PROGRESS AND APPLICATIONS OF THE VARIATIONAL NODAL METHOD*

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This paper summarizes current progress and developments with the variational nodal method (VNM) and its implementation within the DIF3D code suite. After a brief development of the mathematical basis for the VNM, results from two three-dimensional benchmarks are presented for a variety of computers. Then current applications of the VNM are discussed including diffusion theory calculations, burnup calculations, highly heterogeneous cores, higher-order spherical harmonics approximations, perturbation theory and heterogeneous nodes.

I. INTRODUCTION

The variational nodal method is finding increased use for the performance of multidimensional, multigroup transport problems in reactor physics. It is implemented at Argonne National Laboratory as the VARIANT (VARIational, Anisotropic Nodal Transport) module of the DIF3D code system. The module solves multi-energy-group odd-order spherical harmonics equations through the P5 approximation, and several intermediate angular approximations are also available. Nodal calculations may be performed, with anisotropic scattering, in x-y, hexagonal, x-y-z and hexagonal-z geometries. It is used extensively for fast reactor criticality and gamma heating calculation in conjunction with the IFR program and the analysis of EBR-II. More recently, it has been adapted to perform calculations in the French fast reactor code system, ERANOS, at Cadarache, and has also been used for the analysis of thermal reactor experimental configurations.

A number of the variational nodal method's defining features result in the elimination of some of the shortcomings found in other nodal formulations. The method originates from a well-defined variational principle to which numerical approximations are applied with a classical Ritz procedure. Moreover, the construction of the functional ensures nodal balance regardless of the trial functions used in the Ritz procedure. Unlike other interface-current nodal methods, the use of spherical harmonics trial functions in angle creates a clear hierarchy of angular approximations, and unlike SN nodal methods, there are no ray effects. Likewise, the use of complete polynomials in the spatial trial functions eliminates the diagonal depression found in nodal methods based on quasi-one-dimensional DPN approximations. The variational nodal method converges to a well-defined spherical harmonics approximation as the spatial mesh size, h, tends to zero. A more computationally efficient way to reduce truncation error, however, is through p-type convergence in which the order of the polynomial spatial trial functions is increased instead of reducing the dimensions of the spatial nodes.

II. FORMULATION

The Variational Nodal method is based on a functional of the form

\[ F[\psi, \chi] = \sum_v F_v[\psi, \chi] \]  

(1)

where

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The contribution from the node \( v \) is the contribution from the node \( v \). Requiring the functional to be stationary with respect to variations in \( \psi \) and \( \chi \), the even- and odd-parity components of the angular flux, yields the even-parity equation

\[
-\frac{1}{\partial r^2} \psi(r, \Omega) + \sigma \psi(r, \Omega) = \sigma_s \phi(r) + S(r)
\]

within the nodes and continuity conditions on \( \psi \) and \( \chi \) across the nodal interfaces. The functional has been generalized to treat multigroup fixed source and eigenvalue problems and both within-group and group-to-group anisotropic scattering. Vacuum boundaries are also incorporated as modified natural boundary conditions, while reflected boundaries are essential. For brevity and clarity, we utilize the within-group isotropic scattering form of the functional given by Eq. (2) to briefly summarize the method.

The derivation of the equations used in variational nodal computations begins with a classical Ritz procedure. We write the even-parity flux as an expansion of trial functions in space and angle with unknown coefficients. Thus the even-parity flux appears as

\[
\psi(r, \Omega) = f^T(r, \Omega) \zeta, \quad r \in V_v,
\]

and the odd-parity flux at the interfaces take the form

\[
\chi(r, \Omega) = h^T(r, \Omega) \chi, \quad r \in \Gamma_v.
\]

The known trial functions are complete polynomials in space and even and odd spherical harmonics, respectively, in angle. The nodal contribution to the reduced functional is then

\[
F_v[\zeta, \chi] = \zeta^T A \zeta - 2 \zeta^T s + 2 \zeta^T M \chi
\]

where the \( A \) and \( M \) matrices are integrals over the known trial functions, and \( s \) is the group source vector.

Requiring \( F \) to be stationary with respect to a variation of the unknown coefficient vectors, \( \zeta \) and \( \chi \), yields

\[
A \zeta = s - M \chi
\]

within the node, and requires continuity of the quantity

\[
\psi = M^T \zeta
\]

across the interfaces. Combining equations (7) and (8) yields

\[
\psi = M^T A^{-1} s - M^T A^{-1} M \chi.
\]

These equations, coupled with the continuity requirements on \( \psi \) and \( \chi \) across the nodal interfaces may be viewed alternately as a form of hybrid finite-element method or as a generalization of the \( T^{-1} \) form of a response matrix, in which the even-
parity moments at the surface are given in terms of the odd parity moments. To make use of the physical analog of neutrons crossing interfaces, however, we transform these equations by defining vectors of partial current moments:

\[ \mathbf{j} = \frac{1}{2} \mathbf{\psi} \pm \frac{1}{2} \mathbf{\chi} \]  

Eliminating the even- and odd-parity fluxes then yields that conventional response matrix form:

\[ \mathbf{j} = \mathbf{Rj} + \mathbf{B} \]

where

\[ \mathbf{R} = \left[ \frac{1}{2} \mathbf{M}^T \mathbf{A}^{-1} \mathbf{M} + \mathbf{I} \right] \left[ - \frac{1}{2} \mathbf{M}^T \mathbf{A}^{-1} \mathbf{M} - \mathbf{I} \right] \]

and

\[ \mathbf{B} = \left[ \frac{1}{2} \mathbf{M}^T \mathbf{A}^{-1} \mathbf{M} + \mathbf{I} \right]^{-1} \frac{1}{2} \mathbf{M}^T \mathbf{A}^{-1}. \]

The even-parity flux within the node can be recovered from the auxiliary equation

\[ \zeta = \mathbf{A}^{-1} \mathbf{s} - \mathbf{A}^{-1} \mathbf{M}(\mathbf{j} - \mathbf{j}). \]

### III. IMPLEMENTATION

VARIANT, the production implementation of the variational nodal method, has a number of salient features. It makes extensive use of geometry, cross section, editing and other modules of the DIF3D code system, resulting in compatibility for a large number of reactor physics calculations. Extensive use is made of symbolic manipulation to evaluate the large arrays of known space-angle integrals which result from the Ritz procedure used to discretize the equations. The arrays are evaluated using Mathematica and the results stored as data statements in the response matrix generating FORTRAN subroutines of VARIANT. Since the calculations are performed in dimensionless form, each time a new geometry or trial function set is implemented they need be carried out only once, and stored in the appropriate subroutine.

The response matrix equations are solved with a red-black (or in the case of hexagonal geometry a four-color) iterative algorithm. The iterations are accelerated by partitioning the matrices such that only one term per interface, the partial current, is included in the iterations except for periodic updates using the entire response matrix. The code, as originally written for the CRAY XMP, is highly vectorized. More recently it has been ported to IBM RS6000 and SPARC 20/50 work stations, and there the vectorized code seems to work well, often performing at rates in excess of 35 MFLOPS on the RS6000. Limited one-group fixed-source x-y calculations have also been performed using the method on a Connection Machine-5, with indications that the red-black algorithms are highly effective on parallel computers.

The three-dimensional capability of the code is illustrated with two of the Takeda benchmarks, models I and IV. Table 1 shows eigenvalues and rod worths for a variety of methods applied to the model problems. VARIANT results for diffusion and transport (using a P₃ expansion) are presented for several different machines. The advantages of vectorization are obvious from the CPU times, as clearly demonstrated by significantly smaller ratios of transport to diffusion running times on the vector architecture of the CRAY.

### IV. CURRENT WORK

As experience has been gained using the standard form of VARIANT, documented in references 1 and 2, interest has grown in further development to enable the treatment of more complex and physically demanding problems and in further reducing computation costs. In attempting to meet these requirements, current work has also exposed the need for further
theoretical development. Here we review current progress in diffusion theory, burnup calculations, highly heterogeneous cores, higher-order spherical harmonics approximations, perturbation theory and heterogeneous nodes.
A. Diffusion Calculations

The primary thrust of the variational nodal method has been in the development of three-dimensional transport methods for fast reactors. However, interest has increased in using it as an alternative to existing nodal diffusion methods, particularly for the treatment of thermal reactors in hexagonal geometry. Comparisons have been made between VARIANT and the DIF3D-finite-difference and DIF3D-nodal diffusion modules. Representative eigenvalue and power distribution errors are tabulated in Table 2 for three, two-dimensional benchmarks in hexagonal geometry. The results indicate that VARIANT is generally more accurate than DIF3D-nodal diffusion; a conclusion which carried over to comparisons which have thus far been made for three-dimensional hexagonal benchmarks.

Table 2 also indicates that VARIANT does very well relative to DIF3D-nodal in CPU times for two-dimensional problems. At present, however, VARIANT is significantly slower than DIF3D-nodal in three dimensions. The axial sweeping scheme which accounts for this is presently under revision. It should also be noted that VARIANT coding was optimized for vector computers and is most effective for the larger dimensions of transport response matrices. Conversely, DIF3D nodal was optimized to minimize the number of floating point operations. Since the codes are both presently run on workstations, it may be beneficial to configure a version of VARIANT to be optimal to diffusion calculations on scalar machines.

B. Burnup Calculations

Recently, the VARIANT module has been incorporated into the REBUS code system. This allows the performance of three-dimensional burn-up calculations in conjunction with very accurate diffusion solutions and transport capabilities. To illustrate this new application of VARIANT, Tables 3 and 4 list results from two benchmark problems taken from a validation suite for the DIF3D/REBUS package. VARIANT diffusion and transport results are provided and compared to finite difference and transverse integrated nodal methods. In its current implementation, VARIANT is rather inefficient for this application since the entire set of response matrices is recalculated on each REBUS iteration, thus dramatically increasing the cost of the entire burn-up calculation. In addition, only the surface averaged partial current is passed between REBUS iterations, and the higher order moments are lost. This results in VARIANT performing a few extra outer iterations to recover the higher order partial current moments. While correcting the partial current moment problem is straightforward, the problem of recalculating response matrices is more difficult. A first step would involve recalculating response matrices only for those nodes in burn-up regions. A more sophisticated addition might involve the development of an interpolation scheme allowing approximation of new response matrices for small changes in cross section values, thus mitigating the cost of generating new response matrices for each burn-up step. While such developments are not strictly necessary to apply accurate VNM diffusion approximations to burn-up calculations, the utilization of the VNM transport capabilities with realistic reactor configurations motivates examination of interpolation schemes.

C. Highly Heterogeneous Cores

Running times may be divided into the formulation of the response matrices and the solution of the resulting red-black or four color algorithm. In problems where the number of unique node types is small compared to the total number of nodes, the time required to generate the response matrices is insignificant compared to the solution time. For these classes of problems high-order (nearly exact) spatial approximations may be used within the nodes with little cost penalty, since the solution time is dependent only on the response matrix dimension, and therefore on the level of space-angle approximations along the interfaces. For highly heterogeneous reactor cores such as the EBR II, however, there are nearly as many node types as nodes, and thus the generation of response matrices may occupy a substantial fraction of the total computing time. Since the generation time increases rapidly with the number of terms in the within-node space-angle approximation, it becomes important to use the lowest-order space angle approximation which is compatible with the interface approximation.

A number of approaches are being examined for reducing the response matrix formulation effort without a commensurate loss in accuracy. The most ambitious consists of eliminating the present red-black iteration scheme in favor of a matrix splitting technique which operates on Eqs. 7 and 8 directly and thereby does away with the A matrix inversion required to form the response matrix for each node type. Other approaches maintain the solution algorithm but concentrate on reducing the number of internal trial functions, and therefore the dimension of the A matrix which must be inverted. Reduced and simplified spherical harmonics approximations have been formulated. The reduced method has been employed in hexagonal-z problems, while to date simplified P3 has only been implemented for x-y geometry test problems.

Examination was also undertaken to determine the lowest-order complete polynomial spatial approximation which can be used with a given interface approximation. Here, however, examination of diffusion methods indicated that unless the M
matrix which couples the spatial approximation within the node with those at the interface has the same rank as the number of interface basis functions, convergence of the red-black response matrix iterations cannot be guaranteed beyond five or six decimal places. In two-dimensional hexagonal geometry, for example, a sixth order polynomial with 28 terms is required for the twelve-basis-function linear interface approximation. Investigations are being undertaken to find finite-element or other classes of internal trial functions which will allow substantially fewer terms to be used in achieving the required rank and therefore reduce the computational effort required to form the response matrices.

D. General Order Spherical Harmonics Calculations

Until recently, only $P_1$ and $P_3$ approximations have been formulated in the variational nodal methods. In the $P_1$ approximation the odd-parity interface trial function is $P_1(\mu)$ where $\mu$ is the direction cosine perpendicular to the interface. In the $P_3$ approximation, the correct number of odd-parity conditions is obtained by requiring interface continuity of $P_1(\mu), P_1(\eta), P_1(\xi), P_3(\mu), P_3(\eta)$ and $P_3(\xi)$ moments, where $\eta$ and $\xi$ are the direction cosines parallel to the interface. Unfortunately, including the corresponding $P_5$ or higher terms does not yield the correct number of interface conditions necessary to obtain higher order $P_N$ approximations.

To circumvent this difficulty the odd-parity interface conditions have been reformulated in terms of the classical spherical harmonic interface conditions of Rumyantsev. The result is the use of the standard odd-parity spherical harmonic set with the $Y_{n,m}$ terms deleted for all odd $n$. While not identical to the present $P_3$ odd-parity trial functions, the new formulation has very little effect on the accuracy of $P_3$ solutions. However, it does mean that this variational nodal method can be viewed as a nodal formulation which reduces to the classical $P_N$ equations in the absence of spatial discretization errors. Thus far the new trial functions have been implemented in x-y geometry. Figure 1 shows $P_1$, $P_3$ and $P_5$ solutions, with both old and new $P_3$ interfaces included, for the Azmy benchmark problem, along with those obtained from a nodal $S_N$ code.11,19

E. Adjoint and Perturbation Calculations

The ability to carry out both exact and first order perturbation calculations within the framework of the variational nodal method offers a substantial enhancement to its value. This requires as a prerequisite, however, that a code be available to perform adjoint as well as forward neutron transport calculations. With fine mesh diffusion or discrete ordinates codes this poses little difficulty; it can be shown that the mathematical adjoint formed by taking the adjoint of the forward equation, and physical adjoint, formed by discretizing the adjoint equation, are the same. This property allows the same code to be used for forward and adjoint calculations, simply by inverting the energy group ordering. The same property holds for the variational nodal method, allowing the VARIANT code to be used for forward and adjoint calculations.20 This is in sharp contrast to nodal methods based on quasi-one-dimensional solutions of the diffusion or transport equation. There, the mathematical and physical adjoints are not the same, and the mathematical adjoint is required to evaluate the perturbation expressions, while the existing nodal algorithms solve the physical adjoint problem. As a result, similarity transforms or related techniques must be utilized to relate physical and mathematical adjoints. Thus far, these have been developed only for diffusion theory.

A post processing code is under development which takes geometry and cross section files from VARIANT, combines them with the forward and adjoint output flux files, and performs exact or first order perturbation calculations. Work is completed in two-dimensional geometry; the code is being generalized to treat both anisotropic and three-dimensional problems. A companion paper discussing this subject will be presented at this conference. Work on perturbation with anisotropic scattering is also nearing completion.

F. Flux Reconstruction and Homogenization

Heretofore, the variational nodal method has been formulated under the assumption that each node is homogeneous. This is not a fundamental restriction, however, since the Ritz procedure by which the equations are derived can in principle accommodate changes of cross sections within the nodes, and trial functions, such as the piecewise polynomials of finite element methods, to more accurately model the heterogeneity. There is much to do in deciding the optimal tuck to take in blending whole-core variational nodal calculations with treatments of the local heterogeneities which must be modeled in order to derive accurate pin-to-pin power distributions. Work is underway in two-dimensions to examine this problem. A companion paper discussing this subject will be presented at this conference.
CONCLUSION

Previous work has demonstrated the efficacy and flexibility of the variational nodal method. Implementation within the DIF3D code suite allows the use of the VNM for broad classes of problems, and work continues to enlarge the set of VNM applications. Diffusion theory calculations now provide very accurate results for thermal reactor configurations in hexagonal and Cartesian geometries. The VNM also allows accurate handling of pin-power reconstruction, unlike typical transverse leakage methodologies. In conjunction with REBUS, the VNM can now be applied to burn-up calculations using diffusion and transport theory. Alternate solution methods are currently being investigated. One approach involves direct solution of the flux moments, avoiding the response matrix formulation. Other approaches involve finding an improved spatial basis in an attempt to reduce the number of spatial moments required in hexagonal geometries. Investigation of alternate angular bases is also continuing. Expansion of surface fluxes in standard odd-parity spherical harmonics ensures equivalence of the VNM with the P_n equation in the absence of spatial discretization errors, and reduced angular approximations allow near transport accuracy for the cost of diffusion calculations. Completion of a perturbation module for the VNM will round out the capabilities of the method. Further, discretization of heterogeneous subassemblies, when implemented with curvilinear geometries, will put the VNM in direct competition with Monte Carlo codes, and allow more realistic problem representation in complicated geometries. Future work will be directed at improved acceleration and iteration techniques, and implementation of the VNM within a kinetics code for use in solving time dependent problems.

REFERENCES


**TABLE 1. EIGENVALUES AND CONTROL ROD WORTH: TAKEDA BENCHMARKS I AND IV**

<table>
<thead>
<tr>
<th>Method</th>
<th>Takeda I</th>
<th>Takeda IV</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>keff (rod out)</td>
<td>keff (rod in)</td>
</tr>
<tr>
<td>VARIANT P1</td>
<td>.9296</td>
<td>.9328</td>
</tr>
<tr>
<td>VARIANT P3</td>
<td>.9774</td>
<td>.9632</td>
</tr>
<tr>
<td>Pn</td>
<td>.9776 ± .00058</td>
<td>.9630 ± .00078</td>
</tr>
<tr>
<td>S_n</td>
<td>.9772 ± .00007</td>
<td>.9624 ± .00008</td>
</tr>
<tr>
<td>Monte Carlo</td>
<td>.9778 ± .00046</td>
<td>.9623 ± .00048</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Machine Type</th>
<th>CPU Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Takeda I</td>
</tr>
<tr>
<td></td>
<td>VARIANT P1</td>
</tr>
<tr>
<td>SPARC 2</td>
<td>44.4</td>
</tr>
<tr>
<td>SPARC 20/50</td>
<td>15.1</td>
</tr>
<tr>
<td>IBM RS6000</td>
<td>6.4</td>
</tr>
<tr>
<td>CRAY XMP</td>
<td>7.2</td>
</tr>
</tbody>
</table>
### TABLE 2. $K_{eff}$ AND NODE-POWER MAXIMUM DEVIATIONS FOR 2-D HEXAGONAL GEOMETRY TEST CASESA

<table>
<thead>
<tr>
<th>Code/Code Option</th>
<th>ANL Large HWRe</th>
<th>VVER-1000d (0.5 albedo)</th>
<th>IAEAe (0.125 albedo)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$K_{eff}$ (%)</td>
<td>$P_{node}$ (%)</td>
<td>CPUe (s)</td>
</tr>
<tr>
<td>DIF3D-FD (Δ/2)</td>
<td>-0.0004</td>
<td>0.06</td>
<td>155.71</td>
</tr>
<tr>
<td>DIF3D-FD (Δ)</td>
<td>-0.0015</td>
<td>0.25</td>
<td>17.92</td>
</tr>
<tr>
<td>DIF3D-Nodal</td>
<td>-0.0167</td>
<td>1.44</td>
<td>1.32</td>
</tr>
<tr>
<td>ANC-HM</td>
<td>0.0048</td>
<td>0.2</td>
<td>0.035</td>
</tr>
<tr>
<td>VARIANT-40.11</td>
<td>0.0051</td>
<td>0.14</td>
<td>1.52</td>
</tr>
<tr>
<td>VARIANT-41.11</td>
<td>0.0002</td>
<td>0.03</td>
<td>2.43</td>
</tr>
<tr>
<td>VARIANT-61.11</td>
<td>-0.0002</td>
<td>0.01</td>
<td>2.66</td>
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<tr>
<td>VARIANT-62.11</td>
<td>-0.0000</td>
<td>0.00</td>
<td>3.26</td>
</tr>
<tr>
<td>VARIANT-41.33</td>
<td>0.0239</td>
<td>0.71</td>
<td>7.11</td>
</tr>
<tr>
<td>VARIANT-61.33</td>
<td>0.0239</td>
<td>0.71</td>
<td>8.63</td>
</tr>
<tr>
<td>VARIANT-62.33</td>
<td>0.0230</td>
<td>0.69</td>
<td>16.51</td>
</tr>
</tbody>
</table>

- Deviations in all cases are relative to reference fine-mesh diffusion results.
- The VARIANT solution designated as VARIANT-mn.ij employs polynomials of order m for the within-node flux and source and order n for the node-surface currents, and the P$_3$ and P$_j$ (e.g. P$_3$) transport approximations within the node and on the node-surface, respectively.
- The DIF3D-FD(Δ/2) and DIF3D-FD(Δ) solutions were obtained using 384 and 96 triangular cells/hexagon, respectively, and were used to obtain the reference FD solution via Richardson extrapolation.
- The DIF3D-FD(Δ/2) and DIF3D-FD(Δ) solutions were obtained using 864 and 216 triangular cells/hexagon, respectively, and were used to obtain the reference FD solution via Richardson extrapolation.
- CPU time on the IBM RS6000 workstation.

### TABLE 3. REACTIVITY CHANGES FOR TWO THREE-DIMENSIONAL REBUS BENCHMARKS

<table>
<thead>
<tr>
<th>Method</th>
<th>XYZ Benchmark</th>
<th>Hex-Z Benchmark</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Initial $K_{eff}$</td>
<td>Final $K_{eff}$</td>
</tr>
<tr>
<td>VARIANT P$_1$</td>
<td>1.06109</td>
<td>.80719</td>
</tr>
<tr>
<td>VARIANT P$_3$</td>
<td>1.06630</td>
<td>.80237</td>
</tr>
<tr>
<td>DIF3D FD</td>
<td>1.06440</td>
<td>.80739</td>
</tr>
<tr>
<td>DIF3D Nodal</td>
<td>1.06144</td>
<td>.80729</td>
</tr>
</tbody>
</table>
TABLE 4. CPU TIMES FOR TWO THREE-DIMENSIONAL REBUS BENCHMARKS

<table>
<thead>
<tr>
<th>Method</th>
<th>XYZ Benchmark</th>
<th>Hex-Z Benchmark</th>
</tr>
</thead>
<tbody>
<tr>
<td>VARIANT P₁</td>
<td>29.6 (37.32)</td>
<td>34.9 (48.9)</td>
</tr>
<tr>
<td>VARIANT P₃</td>
<td>573. (581.)</td>
<td>1170. (1190.)</td>
</tr>
<tr>
<td>DIF3D FD</td>
<td>11.3 (29.1)</td>
<td>29.4 (62.8)</td>
</tr>
<tr>
<td>DIF3D Nodal</td>
<td>15.9 (34.0)</td>
<td>27.1 (60.1)</td>
</tr>
</tbody>
</table>

* The first time listed corresponds to CPU time spent on neutronics, and the time in parenthesis is the total REBUS job time.

FIGURE 1. AZMY BENCHMARK: FLUX NEAR VACUUM BOUNDARY (Y=9.84 CM)