otimes\mathbf{I}_s$ which, after some simplifications results in Eq. (18).

$$\boldsymbol{\Psi} = \int \mathrm{d}\Omega\,\mathbf{y}(\hat{\Omega})\otimes\mathbf{A}^{-1}(\hat{\Omega})\left[\mathbf{s} - \sum_{\hat{\Omega}\cdot\hat{\mathrm{n}}_\gamma<0} \hat{\Omega}\cdot\hat{\mathrm{n}}_\gamma \mathbf{D}_\gamma\boldsymbol{\psi}_{\lambda\gamma}(\hat{\Omega})\right] \tag{18}$$

2.3 Interface Conditions

As done for the first order spherical harmonics method, the spatial moments of the angular flux on the node surface, must be related to the even- and odd-parity space-angle moments employed in VARIANT. In VARIANT, even-parity spherical harmonics expansions are used to represent the angular flux distribution within the node volume while odd-parity expansions are used upon its surface. These expansions can be combined to express the space-angle distribution of the flux at the nodal surface as

$$\psi(\vec{r},\hat{\Omega}) = \mathbf{y}_+^T(\hat{\Omega}) \otimes \mathbf{f}^T(\vec{r})\boldsymbol{\xi} + \mathbf{y}_-^T(\hat{\Omega})\mathbf{K}_\gamma \boldsymbol{\Lambda} \otimes \mathbf{h}^T(\vec{r})\boldsymbol{\chi}_\gamma, \qquad \vec{r} \in \Gamma_\gamma. \tag{19}$$

Here, $\mathbf{f}(\vec{r})$ and $\mathbf{h}(\vec{r})$ are the same vectors of continuous trial functions defined for $\vec{r} \in V$ and $\vec{r} \in \Gamma$, respectively. $\mathbf{y}_+(\hat{\Omega})$ and $\mathbf{y}_-(\hat{\Omega})$ are vectors of the even- and odd-parity spherical harmonics.

In VARIANT, the odd-parity spherical harmonics are rotated to align the polar angle with the outgoing normal which is done such that the boundary condition implementation is the same on all surfaces. The square matrix $\mathbf{K}_\gamma$ is defined in Eqs. (20) and (21) such that it is the rotation from $\hat{n}_\gamma$ to the reference direction $\hat{n}_o$.

$$\mathbf{y}_-(\hat{\Omega}) = \mathbf{K}_\gamma \mathbf{y}_{\gamma-}(\hat{\Omega}) \tag{20}$$

$$\mathbf{K}_\gamma = \int d\Omega\, \mathbf{y}_-(\hat{\Omega})\mathbf{y}_{\gamma-}^T(\hat{\Omega}) \tag{21}$$

Since there are more odd-parity moments in a complete angular approximation than even-parity ones, we must truncate the series such that one to one moment matching is achieved. In VARIANT, two sets of angular interface functions have been defined: the LI (linearly independent) set [5] and the Rumyantsev set [6]. In the previous work on the first order spherical harmonics method, it was found that the LI truncation approach was inaccurate and thus it is not considered in this work. To apply the Rumyantsev conditions, we introduce the $\boldsymbol{\Lambda}$ matrix to extract the necessary linear combinations of the odd-parity flux moments.

The hybrid nodal method, upon which the VARIANT code is based, requires both $\boldsymbol{\chi}_\gamma$ and $\boldsymbol{\varphi}_\gamma$ to be continuous across nodal interfaces, where $\boldsymbol{\varphi}_\gamma$ is given by Eqs. (22) and (23).

$$\boldsymbol{\varphi}_\gamma = \boldsymbol{\Lambda}^T \mathbf{K}_\gamma^T \mathbf{E}_\gamma^T \otimes \mathbf{D}_\gamma^T \boldsymbol{\xi} \tag{22}$$

$$\mathbf{E}_\gamma = \int d\Omega\, \hat{\Omega} \cdot \hat{n}_\gamma \mathbf{y}_+(\hat{\Omega})\mathbf{y}_-^T(\hat{\Omega}) \tag{23}$$

The boundary flux $\boldsymbol{\psi}_{\lambda\gamma}(\hat{\Omega})$ in Eq. (18) can be expressed in terms of $\boldsymbol{\varphi}_\gamma$ and $\boldsymbol{\chi}_\gamma$ as shown in Eq. (24).

$$\boldsymbol{\psi}_{\lambda\gamma}(\hat{\Omega}) = \mathbf{y}_+^T(\hat{\Omega})(\boldsymbol{\Lambda}^T \mathbf{K}_\gamma^T \mathbf{E}_\gamma^T)^{-1} \otimes \mathbf{I}_\gamma \boldsymbol{\varphi}_\gamma + \mathbf{y}_-^T(\hat{\Omega})\mathbf{K}_\gamma \boldsymbol{\Lambda} \otimes \mathbf{I}_\gamma \boldsymbol{\chi}_\gamma \qquad \hat{n}_\gamma \cdot \hat{\Omega} < 0 \tag{24}$$

Eq. (24) can be multiplied by $\mathbf{D}_\gamma$ and the properties of $\otimes$ used to obtain

$$\mathbf{D}_\gamma \boldsymbol{\psi}_{\lambda\gamma}(\hat{\Omega}) = \mathbf{y}_+^T(\hat{\Omega})(\boldsymbol{\Lambda}^T \mathbf{K}_\gamma^T \mathbf{E}_\gamma^T)^{-1} \otimes \mathbf{D}_\gamma \boldsymbol{\varphi}_\gamma + \mathbf{y}_-^T(\hat{\Omega})\mathbf{K}_\gamma \boldsymbol{\Lambda} \otimes \mathbf{D}_\gamma \boldsymbol{\chi}_\gamma. \tag{25}$$

Substituting Eq. (25) into Eq. (18) results in the following expression.

$$\boldsymbol{\Psi} = \mathbf{N}\, \mathbf{s} - \mathbf{M}_\gamma^+ \boldsymbol{\varphi}_\gamma - \mathbf{M}_\gamma^- \boldsymbol{\chi}_\gamma \tag{26}$$

where an implicit sum is assumed over each interface of the node. The new matrices are defined as

$$\mathbf{N} = \int \mathrm{d}\Omega\, \mathbf{y}(\hat{\Omega}) \otimes \mathbf{A}^{-1}(\hat{\Omega}), \tag{27}$$

$$\mathbf{M}_{\gamma}^{+} = \int \mathrm{d}\Omega \hat{\Omega}\cdot \hat{\mathrm{n}}_{\gamma}\ \mathbf{y}(\hat{\Omega})\mathbf{y}_{+}^{\mathrm{T}}(\hat{\Omega})(\mathbf{\Lambda}^{\mathrm{T}}\mathbf{K}_{\gamma}^{\mathrm{T}}\mathbf{E}_{\gamma}^{\mathrm{T}})^{-1} \otimes \mathbf{A}^{-1}(\hat{\Omega})\mathbf{D}_{\gamma}, \tag{28}$$

and

$$\mathbf{M}_{\gamma}^{-} = \int \mathrm{d}\Omega \hat{\Omega}\cdot \hat{\mathrm{n}}_{\gamma}\ \mathbf{y}(\hat{\Omega})\mathbf{y}_{-}^{\mathrm{T}}(\hat{\Omega})\mathbf{K}_{\gamma}\mathbf{\Lambda} \otimes \mathbf{A}^{-1}(\hat{\Omega})\mathbf{D}_{\gamma}. \tag{29}$$

where an angular quadrature is used to numerically invert and integrate the matrices.

2.4 Response Matrix Form

To obtain response matrices, continuity conditions must be imposed on the angular flux across the interfaces. Recall that the boundary condition given by Eq. (19), which specifies the angular distribution of the incoming flux (for $\hat{n}_{\gamma}\cdot\hat{\Omega} < 0$) in terms of $\boldsymbol{\varphi}_{\gamma}$ and $\boldsymbol{\chi}_{\gamma}$, is the approximation to Eq. (2).

In previous work, studies were undertaken to ascertain the appropriate projection needed to obey the continuity conditions. In that work the interface condition defined by

$$\boldsymbol{\varphi}_{\gamma} = \mathbf{\Lambda}^{T}\mathbf{K}_{\gamma}^{T}\mathbf{E}_{\gamma}^{T}\Xi_{+} \otimes \mathbf{D}_{\gamma}^{T}\mathbf{\Psi}. \tag{30}$$

$$\Xi_{+} = \int d\Omega\ \mathbf{y}_{+}(\hat{\Omega})\mathbf{y}^{T}(\hat{\Omega}) \tag{31}$$

was the only one found to provide accurate solutions. As a consequence, only it is used in this work leading to

$$\begin{aligned}\boldsymbol{\varphi}_{\gamma} &= \mathbf{\Lambda}^{T}\mathbf{K}_{\gamma}^{T}\mathbf{E}_{\gamma}^{T}\Xi_{+} \otimes \mathbf{D}_{\gamma}^{T}\left[\mathbf{N}\ \mathbf{s} - \mathbf{M}_{\gamma'}^{+}\boldsymbol{\varphi}_{\gamma'} - \mathbf{M}_{\gamma'}^{-}\boldsymbol{\chi}_{\gamma'}\right] \\ &= \mathbf{C}_{\gamma}\mathbf{s} - \mathbf{G}_{\gamma\gamma'}^{+}\boldsymbol{\varphi}_{\gamma'} - \mathbf{G}_{\gamma\gamma'}^{-}\boldsymbol{\chi}_{\gamma'}\end{aligned}. \tag{32}$$

where an implicit sum is assumed over γ'.

The same variable transformation implemented in VARIANT, defined as

$$\mathbf{j}^{\pm} = \tfrac{1}{4}\boldsymbol{\varphi} \pm \tfrac{1}{2}\boldsymbol{\chi}, \tag{33}$$

can be implemented into Eq. (32) after it is partitioned over all surfaces of the domain leading to

$$\mathbf{j}^{+} + \mathbf{j}^{-} = \tfrac{1}{2}\mathbf{C}\,\mathbf{s} - \left(\mathbf{G}^{+} + \tfrac{1}{2}\mathbf{G}^{-}\right)\mathbf{j}^{+} - \left(\mathbf{G}^{+} - \tfrac{1}{2}\mathbf{G}^{-}\right)\mathbf{j}^{-}. \tag{34}$$

Solving for $\mathbf{j}^{+}$, the response matrix equation given by Eq. (35) is obtained, where the new matrices are defined in Eqs. (36) and (37).

$$\mathbf{j}^{+} = \mathbf{R}\,\mathbf{j}^{-} + \mathbf{B}\,\mathbf{s} \tag{35}$$

$$\mathbf{R} = \left[\mathbf{I} + \mathbf{G}^{+} + \tfrac{1}{2}\mathbf{G}^{-}\right]^{-1}\left[-\mathbf{I} - \mathbf{G}^{+} + \tfrac{1}{2}\mathbf{G}^{-}\right] \tag{36}$$

$$\mathbf{B} = \tfrac{1}{2}\left[\mathbf{I} + \mathbf{G}^{+} + \tfrac{1}{2}\mathbf{G}^{-}\right]^{-1}\mathbf{C} \tag{37}$$

3. Even-order Spherical Harmonic Interface Conditions

The preceding integral formulation was initially implemented into MathCAD [7] and followed by a more general implementation into the VARIANT code, called VARIANT-FI. Both implementations were thoroughly tested for stability and accuracy, and in all of the problems solved, the first-order integral method conserved neutrons and performed well. With regard to the constraints on the angular approximation, the same issues seen with the second order integral method were seen in the first order integral method. It is for this reason that we choose to discuss the issues seen with these methods in this paper.

The standard approach implemented for the second order even-parity transport equation is to use a complete even-order spherical harmonics expansion within the domain. For the first order

spherical harmonics equation, a full expansion of even and odd-parity spherical harmonics is used within the domain. For both equations the spherical harmonics expansion within the domain is measured in odd numbers that describe the order of the system of equations satisfied by the angular expansion (for P_1, all terms higher than first order are truncated). Justifications for this requirement can be shown by mathematical analysis which are beyond the scope of this paper, but have been carried out previously [6]. The same mathematical analysis is appropriate for the integral methods and thus all four methods to be discussed in this section: second order P_N, first order P_N, second order integral, and first order integral all fundamentally use an odd-order expansion of spherical harmonics internal to the domain (P_1, P_3, P_5, …).

If the problem domain is split into nodes and solved in separate pieces, as done in the VARIANT code, a truncated set of spherical harmonics is used along the interface to couple the pieces together as outlined in [5]. Rumyantsev initially showed the general equations which must be satisfied for continuity to be maintained along the interface. We have extended that work [6] for the ongoing research needs of the VARIANT code, such as the first order integral method. For odd-order N interface expansions, we have shown that continuity of the following expansion functions is required along the boundary.

$$\psi_{n,m}, \quad n = 0,2,4,\cdots,N-1, \quad -n \le m \le n \tag{38a}$$

$$\psi_{n,m}, \quad n = 1,3,5,\cdots,N, \quad |m| = 0,2,4,\cdots,n-1 \tag{38b}$$

$$(2n+1)a_{n,m}\psi_{n,m} + (2n+5)a_{n+1,m}\psi_{n+2,m}, \quad n = 1,3,5,\cdots,N-2, \quad |m| = 1,3,5,\cdots,n \tag{38c}$$

For even-order N interface expansions, the continuity of the following expansion functions is required.

$$\psi_{n,m}, \quad n = 1,3,5,\cdots,N-1, \quad -n \le m \le n \tag{39a}$$

$$\psi_{n,m}, \quad n = 2,4,6,\cdots,N, \quad |m| = 1,3,5,\cdots,n-1 \tag{39b}$$

$$(2n+1)a_{n,m}\psi_{n,m} + (2n+5)a_{n+1,m}\psi_{n+2,m}, \quad n = 0,2,4,\cdots,N-2, \quad |m| = 0,2,4,\cdots,n \tag{39c}$$

Note that in Eqs. (38) and (39), the linkage between the interface set of spherical harmonics and the set of spherical harmonics used within the node is implicitly defined. These equations simply state the continuity conditions between nodes for the set of spherical harmonics within each node of order N.

In the production VARIANT code (second order P_N), the spherical harmonics order used along the interface matches that used within the node (P_1 interface conditions for a P_1 nodal expansion). Some earlier work attempted reduced order approximations [8], but only a P_1 reduced order interface condition was considered for an nodal P_3 angular approximation ($P_{3\text{-}1}$). Although this approach did achieve some success, extension to higher order angular approximations ($P_{5\text{-}3}$, $P_{5\text{-}1}$, etc…) was found to be problematic and prone to convergence problems.

With the recent development of the second order integral formulation, the odd-order interface spherical harmonics prescribed by the original VARIANT code [5] were found to be completely inappropriate. Without access to the interface spherical harmonic expansions given by Eqs. (38) and (39), a trial and error process was used to determine a set of functions which was effective. It is for this reason that the set of spherical harmonics used in the second order integral work [4] were improperly termed odd-order spherical harmonic conditions. Later, after Eqs. (38) and (39) were obtained, it was clear that the set of interface spherical harmonics used in the second order integral form were in fact even-order rather than odd-order.

Given this finding, the reduced order spherical harmonics method used in the production VARIANT code (second order P_N) was revisited and reliable success was achieved by implementing even-order interface spherical harmonic expansions. Those results have not been published primarily due to the fact that they did not provide any substantial achievements in accuracy or computational speed. As expected though, the reduced order spherical harmonics expansions were consistent with those used for the first and second order integral forms along with the first order P_N method ($P_{3\text{-}2}$, $P_{5\text{-}2}$, $P_{5\text{-}4}$, etc…).

With this consistency determined for all four methods, inspection of the system of equations was carried out to ascertain why even-order expansions were appropriate for the continuity conditions while odd-order expansions were not. From Eq (38) we know that each refinement in the interface set of spherical harmonics will fully constrain a complete set of spherical harmonics used internal to the node. This is why we initially expected the odd-order interface conditions to work in the reduced order methods; however, from further inspection one finds that the nodal even and odd-parity spherical harmonic terms within the above the order used for the interface conditions are completely unconstrained by the interface set of spherical harmonics. We have identified this as the primary problem since we are effectively applying boundary conditions to these moments when they are not explicitly constrained by the interface set of spherical harmonics.

For most of these spherical harmonic moments these boundary conditions can be shown to be standard reflected boundary conditions applied to each node. But, for even *n*, odd *m* spherical harmonics moments and odd *n*, even *m* spherical harmonic moments, these boundary conditions are undefined. As a consequence, we believe that these terms with undefined boundary conditions are the source of instability in the system of equations along with the lack of neutron conservation. Note that a general failure of neutron balance was observed when high order expansions of odd-order interface spherical harmonics were used in the second order integral formulation. No such problem has been found with the even-order interface spherical harmonic conditions.

From Eq. (39), the even-order expansions along the interface implicitly include all those terms used in the odd-order expansion, thus one can assume that the internal spherical harmonics expansion of order *N-1* is fully constrained (a P_2 interface set fully constrains a P_1 set internal to the domain; P_4 fully constrains P_3, etc…). The purpose of the additional terms in Eq. (39) relative to Eq. (38) is difficult to state clearly since they lead to different coupling schemes in all four methods. The only common trend is that the additional terms in the even-order interface expansions directly constrain the higher order spherical harmonics which have the undefined boundary conditions (i.e. the even *n*, odd *m* or odd *n*, even *m* moments). This is likely the reason that the method is stable, although a lack of complete coupling in the spherical harmonics methods still requires more mathematical analysis.

There is a physical interpretation which can be made from the even-order interface conditions. All of the proposed even-order expansions along the boundary fundamentally constrain all of the moments of the current ($\psi_{1,-1}, \psi_{1,0}, \psi_{1,1}$). Further, any refinements in the interface angular approximation above P_2 (i.e. P_4, P_6, P_8,…) can be considered complete order refinements of the current along the interface. With this progression, one can easily see that the even-order expansions enforce the requirement that no neutrons be lost between nodes via the continuity conditions. Since we are not explicitly constraining the spherical harmonic terms above the reduced order ones along the boundary, it would appear as though we are required to

impose a constraint on the current such that no neutrons are lost and stability of the system of equations can be maintained.

4. Modified Watanabe-Maynard Benchmark Problem

As mentioned, several benchmark problems were used to test the first order integral formulation. The only ones of interest are those with void regions since the second order integral method can be shown to computationally superior to that of the first order integral (the spatial interface approximation requires the same spatial expansion order internally). It is for this reason that we focus the results obtained with the first order integral method on a simplification of a Watanabe-Maynard benchmark [9,10], shown in Fig. 1. This benchmark displayed the largest errors and was previously used to display the accuracy of the first order spherical harmonics method. The original benchmark defined a larger source region (shaded region) and smaller source magnitude than that shown in Fig. 1. The benchmark dimensions were simplified for the first order spherical harmonics work to reduce the computational burden in MATHCAD, but are unnecessary for the first order integral method. Nevertheless, the modified benchmark is used to allow comparison with the first order spherical harmonics method.

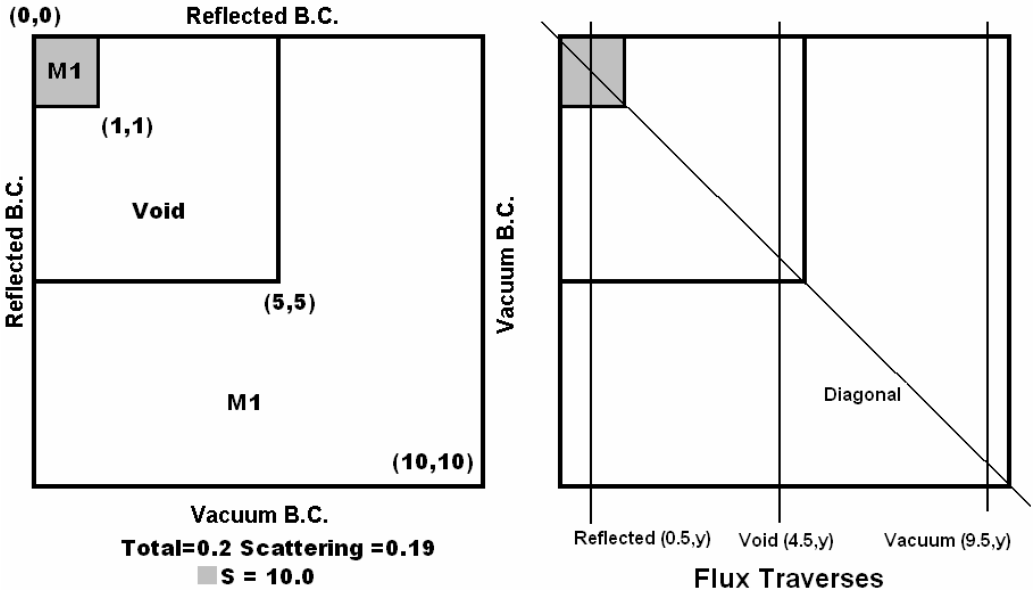

Fig. 1. Modified Watanabe-Maynard Benchmark Geometry

The average flux within each node was used to assess the accuracy of the method rather than relying upon a rigorous reconstruction of the flux. This is done primarily because it is very difficult to obtain a detailed reference flux solution. All four flux traverses shown on the right hand side of Fig. 1 were investigated, but only a few are necessary here to show the accuracy of the method. The reference solution was obtained using the collision probability code DRAGON [10]. For perspective, discrete ordinate solutions were obtained using TWODANT [11].

Figure 2 gives the void flux traverse (at x = 4.5 cm) solutions for VARIANT-FI along with a TWODANT S_{12} solution for comparison purposes. In all of these calculations, a sufficiently high enough angular quadrature was used to ensure accuracy of the angular integrals in Eqs. (27) through (29). The P_2 VARIANT-FI solution corresponds to the use of a P_2 interface conditions

along the boundary and is generally the most inaccurate of those plotted. As expected, though, as the angular order of the interface condition is refined, the VARIANT-FI solutions are seen to converge towards the reference DRAGON solution. Around P_{22}, the VARIANT-FI and DRAGON solutions are nearly indistinguishable although it is important to note that some measurable amount of error exists. Given that the error between two consecutive refinements in the reference DRAGON code shows errors similar to those between VARIANT-FI and DRAGON, no further effort was done to obtain higher order VARIANT-FI solutions.

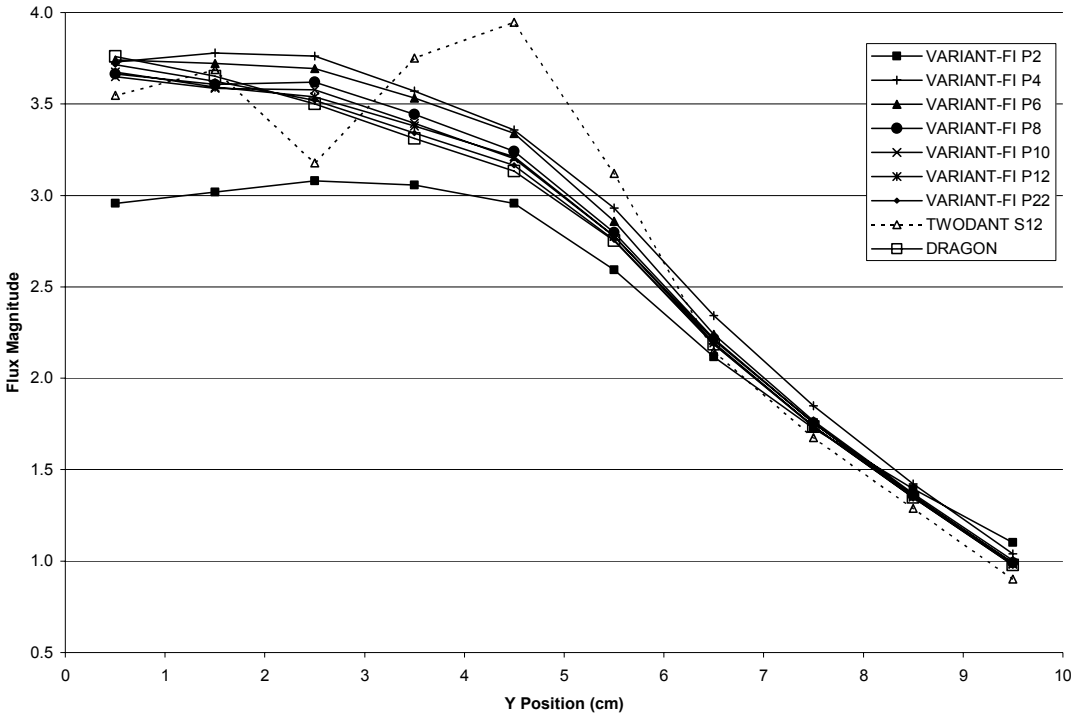

Fig. 2. VARIANT-FI Void Traverse Solution

5. Conclusions

The VARIANT-FI code was able to solve the Watanabe-Maynard benchmark with a reasonable amount of error. Clearly problems such as this are known to require high order angular approximations and thus additional refinements of the angular variable are likely necessary to eliminate all of the error. Regardless, the VARIANT-FI was able to produce flux solutions which were reasonably plausible when compared with the reference solution after a P_6 interface condition was imposed. This contrasts quite well against the discrete ordinates code, which requires a significantly higher angular approximation to eliminate the ray effect problems. Unfortunately, a more refined collision probability reference solution was not possible due to the rapidly increasing number of source regions.

When compared with the first order spherical harmonics method of earlier work, the first order integral method is more efficient for obtaining response matrices. The massive size of the A matrix that has to be formed and inverted in the first order spherical harmonics method was the primary limitation of that method. This result is quite similar to the second order even-parity forms where the integral method greatly out performed the standard spherical harmonics method when high order angular results were required.

Although the first order integral method is computationally more expensive than either of the second order even-parity forms, the ability to treat void regions presents a distinct advantage. Given that the second order forms can quite easily be used in conjunction with the first order integral form, one can easily conceive of a code which contains all three forms. In future work, the goal is to determine whether or not direct application of reflected boundary conditions in the first and second order integral forms will allow odd-order interface conditions to be used. If this can be achieved, then both the first and second order integral forms can be directly coupled with the production VARIANT code. This would eliminate the substantial changes to the code infrastructure which are currently required. With the first and second order integral forms, the new VARIANT code should be able to directly treat beam tubes such as those proposed for accelerator driven systems along with other problems that require high order angular treatments.

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