INTERFACE-FLUX NODAL TRANSPORT METHOD

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ABSTRACT

The development of the interface-flux nodal (IFN) method is presented to determine the flux distribution in reactor cells, cores and shielding. The method offers geometric flexibility, high order of spatial expansions of the node-interior sources and the node surface quantities.

The surface-integral formulation is reduced to response-matrix-like global equations through coupling coefficients which are generalized expressions for escape and transmission probabilities. The spatial distribution of the neutron flux may be represented by high order polynomials using geometric basis functions determined by a least-square minimalization technique. The angular dependency of the outgoing/incoming surface flux components is treated using a general DP_n expansion and the spatial variation is handled with a boundary element technique. The scattering iterations are eliminated by using an explicit expansion of the scalar fluxes.

Based on the IFN method a computer code has been developed capable of calculating fixed-source and eigenvalue problems. Test problems for 1-D and 2-D X-Y and hexagonal geometries are presented including comparison with other techniques to demonstrate the validity and accuracy of the IFN method.

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1. INTRODUCTION

The integral form of the neutron transport equation is very well suited and is widely used to analyze neutron transport in tightly coupled, relatively small heterogeneous medium. The integral formulation can also be extended to large geometries by applying nodal techniques providing the basis for the early development of the nodal transport methods.

The nodal transport methods solve the neutron transport problem in large geometries by dividing the domain into regions and derive coupling equations to describe the transfer between the nodes. The node interior solutions are coupled to the adjacent ones through the angular flux components entering and leaving the nodes. Various approximations are utilized to describe the nodal coupling depending on the angular and spatial representations of the unknown flux components.

Most of the early techniques were based on the interface-current method¹⁻⁴ and were extremely successful in solving complex geometries on the fuel assembly level, generally employing flat or linear spatial expansions of the node interior sources and surface currents. The integral equations are projected onto the expansion functions resulting in a system of coupled equations for each cell with matrix coefficients which are closely related to various probability expressions (transmission and escape probabilities).

The principal advantage of these methods is their relative efficiency due to the decoupling of the regions resulting in relatively small, but dense matrices. The use of the flat flux approximation and the general limitation on the low order spatial expansions of the node interior sources and the surface angular fluxes limits the node sizes especially in regions where the flux varies rapidly.

The recently developed nodal transport methods circumvent these limitations using the highly successful transverse integration technique originally applied to neutron diffusion problems. In these methods high order spatial approximations of the node interior fluxes and sources are possible including the angular surface fluxes and multidimensional regular geometries can easily be accommodated.

In most of these nodal methods⁵⁻⁶, quasi-one-dimensional transport equations are derived in each cell which are coupled through the transverse leakage terms.

The node interior one-dimensional equations may be solved with a variety of techniques such as integral or S_n methods. The global equations are obtained by taking the spatial moments of the transverse flux components both inside and on the node surface.

The node interior solution is decoupled from the surface angular representation leading to inconsistencies with regard to the type and level of angular approximations applied within the node and on the cell interfaces. In addition, the various approximations used in these methods usually lead to the inconsistent formulation of the directional coupling terms or to the introduction of additional unknowns increasing the computational complexity.

In the second class of these modern methods,⁷⁻⁹ the powerful nodal techniques are applied to the spatial differencing of the discrete ordinate equations. The angular dependencies are approximated by using the discrete ordinate technique resulting in a consistent treatment of the angular approximations both inside and on the surface of the nodal cell. The methods employ spatial marching techniques combined with the iteration on the scattering source.

A third class of these nodal methods utilizes a variational approach to the solution of the neutron transport equation^{10,11}. A variational functional is written that guarantees nodal balance for the even-parity form of the neutron transport equation. Complete polynomial trial functions are considered for the spatial and angular distributions allowing the utilization of the classical Ritz-procedure to reduce the transport equation into algebraic forms. The final equations are rearranged to obtain a matrix equation describing the spatial and angular moments of the outgoing partial currents in terms of the incoming moments and the interior group source values.

The method avoids the arbitrary approximation of the transverse leakages found in the previous nodal methods. The angular representation functions and the use of the high order complete polynomials for spatial expansion make this scheme very accurate and allow for geometric flexibility. The extension of the method to three-dimensional geometries is primarily limited by the numerical problems due to the large increase in the dimension of the nodal matrix.

The work on the variational formulation of the nodal transport problem indicates that the early surface-integral techniques (interface-current schemes) may also offer viable approaches in deriving a modern nodal transport scheme offering geometric flexibility, high order of spatial and angular expansions of the node-interior sources and the surface components, and the elimination of the scattering iteration through an explicit expansion.

In the main sections of this study, the development of the interface-flux nodal (IFN) method is presented. The method offers geometric flexibility and as such is not confined to any particular geometry. It is capable of high order spatial expansions of the node-interior fluxes and the node surface quantities and by using an explicit expansion of the scalar fluxes the iteration on the scattering source is eliminated.

The method is based on the surface-integral formulation of the transport problem and employs an approach of a point-to-point transport on each nodal surface. The coupling coefficients are similar to the probability expressions of the interface current schemes, but are simpler to calculate and may even be reduced to analytical expressions in special cases. The spatial dependence of the node interior sources may be expanded by high order complete polynomials.

The resulting compact nodal equations are assembled into a response-matrix-like global equations through the application of the interface constraints. The matrix coefficients are independent of the eigenvalue obviating the need for recurrent evaluation during the iterative process.

Section 2 will present the theoretical development of the IFN method including the detailed description of the various approximations applied at each step. The numerical techniques are briefly discussed in Section 3. Based on the theoretical development a computer code was written to implement the IFN method for numerical calculations. The results of the analysis of various one and two dimensional test problems are discussed in Section 4.

2. THEORETICAL DEVELOPMENT

The interface-flux nodal method is derived by considering the neutron transport problem in a spatial region composed of several homogeneous nodes. For each subsystem of cells the transport problem is reduced to a system of equation giving the outgoing angular interface-flux components in terms of the node interior sources and the incoming angular fluxes. The interaction between the nodes are included through the appropriate interface coupling conditions.

The angular flux inside a node is given by the integral transport equation as

$$\psi(r, \Omega) = \int_0^{R_s} \frac{1}{4\pi} F(r') e^{-\tau} dR + \psi^{in}(r_s, \Omega) e(-\tau_s) , \quad (1)$$

where each variable has the usual meaning i.e., $\psi(r, \Omega)$ is the angular flux, $r' = r - R\Omega$, τ is the optical length, the subscript s indicates a point on the nodal surface and $F(r')$ is the neutron emission density that includes the contribution from scattering and any internal or fission sources,

$$F(r) = \Sigma_s \phi + Q. \quad (2)$$

By locating the point of interest on the node boundary, $r = r_s$, and integrating the surface-integral equation for the outgoing angular flux components over $\Omega \cdot n > 0$ leads to

$$\begin{aligned} \phi^{\text{out}, l}(r_s) = & \int_{\Omega \cdot n > 0} \int_0^{R_s} \frac{1}{4\pi} F(r) e^{-\tau} (\Omega \cdot n)^l dR d\Omega + \\ & + \int_{\Omega \cdot n > 0} \psi^{\text{in}}(r_s, \Omega) e(-\tau_s) (\Omega \cdot n)^l d\Omega. \end{aligned} \quad (3)$$

The indices out/in indicates the outgoing/incoming angular flux components and l refers to the order of angular expansion.

The surface-integral equation cannot be solved without an appropriate coupling of the surface components to the neutron emission density. This may easily be accomplished if the node-interior scalar flux is expanded in terms of the node-surface values with the boundary supports at the same nodal surface points i.e.,

$$\phi(r) = \sum_j f(r'/r_j) \phi_j, \quad (4)$$

where, $f(r'/r_j)$ is the polynomial basis function at point r_j . The basis functions are two-dimensional high degree polynomials and are determined by using a least-squares minimalization approach. The singular value decomposition technique¹², used to generate the functions $f(r'/r_j)$, avoids the inversion of the usual normal equations which are usually ill-defined for most geometric configuration.

The surface angular components are expanded in the double P_n angular expansions i.e.,

$$\psi_i^{\text{out/in}, l}(r_s, \Omega) = \sum_{m=1, l} f_i^{\text{out/in}, m} (\Omega \cdot n)^l. \quad (5)$$

The expansion coefficients, $f_i^{\text{out/in},m}$, and the surface-flux components, $\phi^{\text{out/in},l}(r)$, are interrelated and a simple moments weighting scheme may be used to determine their relationships i.e.;

$$f_i^{\text{out/in},m} = \sum_l G_{ml} \phi^{\text{out/in},l} \quad , \quad (6)$$

where G_{ml} 's are the coefficients of the geometric matrix representing the relations of the nodal surface with respect to the normal directions.

The spatial variation of the surface flux components are incorporated by utilizing a boundary element technique, where the incoming components of the surface angular fluxes are expanded in basis function defined along the boundary of the node:

$$\psi^{\text{in}}(r_s, \Omega) = \sum_j h(r_s) \psi^{\text{in}}(\Omega) \quad . \quad (7)$$

Inserting the representations embodied in (4), (5) and (6) into the surface-integral equation (3), and utilizing the relation indicated in (7), leads to a system of approximate equations for each of the nodal surface points:

$$\phi_i^{\text{out},l} = \sum_j P_{ij}^l F_j + \sum_j \sum_m T_{ij}^{m,l} \phi_j^{\text{in},m} \quad . \quad (8)$$

The matrix coefficients P_{ij}^l and $T_{ij}^{m,l}$ are closely related to the escape and transmission probabilities and may be expressed as the basis function-weighted integrals of the Ki_n functions:

$$P_{ij}^l = \frac{1}{2\pi} \int_{\varphi} f(r'/r_j) \int_0^{\omega_s} (\Omega \cdot n)^l Ki_{l+1}(\Sigma_T \omega) d\omega d\varphi \quad , \quad (8a)$$

and

$$T_{ij}^{m,l} = 2 \int_{\Omega n} \sum_j h(r_{j,j+1}) (\Omega \cdot n)^l \alpha_j^m \psi_j^{\text{in},m} Ki_{l+2}(\Sigma_T \omega_1) d\Omega \quad . \quad (8b)$$

The nodal system of Eq.(8) may be coupled to global system equations through the node-surface boundary conditions. These conditions reflect the continuity of the angular flux at the boundary points and may be generalized by writing

$$\phi_i^{\text{in},1} = \sum_k \int_{\Omega_{ik}} \psi_k^{\text{out},1} (\Omega \cdot n)^1 d\Omega, \quad (9)$$

where k indicates adjacent nodal points and the angular integration extends over only the incoming directions.

The inclusion of Eq. (9) into (8) leads to the final equation for the nodal points as

$$A_i^1 \phi_i^{\text{out},1} = \sum_j P_{ij}^1 (\sum_s \phi_j^s + \sum_k C_{kj} \sum_s \phi_k^{\text{in},1} + \sum_k D_{kj} \sum_s \phi_k^{\text{out},1} + Q_j) + \sum_j \sum_{m=1,1} T_{ij}^{m,1} \phi_j^{\text{in},1}, \quad (10)$$

where the matrix coefficients C_{kj} and D_{kj} contain terms representing the coupling between neighbouring nodal points which may or may not overlap the incoming/outgoing angular directions.

The global system matrix equation may be written as,

$$A \phi^{\text{out}} = P (\phi^{\text{in}} + Q + \phi_k) + \sum_l T^l \phi^{\text{in},l}. \quad (10)$$

The diagonal elements of A contain the ingroup scattering terms eliminating the iteration on the scattering source. The matrices P and T^l are the nodal coupling coefficients and the coupling between adjacent nodal surface points are included in ϕ_k .

The global system equation (10) is treated on the sub-system level solving the nodal equations, represented by (8), utilizing the boundary conditions of (9) which connects the interface-flux angular moment components of the adjacent nodes.

3. NUMERICAL TECHNIQUES

The matrix coefficients of Eq. (8) are to be precalculated before the iteration on the flux components for each material and geometric configuration. The expression of (8a) may be simplified and actually is analytical for one variable along the particle tracking length. The integration over the angular variable has to be performed numerically and a simple Gaussian integration procedure is utilized.

The coefficients in (8b) are calculated also numerically assuming a linear spatial dependence along the nodal surface.

The integration between the nodal points also used a gaussian integration procedure. There are symmetry conditions based on the geometric configuration of the node which were utilized to reduce the number of calculations.

The global system of (10) and (8) are solved using the normal inner/outer iteration strategy. First, the nodal subsystem is solved by inverting A^1 using Gaussian elimination, and then the calculated outgoing components are used through Eq.(9) as the incoming values for the adjacent nodes. The SOR method is used in the outer iteration loop once an estimate is obtained for the eigenvalue. The average nodal flux may be determined through the balance equations.

4. TEST RESULTS

Based on the previously developed theory a computer code has been written to implement the IFN method for numerical calculations. A number of one- and two-dimensional test problems were analyzed to test the validity and accuracy of the proposed technique. The code can calculate fixed-source or eigenvalue problems employing the usual inner-outer iteration algorithm.

Figure 1 shows a fixed source one-dimensional slab problem that was used to examine the accuracy of the pointwise prediction of the surface-flux values at the node boundaries. Table 1 indicates the calculated scalar fluxes at the interval boundaries as compared to the discrete ordinate code ANISN. The maximum deviation is about 1% or less even at the vacuum boundary which is difficult to calculate.

In order to check the eigenvalue calculations, the k_{∞} value has been calculated for a homogeneous slab problem also analyzed in Ref. 13. The results indicate that for equal order of spatial polynomial expansions (linear for 1-D) the IFN method calculates k_{∞} values that are similar to the very accurate SURCU results (less than .01% deviation). In addition the analysis require far fewer spatial divisions than the ANISN discrete ordinate calculations indicating the potential for large spatial meshes without the loss of accuracy.

Table 3 list the results of a somewhat more complicated 1D heterogeneous, multigroup problem as compared with other analysis from Ref.4 again indicating good accuracy.

The X-Y fixed-source two-dimensional problem⁸, shown in Figure 2, is a highly absorbing model representing a difficult test to reproduce the interface fluxes far from the source region. The problem was solved on a sequence of different mesh sizes and order of spatial polynomial approximations. A pointwise relative error convergence of 10^{-4} was used on the interface-flux components. The zone-wise average fluxes, listed in Table 4, were calculated through the balance conditions once convergence was achieved.

For comparison the same problem was also calculated using the two-dimensional discrete ordinate code DOT with different spatial meshes and quadrature sets listing in Table 4 only the spatially converged results. The results indicate that accurate results can be obtained with increasing spatial polynomial expansions with relatively few spatial meshes. For comparison the result of a nodal transport calculation is also shown that uses S₄ quadrature set.

In order to test the geometric flexibility of the code, a hexagonal homogeneous problem¹⁴, shown on Figure 3, was also analyzed. The eigenvalue was calculated with different mesh sizes using equilateral triangles of varying sizes and different spatial polynomial expansions. The convergence criteria were 10^{-3} for the k_{∞} and 10^{-4} for the interface-fluxes. The results of the calculations are listed in Table 5a comparing them with those of Ref.14. The DITRI scheme is based on the characteristic method¹⁵ of solving the neutron transport equation. The TLC method is basically a nodal transport method with some features typical for characteristic methods.

The different schemes do not produce or converge to the same results, because the DITRI and TLC methods use low-order quadrature sets while the IFN technique does not employ discrete ordinate angular representations. The results indicate that accurate eigenvalues may be calculated with relatively coarse meshes.

The essential feature of the IFN method is the number of point used on the nodal surface. In order to examine the stability of the predicted k_{∞} , a sensitivity calculation was also conducted with regard to the number of surface points. Table 5b lists the obtained eigenvalues as a function of nodal points for a triangle of 4 cm height. The relative stability of the k_{∞} as the nodal points increase also indicates that the nodal matrix may be minimized reducing the calculational time.

In summary, the IFN method presented in this paper offers geometric flexibility combined with coarse-mesh capabilities.

5. References

1. R.SANCHEZ, *Nucl.Sci.Eng.*, **64**, 384(1977).
2. P.MOHANAKRISHNAN, *Prog.in Nucl.Energy*, Vol.7, 1-10(1981).
3. H.S.CHENG, et al., "A Nodal Integral Transport Method for Calculation of Two-Dimensional Power Distributions in Non-Uniform Lattices," *Proc. Conf. New Developments in Reactor Mathematics and Applications*, Idaho, CONF-710302, p. 655, (1971).
4. H.HAGGBLOM, *Nucl.Sci.Eng.*, **56**, 411(1975).
5. R.D.LAWRENCE, *Prog.in Nucl.Energy*, Vol.17, 271-301(1986).
6. M.R.WAGNER, "A Nodal Discrete-Ordinates Method for the Numerical Solution of the Multi-Dimensional Transport Equation," *Proc. Topl. Mtg. Computational Methods in Nucl. Eng.*, Williamsburg, Virginia, 1979, Vol.2,p.4, ANS(1979).
7. W.F.WALTERS, R.D.O'DELL, "Nodal Methods for Discrete-Ordinates Transport Problems in X-Y Geometry," *Proc.Int.Topl.Mtg.Advances in Mathematical Methods for the Solution of Nucl.Eng. Problems*, Munich, FRG, 1981, Vol.1, p.115, Kernforschungszentrum Karlsruhe (1981).
8. Y.Y.AZMY, *Nucl.Sci.Eng.*, **98**, 29(1988).
9. H.KHALIL, *Nucl.Sci.Eng.*, **90**, 263(1985).

10. I.DILBER, E.E.LEWIS, *Nucl.Sci.Eng.*, **91**, 132(1985).
11. E.E.LEWIS, *Nucl.Sci.Eng.*, **102**, 140-152(1989).
12. G.H.GOLUB, C.REINSCH, "Singular Value Decomposition and Least Squares Solutions," in *Handbook for Automatic Computation*, Volume II, *Linear Algebra*, edited by J.E.Wilkinson, C.Reinsch, Springer-Verlag, New York (1971).
13. J.STEPANEK, *Nucl.Sci.Eng.*, **78**, 53-65(1981).
14. W.F.WALTERS, "The TLC Scheme for Numerical Solution of the Transport Equation on Equilateral Triangular Meshes," *Proc. Topl.Mtg.Advances in Reactor Computations*, Salt Lake City, March 28-31, 1983, Vol.1.
15. E.W.LARSEN, R.E.ALCOUFFE, "The Linear Characteristic Method for Spatially Discretizing the Discrete-Ordinates Equation in (x,y)-Geometry," *Proc. ANS/ENS Joint Topical Meeting, Advances in Mathematical Methods for the Solution of Nuclear Engineering Problems*, April 27-29, 1981, Munich, **1**, 99(1981).

Figure 1. Test #1, fixed-source slab

REFL.

Figure 2. Test #4, X-Y fixed source

MATERIALS

$$\sum_T = .15$$

$$\sum_S = .14$$

$$v \sum_f = .03$$

Figure 3. Test #5, hexagonal eigenvalue problem

TABLE 1. TEST #1, BOUNDARY FLUXES

DISTANCE FROM BOUNDARY (cm)	ANISN	IFN	%
0.0	.04179	.04182	.06
.25	.06473	.06533	.90
.5	.08533	.08631	1.15
1.0	.12801	.12953	1.19
3.0	.39965	.40508	1.36
5.0	1.13650	1.13510	-.12
7.5	1.78347	1.77320	-.58

TABLE 2. TEST #2, EIGENVALUES

ANISN		SURCU		IFN	
S/N	k	M/N	k	M/N	k
4/100	.95207	0/20	.94984	1/1	.96161
8/100	.95316	1/20	.95348	1/20	.95706
16/100	.95343	3/2	.95345	1/24	.95337

Notes: S - quadrature set
 N - spatial intervals
 M - spatial polynomial expansion

TABLE 3. TEST #3, 1-D HETEROGENEOUS CELL, EIGENVALUES

METHOD	k
DTF-S4	.32759
DTF-S16	.32771
CASMO	.33111
IFN	.32093

TABLE 4. TEST #4, X-Y FIXED-SOURCE, ZONE AVERAGE FLUXES

METHOD	MESH	POLYNOMIAL ORDER	ZONE		
			I	II	III
INF	4x4	2	1.700	.3864-1*	.1778-2
		4	1.693	.3941-1	.1882-2
		6	1.691	.3949-1	.2081-2
	8x8	2	1.689	.4009-1	.1726-2
		4	1.686	.4049-1	.1768-2
		6	1.685	.4054-1	.1780-2
DOT	22x22	S4	1.679	.4127-1	.1908-2
		S8	1.682	.4095-1	.1849-2
		S16	1.683	.4074-1	.1807-2
NODAL		S4	1.676	.4159-1	.1992-2

* Read as 0.3864×10^{-1}

TABLE 5a, TEST #5, HEXAGONAL REACTOR, EIGENVALUE

TRIANGLE HEIGHT (cm)	METHOD			
	IFN	DITRI-S6	TLC-S4	DOT (DIFF.TH)
12	.5471	.5398	.6236	.5631
6	.5962	.5892	.6011	
4	.5999	.5980	.5995	
2	.5969	.6042	.5989	
1				

TABLE 5b, TEST #5, EIGENVALUE AS THE FUNCTION OF
THE NODAL POINTS

NODAL POINTS	k
5	.6053
10	.6052
20	.5928
30	.5999