

ANL/RA/CP--89399
CONF-9606116--20

Anisotropic Scattering in the Variational Nodal Simplified Spherical Harmonics Formulation

by

Elmer E. Lewis
Giuseppe Palmiotti

Reactor Analysis Division
Argonne National Laboratory
9700 South Cass Avenue
Argonne, Illinois 60439

The submitted manuscript has been authored
by a contractor of the U. S. Government
under contract No. W-31-109-ENG-38.
Accordingly, the U. S. Government retains a
nonexclusive, royalty-free license to publish
or reproduce the published form of this
contribution, or allow others to do so, for
U. S. Government purposes.

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

*Work supported by the U.S. Department of Energy, Nuclear Energy Programs under
Contract W-31-109-ENG-38

MASTER

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED *JK*

DISCLAIMER

**Portions of this document may be illegible
in electronic image products. Images are
produced from the best available original
document.**

Anisotropic Scattering in the Variational Nodal Simplified Spherical Harmonics Formulation

E. E. Lewis & G. Palmiotti

Under the assumption of isotropic scattering, the simplified spherical harmonics method (SP_N) was recently formulated in variational nodal form¹ and implemented successfully as an option of the VARIANT code.² We here remove the isotropic scattering restriction. The variational nodal form of the SP_N approximation is formulated and implemented with both within-group and group-to-group anisotropic scattering. Results are presented for a model problem previously utilized with the standard P_N variational nodal method.

The derivation of the SP_N equations with anisotropic scattering added parallels the isotropic case.¹ We first write the slab geometry P_N approximation for odd-order N . Let Ψ and χ be vectors of length $(N+1)/2$ of the even- and odd-parity moments. Then the P_N approximation may be written as the pair of equations

$$E \frac{d}{dx} \chi + \Sigma_e \Psi = s^+$$

and

$$E^T \frac{d}{dx} \Psi + \Sigma_o \chi = s^- ,$$

where E is a two-stripe lower triangular coefficient matrix,

$$E_{mm'} = (2m-1)\delta_{mm'} + 2m\delta_{m,m'+1} , \quad 1 \leq m, m' \leq (N+1)/2$$

and the within-group anisotropic cross sections appear in the diagonal matrices

$$[\Sigma_e]_{mm'} = (4m-3)(\sigma - \sigma_{2m-2})\delta_{mm'} , \quad 1 \leq m, m' \leq (N+1)/2$$

and

$$[\Sigma_o]_{mm'} = (4m-1)(\sigma - \sigma_{2m-1})\delta_{mm'} , \quad 1 \leq m, m' \leq (N+1)/2 .$$

The even- and odd-parity group-to-group anisotropic cross sections appear in the group source terms. s^+ and s^- respectively. Eliminating χ yields the even-parity equation

$$-\frac{d}{dx} \mathbf{E} \Sigma_o^{-1} \mathbf{E}^T \frac{d}{dx} \psi + \Sigma_e \psi = s^+ - \frac{d}{dx} \mathbf{E} \Sigma_o^{-1} s^- ,$$

along with the auxiliary relationship

$$\chi = -\Sigma_o^{-1} \mathbf{E}^T \frac{d}{dx} \psi + \Sigma_o^{-1} s^- .$$

The simplified spherical harmonics approximation is obtained simply by making the replacement $\frac{d}{dx} \rightarrow \vec{\nabla}$, letting the even-parity quantities become functions of three spatial dimensions: $\psi(x) \rightarrow \psi(\vec{r})$, $s^+(x) \rightarrow s^+(\vec{r})$, and ordering the odd-parity quantities into spatial vectors in the three dimensions: $\chi(x) \rightarrow \vec{\chi}(\vec{r})$, $s^-(x) \rightarrow \vec{s}^-(\vec{r})$. The even-parity form of the simplified spherical harmonics equation is then

$$-\vec{\nabla} \cdot \mathbf{E} \Sigma_o^{-1} \mathbf{E}^T \vec{\nabla} \psi + \Sigma_e \psi = s^+ - \vec{\nabla} \cdot \mathbf{E} \Sigma_o^{-1} \vec{s}^- , \quad (1)$$

with the auxiliary relationship

$$\vec{\chi} = -\Sigma_o^{-1} \mathbf{E}^T \vec{\nabla} \psi + \Sigma_o^{-1} \vec{s}^- . \quad (2)$$

The SP_N approximation may be expressed variationally by writing a global functional which is a superposition of nodal contributions of the form

$$\begin{aligned} F_v[\psi, \chi] = \int_v dV [(\vec{\nabla} \psi^T) \mathbf{E} \Sigma_o^{-1} \mathbf{E}^T (\vec{\nabla} \psi) + \psi^T \Sigma_e \psi - 2 \psi^T s^+ \\ - 2(\vec{\nabla} \psi^T) \cdot \mathbf{E} \Sigma_o^{-1} \vec{s}^-] + 2 \int_v d\Gamma \psi^T \mathbf{E} \hat{n} \cdot \vec{\chi} \end{aligned}$$

This may be shown to yield Eqs. (1) and (2) as the Euler-Lagrange equations in the nodes and at the interfaces respectively.

The procedure for obtaining within-group response matrix equations is identical to that published previously.³ Spatial polynomials approximate the element of ψ and χ ; a Ritz procedure is applied, and the resulting equations are converted to response matrix form. The same spatial approximations are applied to the group source vectors. These have the form

$$s_g^+ = \frac{1}{K} \chi_g \sigma_{fg} \Phi_g + \Sigma_{egg'} \Psi_{g'}$$

and

$$\vec{s}_g^- = \Sigma_{ogg'} \Sigma_{og}^{-1} (\vec{s}_{g'}^- - E \vec{\nabla} \Psi_{g'}) ,$$

where repeated subscripts signify summation, and the group-to-group anisotropic scattering cross sections are contained in the diagonal matrices

$$[\Sigma_{egg'}]_{mm'} = (4m-3) \sigma_{2m-2,gg} \delta_{mm'}$$

and

$$[\Sigma_{ogg'}]_{mm'} = (4m-1) \sigma_{2m-1,gg} \delta_{mm'} .$$

Note that the need to store the χ_g is eliminated by writing the odd-parity source as a recursive relationship. These forms allow the SP_N approximation with anisotropic scattering to be incorporated into the variational nodal code VARIANT in a relatively straight-forward manner.

Eigenvalue results are shown in Table I for the two-group, two-composition, x-y geometry benchmark described elsewhere.³ The P₃ results with linear interface conditions may be considered to be reference values. All of the calculations utilize fourth-order complete polynomial approximations within the nodes. Even in the presence of anisotropic scattering, the deviations between SP₃ and P₃ results are roughly a tenth of a percent or less. In some cases the SP_N approximation with flat interface approximation may display less error than the companion linear approximation. This results from truncation error cancellation between spatial and angular approximations. The substantial CPU savings accrued from SP₃ approximations is apparent; as discussed elsewhere,¹ P₃ approximations with flat interface conditions result in unacceptable truncation errors.

References:

1. E. E. Lewis and G. Palmiotti, "Comparison of Simplified and Standard Spherical Harmonics in the Variational Nodal Method," *Trans. Am. Nucl. Soc.* **73**, 200 (1995)
2. G. Palmiotti, E. E. Lewis and C. B. Carrico, VARIANT: VARIational Anisotropic Nodal Transport for Multidimensional Cartesian and Hexagonal Geometry Calculation, ANL-95/40, Argonne National Laboratory, 1995.
3. G. Palmiotti, C. B. Carrico and E. E. Lewis, "Variational Nodal Transport Methods with Anisotropic Scattering," *Nucl. Sci. Eng.* **115**, 233 (1993)

Table I
Eigenvalues and CPU Times
for Model Problem

Scattering	SP ₃ -flat	SP ₃ -linear	P ₃ - linear
P ₀	1.30339 1.33 sec.	1.30618 2.21 sec.	1.30465 4.82 sec.
P ₁	1.30074 1.54 sec.	1.30219 3.39 sec.	1.30196 6.26 sec.
P ₃	1.30232 1.74 sec.	1.30438 3.82 sec.	1.30346 10.22 sec.