VARIATIONAL NODAL PERTURBATION THEORY
WITH ANISOTROPIC SCATTERING

Kirsten F. Laurin-Kovitz
Reactor Analysis Division
Argonne National Laboratory
Argonne, IL 60439
(630)252-4143
kkovitz@anl.gov

G. Palmiotti
Reactor Analysis Division
Argonne National Laboratory
Argonne, IL 60439
(630)252-2858
GPalmiotti@anl.gov

E.E. Lewis
Northwestern University
Department of Mechanical Engineering
Evanston, IL 60208
(847)491-3579
e-lewis@nwu.edu

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Kirsten F. Laurin-Kovitz and G. Palmiotti
Reactor Analysis Division
Argonne National Laboratory
Argonne, IL 60439
(630)252-4143

E.E. Lewis
Northwestern University
Department of Mechanical Engineering
Evanston, IL 60208
(847)491-3579

ABSTRACT

The variational nodal perturbation method previously developed in two- and three-dimensional Cartesian and hexagonal geometries using the diffusion and full or simplified spherical harmonics transport approximations, is extended to treat problems with anisotropic scattering. The requisite solution to the adjoint transport equation with anisotropic scattering is formulated and incorporated into the VARIANT (VARIational Anisotropic Nodal Transport) option of the Argonne National Laboratory DIF3D production code. The method, which calculates changes in the critical eigenvalue due to perturbations arising from changes in the material cross sections, is demonstrated by applying perturbations to an anisotropic hexagonal benchmark. Exact and first order perturbation theory are used to calculate changes in the critical eigenvalue and compared to the change obtained by direct calculation in VARIANT. The time savings obtained by using perturbation theory is substantial; times for base forward and adjoint calculations are much greater than the times for perturbation calculations.

I. INTRODUCTION

Perturbation methods are useful for a variety of calculations such as changes in reactivity and sensitivity studies. The variational nodal method has been shown to be ideally suited for perturbation calculations; both diffusion and higher order transport calculations may be performed, and substantial computational savings over traditional fine mesh methods are obtained while maintaining comparable accuracy. Equally important, unlike other nodal methods, the physical adjoint obtained from discretizing the continuous adjoint transport equation is identical to the mathematical adjoint obtained by transposing the discretized forward adjoint equation.

Thus far variational nodal perturbation theory has been applied with the assumption of isotropic scattering using spherical harmonics and, more recently, simplified spherical harmonics angular approximations. In the following section, we extend the formulation to include both within-group and group-to-group anisotropic scattering. In section III numerical results are given for problems in two-dimensional hexagonal geometry. Detailed descriptions of the inclusion of anisotropic scattering in variational nodal methods using both spherical harmonics ($P_n$) and simplified spherical harmonics ($SP_n$)

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approximations are given in references 3 and 4 respectively. Thus for brevity we utilize the notation which is common to these two papers to present a unified derivation of the perturbation equations with anisotropic scattering.

II. THEORY

The defining feature of the variational nodal method (VNM) is a variational principle for the even-parity form of the within-group transport equation in which odd-parity Lagrange multipliers along nodal interfaces guarantee neutron conservation for each node. Even- and odd-parity components of the angular flux may be represented with either $P_N$ or $S_{PN}$ approximations, and complete polynomials approximate the spatial dependence of the even- and odd-parity components within the nodes and along the interfaces respectively. The VNM functional consists of a superposition of nodal functionals. After applying the Ritz procedure within the VNM, these nodal functionals for node $V$, reduce to the algebraic form

$$ F_V \left[ \zeta_V, \chi_V \right] = \zeta_V^T A_V \zeta_V - 2 \zeta_V^T s_V + 2 \zeta_V^T M_V \chi_V . \tag{1} $$

Here $\zeta_V$ and $\chi_V$ are the unknown coefficients of the even- and odd-parity flux components within the node and along the interface, respectively, and $s_V$ is the group source. The elements of the $A$ and $M$ matrices are space-angle integrals over the known trial functions; $A$ also contains cross sections. While the forms of the matrices are similar, the dimension is quite different for $P_N$ and $S_{PN}$ approximations owing to the fact that in three dimensions there are $N(N+1)/2$ even-parity angular trial functions in a $P_N$ approximation but only $(N+1)/2$ in an $S_{PN}$ approximation. Since $A$ is symmetric, the adjoint functional corresponding to (1) may be written simply as

$$ F_V \left[ \zeta_V^*, \chi_V^* \right] = \zeta_V^* T A_V \zeta_V^* - 2 \zeta_V^* T s_V^* - 2 \zeta_V^* M_V \chi_V^* , \tag{2} $$

where $s^*$ is the group source term.

The foregoing functionals have the same form for isotropic or anisotropic scattering. However, as detailed in References 3 and 4, inclusion of within-group anisotropic scattering modifies the elements of $A$, but does not destroy its symmetry. Likewise, with the inclusion of anisotropic scattering, the group source $s$, no longer carries only isotropic moments, and is divided into even- and odd-parity components

$$ s_V = s_V^+ + T_V s_V^- \tag{3} $$

where $T_V$ is a matrix coupling even- to odd-parity within node moments. Likewise for the adjoint

$$ s_V^* = s_V^* + T_V s_V^* . \tag{4} $$

In variational nodal codes the within-group equations are solved by requiring the functional to be stationary with respect to variations in $\zeta_V$ and $\chi_V$. A change in variables is made to cast the resulting equations in response matrix form. This procedure does not concern us here, other than to note that is has been successfully implemented with anisotropic scattering for both the forward and adjoint forms of the equations. Our task is to first assemble the functionals in global form and then incorporate the resulting equations in a multigroup form which allows the necessary perturbation expressions to be obtained.
The global equations are obtained by noting that the global functionals are just the superpositions

\[ F[\zeta, \chi] = \sum_v F_v[\zeta_v, \chi_v], \]  

and

\[ F^*[\zeta^*, \chi^*] = \sum_v F^*_v[\zeta^*_v, \chi^*_v]. \]

First we construct global within-group vectors for the even-parity flux and sources from the corresponding nodal vectors:

\[ \zeta = \begin{bmatrix} \zeta_1 \\ \zeta_2 \\ \vdots \\ \zeta_v \\ \vdots \end{bmatrix}, \quad s = \begin{bmatrix} s_1 \\ s_2 \\ \vdots \\ s_v \\ \vdots \end{bmatrix}, \quad \zeta^* = \begin{bmatrix} \zeta_1^* \\ \zeta_2^* \\ \vdots \\ \zeta_v^* \\ \vdots \end{bmatrix}, \quad s^* = \begin{bmatrix} s_1^* \\ s_2^* \\ \vdots \\ s_v^* \\ \vdots \end{bmatrix} \]

The odd-parity interface fluxes must be mapped onto global vectors \( \chi \) and \( \chi^* \) through transformations of the form

\[ \chi_v = \Pi_v \chi, \quad \chi_v^* = \Pi_v \chi^* \]

where the Boolean operator \( \Pi_v \) is a matrix containing one entry of +1 or -1 per row. Applying these local-global within-group transformations to the forward and adjoint functionals yields, for group \( g \),

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

\[ F^*[\zeta^*, \chi^*] = \zeta^{*T} A^* \zeta - 2\zeta^{*T} s^* - 2\zeta^{*T} M^* \chi^* \]

where

\[ A = \begin{bmatrix} A_1 & 0 & 0 & 0 & 0 \\ 0 & A_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & A_v & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \quad M = \begin{bmatrix} M_1 \Pi_1 \\ M_2 \Pi_2 \\ \vdots \\ M_v \Pi_v \end{bmatrix} \]
Taking the variation of the global forward and adjoint functionals with respect to $\zeta$ and $\chi$ and their adjoints yields the following set of global within-group equations:

$$\begin{bmatrix} A & M \\ -M^T & 0 \end{bmatrix} [\zeta] = [s], \quad (11)$$

and

$$\begin{bmatrix} A & -M^T \\ M^T & 0 \end{bmatrix} [\chi^*] = [s^*]. \quad (12)$$

Since $A$ is symmetric, the adjoint coefficient matrix is the transpose of the forward coefficient matrix as required.

Before forming the multigroup equations, it is necessary to write the global group sources explicitly in terms of their even- and odd-parity components. If we first define

$$s = s^+ + T s^- \quad (13)$$

and

$$s^* = s^{*+} + T s^{*-} \quad (14)$$

Designating these within-group equations with the subscript $g$, we may form a single set of multigroup equations with the following definitions. Let

$$\tilde{A} = \begin{bmatrix} A_1 & 0 & 0 & 0 & 0 \\ 0 & A_2 & 0 & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & A_g & 0 \\ 0 & 0 & 0 & 0 & \cdots \end{bmatrix}, \quad \tilde{M} = \begin{bmatrix} M & 0 & 0 & 0 & 0 \\ 0 & M & 0 & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & M & 0 \\ 0 & 0 & 0 & 0 & \cdots \end{bmatrix}, \quad \tilde{T} = \begin{bmatrix} T_1 & 0 & 0 & 0 & 0 \\ 0 & T_2 & 0 & 0 & 0 \\ 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & T_g & 0 \\ 0 & 0 & 0 & 0 & \cdots \end{bmatrix}$$

where the $-$ notation will henceforth be used to indicate multigroup quantities.
Similarly, the multigroup even- and odd-parity flux and source vectors are defined

\[
\vec{\varphi} = \begin{bmatrix} \zeta_1 \\ \zeta_2 \\ \vdots \\ \zeta_g \\ \vdots \\ \zeta_g \end{bmatrix}, \quad \vec{\chi} = \begin{bmatrix} \chi_1 \\ \chi_2 \\ \vdots \\ \chi_g \\ \vdots \\ \chi_g \end{bmatrix}, \quad \vec{s}^\pm = \begin{bmatrix} s_1^\pm \\ s_2^\pm \\ \vdots \\ s_g^\pm \end{bmatrix},
\]

and their adjoint counterparts are

\[
\vec{\varphi}^* = \begin{bmatrix} \zeta_1^* \\ \zeta_2^* \\ \vdots \\ \zeta_g^* \\ \vdots \\ \zeta_g^* \end{bmatrix}, \quad \vec{\chi}^* = \begin{bmatrix} \chi_1^* \\ \chi_2^* \\ \vdots \\ \chi_g^* \\ \vdots \\ \chi_g^* \end{bmatrix}, \quad \vec{s}^{*\pm} = \begin{bmatrix} s_1^{*\pm} \\ s_2^{*\pm} \\ \vdots \\ s_g^{*\pm} \end{bmatrix}.
\]

From these definitions, we find the multigroup form of equations (11) and (12):

\[
\begin{bmatrix} \tilde{A} & \tilde{M} \\ -\tilde{M}^T & 0 \end{bmatrix} \begin{bmatrix} \vec{\varphi} \\ \vec{\chi} \end{bmatrix} = \begin{bmatrix} I & \tilde{T} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \vec{s}^+ \\ \vec{s}^- \end{bmatrix}. \tag{15}
\]

and

\[
\begin{bmatrix} \tilde{A} & -\tilde{M} \\ \tilde{M}^T & 0 \end{bmatrix} \begin{bmatrix} \vec{\varphi}^* \\ \vec{\chi}^* \end{bmatrix} = \begin{bmatrix} I & -\tilde{T} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \vec{s}^{*+} \\ \vec{s}^{*-} \end{bmatrix}. \tag{16}
\]

The group-to-group anisotropic scattering somewhat complicates the source vectors. For the even-parity term

\[
\vec{s}^+ = \left[ \frac{1}{k} \tilde{F} + \tilde{C}^+ \right] \vec{\varphi}, \tag{17}
\]
where $\bar{F}$ is the fission operator and (in the absence of upscattering) $\bar{C}^+$ is the strictly lower triangular matrix containing the even-parity components of the group-to-group scattering cross sections. Likewise

$$\bar{s}^{+} = \left[ \frac{1}{\tilde{k}} \bar{F}^T + \bar{C}^+ \right] \bar{\zeta}^* .$$

(18)

The odd-parity source is obtained from a recursive relationship of the form

$$\bar{s}^- = \bar{C}^- \bar{D} \bar{s}^-- \bar{C}^- \bar{T}^T \bar{\zeta}$$

(19)

where $\bar{C}^-$ (in the absence of upscattering) is the strictly lower triangular matrix containing the odd-parity group-to-group scattering cross sections, and $\bar{D}$ is a diagonal matrix containing $(\sigma_g - \bar{\sigma}_{gm})^{-1}$ as its elements. Thus we have

$$\bar{T} \bar{s}^- = - \bar{T} \left[ I - \bar{C}^- \bar{D} \right]^{-1} \bar{C}^- \bar{T}^T \bar{\zeta} ,$$

(20)

and the corresponding adjoint source contribution is

$$\bar{T} \bar{s}^* = - \bar{T} \left[ \bar{T} \left[ I - \bar{C}^- \bar{D} \right]^{-1} \bar{C}^- \right]^T \bar{T} \bar{\zeta}^* .$$

(21)

Now we are prepared to write the forward and adjoint equations in a form which will serve as the basis for the perturbation calculations. First, for brevity we consolidate the group-to-group scattering terms as

$$\bar{C} = \bar{C}^+ - \bar{T} \left[ I - \bar{C}^- \bar{D} \right]^{-1} \bar{C}^- \bar{T}^T ,$$

thus from equations (15) and (16) we obtain

$$\begin{bmatrix} \tilde{A} & \tilde{M} \\ -\tilde{M}^T & 0 \end{bmatrix} [\tilde{\zeta}] = \frac{1}{\tilde{k}} \begin{bmatrix} \bar{F}^T & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \tilde{\zeta} \\ \tilde{\chi} \end{bmatrix} + \begin{bmatrix} \bar{C}^+ & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \bar{\zeta} \\ \bar{\chi} \end{bmatrix}. $$

(22)

And

$$\begin{bmatrix} \tilde{A} - \tilde{M} \\ \tilde{M}^T & 0 \end{bmatrix} [\tilde{\zeta}^*] = \frac{1}{\tilde{k}} \begin{bmatrix} \bar{F}^T & 0 \\ 0 & 0 \end{bmatrix} [\tilde{\zeta}^*] + \begin{bmatrix} \bar{C}^- & 0 \\ 0 & 0 \end{bmatrix} [\bar{\zeta}^*].$$

(23)

Perturbation expressions can now be derived from the global form of the forward and adjoint variational nodal equations. The perturbed state is indicated by adding primes to the forward equation

$$\begin{bmatrix} \tilde{A}' & \tilde{M}' \\ -\tilde{M}'^T & 0 \end{bmatrix} [\tilde{\zeta}'] = \frac{1}{\tilde{k}} \begin{bmatrix} \bar{F}' & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \tilde{\zeta}' \\ \tilde{\chi}' \end{bmatrix} + \begin{bmatrix} \bar{C}' & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \bar{\zeta}' \\ \bar{\chi}' \end{bmatrix}. $$

(24)
We next premultiply the perturbed forward equation (24) by the unperturbed adjoint flux vectors, 

\[
[\tilde{\varphi}' \tilde{\chi}']^T
\]

yielding

\[
\tilde{\varphi}'^T \tilde{A} \tilde{\varphi} - \tilde{\chi}'^T \tilde{M} \tilde{\varphi} = \tilde{\varphi}'^T \left( k \tilde{F} + \tilde{C} \tilde{\gamma} \right) + \tilde{\chi}'^T \tilde{C} \tilde{\gamma}'.
\] (25)

Transposing the adjoint equation (23) and postmultiplying by the perturbed forward flux, 

\[
[\tilde{\varphi}' \tilde{\chi}']^T
\]

yields

\[
\tilde{\varphi}'^T \tilde{A} \tilde{\varphi} + \tilde{\chi}'^T \tilde{M} \tilde{\varphi} - \tilde{\chi}'^T \tilde{M} \tilde{\varphi} = \tilde{\varphi}'^T \left( k \tilde{F} \tilde{\gamma}' + \tilde{\chi}'^T \tilde{C} \tilde{\gamma}' \right).
\] (26)

The perturbed state consists of changes in the material cross sections contained in the \( \tilde{A} \), \( \tilde{F} \) and \( \tilde{C} \) matrices and can be written as \( \tilde{A}' = \tilde{A} + \delta \tilde{A} \), \( \tilde{F}' = \tilde{F} + \delta \tilde{F} \), and \( \tilde{C}' = \tilde{C} + \delta \tilde{C} \). Since \( \tilde{M} \) contains no cross sections, \( \delta \tilde{M} = 0 \). To obtain an exact expression for the change in the eigenvalue, \( \delta k = k' - k \), that results from these cross section perturbations, we subtract equation (26) from (25) and rearrange terms,

\[
\frac{\delta k}{k'k} = \frac{1}{k'} \tilde{\varphi}'^T \delta \tilde{F} \tilde{\varphi}' + \tilde{\varphi}'^T \delta \tilde{C} \tilde{\gamma}' - \tilde{\varphi}'^T \delta \tilde{A} \tilde{\gamma}'.
\] (27)

The first order approximation of the eigenvalue perturbation is obtained by setting \( k' = k \), expanding \( \tilde{\gamma}' \) into \( \tilde{\gamma} + \delta \tilde{\gamma} \) and eliminating all second order terms. This is equivalent to replacing the perturbed quantities, \( \tilde{\gamma}', k' \) and \( \sigma' \) with the corresponding unperturbed quantities. The first order expression for the change in the eigenvalue becomes

\[
\frac{\delta k}{k^2} = \frac{1}{k} \tilde{\varphi}'^T \delta \tilde{F} \tilde{\varphi}' + \tilde{\varphi}'^T \delta \tilde{C} \tilde{\gamma} - \tilde{\varphi}'^T \delta \tilde{A} \tilde{\gamma}.
\] (28)

III. RESULTS

The theory developed here has been implemented in conjunction with the VARIANT's module of the DIF3D6 code at Argonne National Laboratory. The adjoint solution algorithm for anisotropic scattering has been incorporated within VARIANT. To verify the accuracy of the adjoint solutions for anisotropic scattering problems, comparison was made between VARIANT forward and adjoint eigenvalues. The forward and adjoint eigenvalues were in agreement for all cases to within convergence criteria.

A post-processor to VARIANT has been written to perform perturbation calculations and the extensions for anisotropic scattering have been incorporated. This code combines cross section and geometry files with the forward and adjoint flux files from VARIANT to calculate first-order and/or exact eigenvalue perturbations. Here we present results for perturbations applied to an anisotropic two-dimensional hexagonal benchmark using P1, SP3 and P3 approximations.
The Anisotropic Hexagonal Benchmark depicted in Figure 1 was used to test the adjoint solution algorithm and the perturbation method for problems with anisotropic scattering. The cross sections and two-group structure are given in Reference 3. The perturbations applied to the benchmark consist of increasing the scattering cross sections in the outer ring of the core. Both isotropic and anisotropic scattering cross sections were perturbed by the same relative amount. Table 1 and Figure 2 show the results of these perturbations.

The values in Table 1 show that in the diffusion and SP₃ approximation, the reactivity change predicted by exact theory perturbation exactly matches the actual change computed from the VARIANT eigenvalues. However, in the presence of group-to-group anisotropic perturbations, slight differences exist between the VARIANT eigenvalue change and the exact theory perturbation calculations in the full P₃ transport approximation. The differences, possibly due to round-off or finite convergence in the code, are under investigation. In Figure 2, the P₃ and SP₃ results are virtually indistinguishable. First order results in P₁, SP₃ and P₃ approximations hold well for the scattering increases since the effect of the perturbation is nearly linear.

Typical runs times for the two-dimensional hexagonal benchmark considered here ranged from 16 seconds (P₁) to 140 seconds (P₃) for the base forward and adjoint calculations and from 10 seconds (P₁) to 60 seconds (P₃) for the perturbation calculations. The same polynomial expansions were used in all cases: sixth order expansion within the node and linear expansion on the nodal interfaces. The eigenvalue convergence criteria was 10⁻⁷.

![Figure 1. Anisotropic Hexagonal Benchmark Configuration](image-url)
Table 1. -- Anisotropic Hexagonal Benchmark Scattering Perturbation Results

<table>
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<tr>
<th>VARIANT approx.</th>
<th>% increase in scattering</th>
<th>Eigenvalues</th>
<th>Change in Reactivity (δ(k/k'))</th>
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<td>VARIANT</td>
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<td>P₁ diffusion</td>
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Figure 2. Anisotropic Hexagonal Benchmark Scattering Perturbation with Group to Group Scattering
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