FINITE ELEMENTS IN NEUTRON
TRANSPORT THEORY

E. H. Bareiss and I. K. Abu-Shumays
Northwestern University
Evanston, Illinois

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Abstract

An assessment of current multidimensional neutron transport theory calculations is made with respect to the use of large computational cells or finite elements. It is shown that many variational methods exist to accomplish a given job. The symmetrization processes are compared, and the Vladimirov-Lagrange Functional is derived. The numerical behavior is discussed, and illustrated by examples in tables and graphs, together with finite difference calculations for identical problems. Because of the great variety of numerical techniques to solve neutron transport problems, a rating of these methods is necessary to minimize development and user's cost. A general, systematic evaluation procedure is described of which a computerized version is under development at Northwestern University. The importance of knowing the analytic behavior of the mathematical solution to achieve computational efficiency is demonstrated by numerical examples and the behavior at corners is analyzed in phase-space. Using the S_N - methods as an example it is shown that the global behavior of the numerical solutions can be predicted from individual matrix blocks. Also by example it is shown that great computational economy can be achieved by using space and angular approximations in a predetermined appropriate relationship.

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1. Introduction

The words "Finite Element Method" (FEM) leave some mystic connotation associated with them. To give a precise definition of FEM is hard. In structural mechanics, the definition used to be simple: To minimize the energy functional for piecewise continuous (conforming) and nonconforming multivariate polynomial trial functions. A generalization of this concept would be to minimize the Lagrange functional of a given Euler equation for conforming and nonconforming rational finite element trial functions. But the use of the word FEM also appears in connection with projection and collocation methods, the use of irrational trial functions, different functionals, and in approximation theory. Babuska and Aziz (1927) define the "general finite element method" as the use of variational principles to solve given equations by trial functions with base functions of small support.

There is however a basic philosophical difference between the finite element approach and the finite difference approximation method. In the finite element method, we look at a given problem as the collection of individual smaller problems over a (preassigned) number of finite elements, each finite element being considered as an entity by itself. The union of the finite elements covers the domain of the global problem, but the intersection of the finite elements is restricted to boundary points of contiguous elements. The final stage in a FEM approximation is characterized by the term "assembling the finite elements".

In the finite difference methods (FDM), the given problem is considered over (predetermined) overlapping neighborhoods of (usually preassigned)

net points. The elements for the matrix equation are generated by moving from net point to net point in a given sequence. This difference is illustrated in Figure 1.1. for a quadratic approximation over a linear domain. By imposing boundary conditions to the finite elements in FEM, the distinction between FEM and FDM becomes blurred.

Courant and Hilbert (1931) mention that Euler (1707-83) created the variational calculus to approximate continuously differentiable functions by only piecewise continuous functions. Medelung (1922) introduced the "Approximation durch gebrochene Linienzüge" i.e. approximation by line segments. In short, he approximates the stationary functional by

$$S = \int_a^b V(t, x, \dot{x}) dt \approx \sum_{i=0}^n (t_i, x_i, \frac{x_{i+1} - x_i}{\Delta t}) \Delta t = \sum_{i=0}^n V_i \Delta t$$

and obtains from

$$\frac{\partial S}{\partial x_i} = 0$$

a system of difference equations

$$\frac{\partial V}{\partial x_i} - \frac{1}{\Delta t} \left(\frac{\partial V_i}{\partial \dot{x}_i} - \frac{\partial V_{i-1}}{\partial \dot{x}_{i-1}} \right) = 0.$$

which replaces the Euler-Lagrange differential equations. This is obviously FEM, and it was already used by A. L. Cauchy (1789-1857).

Francis, Stewart, Bohl and Krieger (1958) pointed out the many advantages of using the Schwinger variational expressions to obtain "almost all quantities needed in reactor design" from the transport equation. Among the many examples, the scalar flux was calculated by a step function approximation (Fig. 1.2) which probably represents the first example of FEM in transport theory and also the first use of "non-conforming" elements.

The first (and at this time the only) space-angle transport FEM codes

a. Assembly of Two Finite Elements

b. Quadratic Finite Difference Approximation

Figure 1.1 Original Geometric Interpretations of Finite Element Method and Finite Difference Method

were developed and brought into operation at Northwestern University in 1970 (x, μ) and 1971 (r, μ), (x, y, φ, θ), (r, z, φ, θ) by Miller, Lewis and Rossow (1972, 1973). The latest codes are four times as fast as those reported in the literature. Other codes have been proposed by Ohnishi (1971, 1972) and Reed (1972) who use FEM in space only combined with a projection method and discrete ordinates in angle. Reed (1973) has a working code. Work on a 2-D transport code is also in progress at ANL using the Galerkin method on triangular elements in space and spherical harmonics in angle (unpublished 1973). A survey on the discrete ordinate methods in transport theory and their applications with emphasis on work done at Los Alamos was given by Lathrop (1972). Similarly, an excellent survey on variational methods in nuclear engineering was written by Kaplan (1969) and a survey by Steele (1970). Hence, we shall not repeat the mathematics derived there. We shall concentrate on new issues important to the numerical analyst to assess the future development of transport theory codes. The first author (1955) devised and implemented the first discrete ordinate neutron transport codes (RDR1 to RDR4) as opposed to the S_N -codes and proposed "Multi-polynomial" approximations (1958) and partially implemented them in research codes. "Multipolynomial" is synonym to "piecewise polynomial", which today means finite elemental with polynomial base functions.

It has been recognized that the mathematical solution of the transport equation for realistic multidimensional neutronics problems exhibit a drastically different structure than for one-dimensional problems (Bareiss and Abu-Shumays 1969). We do not refer here to the ray-effect which is due to the incomplete specifications in the approximation method used (Bareiss, 1971). We refer to the true propagation of singularities which

Using the variational method digital computer code, the average scalar flux has been calculated for various regions in the scatterer and absorber of a repeating lattice. The continuous curve is the result of an exact calculation (RDR-4). $f_T = \bar{\phi}_T / \bar{\phi}_s$ is the ratio of average flux in the absorber to that in the scatterer, calculated using the variational method. It differs from the exact result, f_R , by only 0.03%.

Another example of the comparison of the variational method with an RDR-4 calculation

Figure 1.2 First Examples of FEM in Transport Theory

makes it practically very difficult (i.e. expensive) to obtain accurate strong solutions to the multidimensional problem. This problem begins to get the proper recognition (Arkuszewski, Kulikowska, Mika, 1971, 1972; Babuska, Kellog, 1973; Van Binnebeck, 1973; and others).

The question we shall discuss are the following:

- Why and when should we use variational techniques in transport theory calculations
- How can we test the reliability of proposed methods and predict their performance at reasonable cost
- What approach shall we take to solve the multi-dimensional neutron transport problem.

In many introductions to the finite element method, the flexibility of a triangular mesh is cited as a major advantage of FEM. We should like to remember that Southwell's relaxation method, popular in the forties to solve the Laplace and Helmholtz equations, was routinely done on triangular (or hexagonal) meshes. Finite difference methods for triangular meshes can as easily be constructed and implemented for computers as corresponding FEM (Panov, 1951, 1963 and others).

2. The Numerical Analyst Looks at the Variational Problem

In this section we will discuss the potential gain in using variational methods as opposed to finite difference methods. We shall derive functionals in an abstract way to bring out the main points.

Let C be a (complex) linear space and define an inner product $[u, v]$ which satisfies the conditions

$$[u, v] = \overline{[v, u]}$$

$$[au, v] = a[u, v] \quad (a \text{ any complex number})$$

$$[u_1 + u_2, v] = [u_1, v] + [u_2, v]$$

$$[u, u] \geq 0 \quad (\text{real; semi-norm})$$

Therefore:

$$[u - \tilde{u}, v - \tilde{v}] = [u, v] - [\tilde{u}, v] - [u, \tilde{v}] + [\tilde{u}, \tilde{v}]$$

if $u = \tilde{u}$ and/or $v = \tilde{v}$, this expression is zero.

Define the functional F_1 by

$$F_1(\tilde{u}, \tilde{v}) \equiv [\tilde{u}, v] + [u, \tilde{v}] - [\tilde{u}, \tilde{v}]$$

Let $\tilde{u} = u + \delta u$, $\tilde{v} = v + \delta v$, then

$$\delta F_1 \equiv \delta [u, v] = -[\delta u, \delta v] \gtrless 0 \quad (\text{min, max, saddle})$$

F_1 is stationary for $\tilde{u} = u$, $\tilde{v} = v$, and of second order.

Note, however that $\delta F = 0$ implies only

$$[\delta u, \delta v] = 0$$

Thus, the approximation $\tilde{u}$ is at most accurate of order one. From the numerical analysts point of view, this indicates potential numerical instability. Let $\tilde{u} \rightarrow c\tilde{u}$, $c = [u, \tilde{v}] / [\tilde{u}, \tilde{v}]$. Then

$$F_2 = F_1[c, \tilde{u}, \tilde{v}] = \frac{[\tilde{u}, v][u, \tilde{v}]}{[\tilde{u}, \tilde{v}]} \doteq [u, v] \quad (\text{Schwinger-Levine})$$

This functional is dimensionless in $\tilde{u}$ and $\tilde{v}$, thus only the shapes of $\tilde{u}$ and $\tilde{v}$ are necessary.

Let $v = u$, then (Friedrichs 1929, Diaz 1955)

$$[u-\tilde{u}, u-\tilde{u}] = [u,u] - [\tilde{u},u] - [u,\tilde{u}] + [\tilde{u},\tilde{u}] \geq 0 \quad (\text{least square})$$

$$[u,u] \geq F_3(\tilde{u}) \equiv [u,\tilde{u}] + [\tilde{u},u] - [\tilde{u},\tilde{u}] \quad (\text{Lagrange})$$

$$[u,u] \geq F_4(c\tilde{u}) \equiv \frac{|[u,\tilde{u}]|^2}{[\tilde{u},\tilde{u}]} \quad \text{if } [\tilde{u},\tilde{u}] > 0 \quad (\text{Schwarz})$$

In addition we have

$$[u,u] \leq F_5(\tilde{u}) \equiv [\tilde{u},\tilde{u}] \quad \text{if } [\delta u, u] = 0$$

which follows from $[\tilde{u},\tilde{u}] = [u + \delta u, u + \delta u] \geq [u,u]$.

Again, u being the stationary value of $F(\tilde{u})$, δF is approximated of order two if $\tilde{u} = u + \delta u$ in an approximation of order one. Since it is straight forward to construct functionals which are stationary for almost all design data a nuclear engineer may want, variational methods have been favored by engineers [Francis (1958), Lewins (1965, 1958), Kaplan (1969), Stacey (1972) and others]. Indeed it is possible to write a flexible computer program that is self-adoptive to the engineer's need.

As an example, let $Au = f$ be the given equation. We desire to calculate the weighted value (flux) $\int u g dv \equiv \langle u, g \rangle$. Define A^* by $\langle A\tilde{u}, \tilde{v} \rangle = \langle \tilde{u}, A^* \tilde{v} \rangle$, and let $A^* v = g$. Define $[u, v] = \langle Au, v \rangle = \langle u, A^* v \rangle$. Obviously, $[u, u]^{\frac{1}{2}}$ is the associated natural norm, known as "energy norm". We use $F_2(\tilde{u}, \tilde{v})$ and obtain

$$\langle u, g \rangle \approx F_2 = \langle \tilde{u}, g \rangle + \langle f, \tilde{v} \rangle - \langle A\tilde{u}, \tilde{v} \rangle.$$

If g has small support, this method of calculating u is equivalent to Green's function method. Stacy (1972) and the references given there, report mixed success, while Francis et al. (1958) were very successful using F_2 (Fig. 1.1) for the transport equation. This phenomena is connected with the fact that the transport equation is not self adjoint.

The problem under consideration here is to calculate u in $Au = f$, when A is a transport operator. From the standpoint of numerical analysis,

a positive definite functional is desirable. Therefore we define

$[u, v] = \langle Au, Av \rangle$. Then, in real space,

$$\langle f, f \rangle \geq F_1(\tilde{u}, \tilde{u}) = F_3(\tilde{u}) = 2 \langle f, A\tilde{u} \rangle - \langle A\tilde{u}, A\tilde{u} \rangle \geq 0$$

for $\tilde{u} \rightarrow u$. We note that this method is equivalent to the symmetrization of $Au = f$, i.e. $A^*Au = A^*f$. The advantage of the variational formulation is that F_3 uses only first derivatives, i.e. A , while the symmetrized equation exhibits second order derivatives, i.e. A^*A .

The finite element transport codes implemented at Northwestern University are based on the decomposition of an operator into the sum of a symmetric and antisymmetric operator. We have in general

$$\begin{aligned} 2Au &= (A + A^*)u + (A - A^*)u = 2f \\ 2A^*u^* &= (A + A^*)u^* - (A - A^*)u^* = 2f^* \end{aligned}$$

Addition and subtraction of these equations yield

$$\begin{aligned} (A + A^*)(u + u^*) + (A - A^*)(u - u^*) &= 2(f + f^*) \\ (A + A^*)(u - u^*) + (A - A^*)(u + u^*) &= 2(f - f^*) \end{aligned}$$

Formally, $u - u^*$ can be eliminated. We obtain

$$\begin{aligned} \{A + A^* - (A - A^*)(A + A^*)^{-1}(A - A^*)\}(u + u^*) \\ = 2(f + f^*) - 2(A - A^*)(A + A^*)^{-1}(f - f^*) \end{aligned}$$

The operator in braces $\{\}$ is selfadjoint (symmetric) but it is not necessarily a definite operator. It is definite, if $A + A^*$ is definite.

The above symmetrization process was applied by Vladimirov (1961) to the stationary transport operator

$$A\psi \equiv (L + I - J)\psi = S$$

where

$$L\psi = \Omega \cdot \nabla \psi, \quad J\psi = \frac{c}{4\pi} \int_{\Omega} p(\Omega \cdot \Omega') \psi(\Omega') d\Omega'$$

and

$$S^*(\Omega) = S(-\Omega) = S \quad (\text{isotropic source})$$

Define

$$\begin{aligned} L + L^* &= L^+ & \psi + \psi^* &= 2\psi^+ & S + S^* &= S^+ \\ L - L^* &= L^- & \psi - \psi^* &= 2\psi^- & S - S^* &= S^- = 0 \end{aligned}$$

We note that $S^* = S(-\Omega)$ implies $\psi^*(\Omega) = \psi(-\Omega)$.

Hence $A\psi \pm A^*\psi^*$ yields

$$\begin{aligned} L^-\psi^- + \psi^+ - J\psi^+ &= S^+ & L^+ &= 0 \\ L^-\psi^+ + \psi^- - J\psi^- &= 0 & L^- &= 2\Omega \cdot \nabla \end{aligned}$$

We solve the second equation for ψ^-

$$\psi^- = -(I - J)^{-1} L^-\psi^+$$

and substitute into the first equation:

$$\{-L^-(I - J)^{-1} L^- + I - J\} \psi^+ = S^+$$

Miller, Lewis and Rossow (1971) used this equation to obtain the Lagrange functional $F_3(\psi^+)$ for their FEM codes. The operator on the left hand side of the equation is positive definite if $\|J\| < 1$. This follows from the condition

$$\langle (I - J)^{-1} L^- u, L^- u \rangle + \langle (I - J) u, u \rangle \geq 0.$$

For $c < 1$, this condition is always satisfied. For one group eigenvalue calculations, $c > 1$. For this case saddle points have been observed in the Lagrange functional. The numerical results of the above FEM codes are characterized by the smoothness of the fluxes. Figure 2.1 illustrates the results of FEM calculations and comparable S_N calculations. $E_{i,k}$ means sub-dividing the Lambert projection of the half sphere in ik congruent rectangles, where i refers to $\cos \theta$, k to φ .

Reed and Hill (1973) applied a triangular mesh over the space variable only and used discrete ordinates in angle. Thus, they create a system of differential equations which are solved by a projection method yielding

Fig. 2.1 Scalar flux for the hexagon plate problem along the vacuum boundary.
W. F. Miller, Jr., E. E. Lewis, E. C. Rossow.

an explicit computational algorithm. We shall attempt to explain the oscillatory behavior observed in S_N -calculations. For simplicity's sake, let us take the general computation pattern of the one-dimensional S_N -codes. Lathrop (1972) gives the following iterative scheme

$$a \psi_{i-\frac{1}{2},m} + b \psi_{i,m-\frac{1}{2}} + \psi_{i,m} = C_i$$

$$\psi_{i-\frac{1}{2},m} + 0 - 2\psi_{i,m} + \psi_{i+\frac{1}{2},m} = 0$$

$$0 + \psi_{i,m-\frac{1}{2}} - 2\psi_{i,m} + 0 + \psi_{i,m+\frac{1}{2}} = 0$$

Basically, we have a large linear system of equations with a lower triangular matrix. If we write this matrix in block form as an infinite matrix, the equation with $\vec{\psi}_i^T = [\psi_{i-\frac{1}{2},m}, \psi_{i,m-\frac{1}{2}}, \psi_{i,m}]$ and $\vec{C}_i^T = [C_i, 0, 0]$ becomes

$$\begin{bmatrix} \text{---} & & & \\ & A & B & \\ & & A & B \\ & & & A & B \\ & & & & \text{---} \end{bmatrix} \begin{bmatrix} \vdots \\ \vec{\psi}_i \\ \vec{\psi}_{i+1} \\ \vec{\psi}_{i+2} \\ \vdots \end{bmatrix} = \begin{bmatrix} \vdots \\ \vec{C}_i \\ \vec{C}_{i+1} \\ \vec{C}_{i+2} \\ \vdots \end{bmatrix}$$

and is equivalent to a matrix difference equation. An elementary solution takes the form

$$\vec{\psi}_i^e = \vec{\psi}_i^e = \vec{\lambda}^i \cdot \vec{u}$$

The iterative scheme can be analyzed by the behavior of

$$A \vec{u} \vec{\lambda}^i + B \vec{u} \vec{\lambda}^{i+1} = 0$$

for a homogeneous solution. Therefore we have the condition ("characteristic

equation")

$$\det | A + \lambda B | = 0$$

for λ to be compatible. For the S_N - iteration, this is

$$\det \begin{vmatrix} a & b & 1 \\ 1 + \lambda & 0 & -2 \\ 0 & 1 + \lambda & -2 \end{vmatrix} = (1 + \lambda)^2 + 2(a + b)(1 + \lambda) = 0$$

The eigenvalues of this problem are

$$\lambda_1 = -1, \quad \lambda_2 = -(1 + 2(a + b))$$

Thus we have two sets of elementary solutions, $\lambda_1^i \vec{u}_1$, and $\lambda_2^i \vec{u}_2$ where $\vec{u}_1$ and $\vec{u}_2$ are eigenvectors of $(A + \lambda B) \vec{u} = 0$. The vector

$\vec{\psi}^T = \{ \dots \vec{\psi}_i, \vec{\psi}_{i+1}, \dots \}$ of the homogeneous problem has as its general solution the superposition of the linear elementary solutions, i.e.

$$\vec{\psi}_i = (-1)^i (\alpha_1 \vec{u}_1 + (1 + 2a + 2b)^i \alpha_2 \vec{u}_2)$$

where α_1 and α_2 are scalars. The general solution of the inhomogeneous problem is the superposition of a particular solution and the general homogeneous solution. The parameters α_1 and α_2 are determined by the initial conditions of the iteration. The point to be made is that all S_N - codes lead to oscillating solutions. The same behavior can also be predicted for the propagation of round-off errors in the S_N - method.

This section has shown that there is an abundance of possibilities to create functionals for use in variational methods. If the stationary value of the functional is the desired number, we can expect good answers. There will however be one variational formulation that performs best. No general theory has been developed that would guarantee optimum accuracy with minimum computational complexity. This is an unsolved problem.

A completely different aspect arises if we want to use a variational

formulation of the neutron transport problem to solve pointwise for the angular flux distribution. One can only hope that under given constraints, the variational formulation gives an optimum solution. The numerical analyst looks for functionals which can render numerically stable methods. We have shown that symmetrization of the operator by premultiplication by its adjoint operator is especially attractive for the variational formulation. Symmetrization by addition is tedious for the general transport operator. Semi-variational formulations are relatively easy to obtain. As a new contribution to this section we have shown that the oscillatory behavior of the S_N - solutions can be predicted easily. By such investigations, the expense of code development can be reduced.

So far, we have considered global aspects. We have only touched on the problem of global error analysis. This problem will be investigated later. The important problem, it seems to us, is to answer the question of how to pinpoint the most promising numerical methods at reasonable cost. We shall try to answer this question in the following two sections. Section 3 deals with the systematic search for optimum approximation methods. Section 4 will give new insight into the structure of the mathematical solution of the transport equation.

3. Optimal Operator Approximations

The nuclear engineering community has recognized for some time the importance of unbiased testing of new neutronics codes. This is evidenced by the work of the Benchmark Problem Committee and the Benchmark Problem book, which represents an open set of "exact" and "realistic" problems. I have set the words "exact" and "realistic" in quotation marks because they reflect the proper attitude toward testing, but leave the actual interpretation and implementation open for discussion. I should like to point to the recent practice of comparing finite difference methods which approximate a circle by step functions with finite element methods which approximate a circle by straight line segments. Such comparisons are not fair since two very different problems are solved which differ in boundary and interface area by over 40 percent. A fair comparison would be to use the greater flexibility of the new code and solve identical problems, i.e. a fortiori the step function boundary and interface problem.

I should also like to bring attention to the mathematical tradition of rating approximations by the symbols

$$O(h^k) \leq C h^k \parallel \text{Sobolev Norm} \parallel$$

Any scholar will use them because they establish consistency and the rate of convergence as the diameter of the reference domain, usually the mesh width, approaches zero. We remember now that we deal with finite elements, and not with infinitesimal elements. In fact, we wish to make the finite elements as large as possible and to this end the use of high order polynomials, rational approximations, and a multitude of special tricks have been proposed to achieve the goal of making the diameter (h) as large as tolerable. Practice has taught us that the generic constant C

and the Sobolev norm are hard to estimate, and, if found, are often useless. Instead we can demonstrate that for certain problems a lower order operator approximation (in the $O(h)$ sense) performs as well on a finite domain as a so called higher order approximation. For example, it is generally accepted that in one-dimensional transport theory calculations, double-Gauss approximations yield more accurate results than single-Gauss approximations for multiregion calculations, although the precision for n ordinates in each case is of order $n - 1$ for double-Gauss and of order $2n - 1$ for single-Gauss integrations.

At Northwestern University, four kinds of finite difference approximations to the discrete ordinate method were tested on the same set of twelve two-dimensional benchmark problems. The results are summarized in Table 3.1. Case 1 used forward first order differences, Case 2, backward first order differences with respect to the direction of neutron motion, while Case 3 employed second order central differences. In Case 4, a mixture of first order forward and backward differences was used as indicated by the diagram (Averaging Operator). For the angular approximation symmetric equal weight integration formulas were used in all cases. The interesting fact is, that the averaging operator in spite of being a first order approximation, performed as well as the second order operator and proved much easier to handle than all other operators. The question of optimum performance has not yet been answered, but we shall address this question shortly.

To obtain optimum performance we must consider the shapes of the finite elements and/or the computational cells, their size, the relative approximations in space and angular direction and the implied computational complexity. If the cost of transport theory calculations is to be reduced, finite elements must eventually be made so large as to coincide with

Table 3.1

CONDENSED RESULTS OF 2-D CALCULATIONS

MAXIMUM FLUX ERROR

$$c = 1.273$$

$$\lambda = i+$$

IN UNITS OF 10^{-1}

CASE 1:

No. Angles		Space Mesh $h=n^{-1}$		
θ	ϕ	1	2	4
2	4	.118	.333	.337
2	8	.149	.236	
4	8	.139	.371	
2	16	.145	.350	
4	16	.136		
6	16	.136		
8	16	.136		

CASE 2:

No. Angles		Space Mesh $h=n^{-1}$		
θ	ϕ	1	2	4
2	4	.118	.083	.053
2	8	.149	.113	
4	8	.139	.095	
2	16	.145	.112	
4	16	.136		
6	16	.136		
8	16	.136		

CASE 3:

No. Angles		Space Mesh $h=n^{-1}$		
θ	ϕ	1	2	4
2	4	-	-.0110	-.0042
2	8	-	.0403	
4	8	-	-.0125	
2	16	-	.0400	
4	16	-		
6	16	-		
8	16	-		

CASE 4:

No. Angles		Space Mesh $h=n^{-1}$		
θ	ϕ	1	2	4
2	4	.0332	.0070	.00130
2	8	.0872	.0556	
4	8	.0405	.0118	
2	16	.0911	.0695	
4	16	.0394		
6	16	.0356		
8	16	.0354		

elementary computational cells with arbitrary curved boundaries. With the multitude of possible approximations, methods, elementary cell configurations, and conforming and non-conforming elements, is it possible to systematically analyze these methods and select the best performers at a reasonable cost? The answer is yes. A great deal of this work has already been done. The first step is a systematic elementary cell analysis (by the computer). The second step is the global error and stability analysis (also done by the computer eventually), and the third step is performance prediction (computational complexity). The analysis rests on the representation theorem (Bareiss, Abu-Shumays, 1971) which states in essence the following.

In the space of distributions the general solution $\psi(x, \Omega)$ of

$$(\Omega \cdot \Delta + 1) \psi = \frac{c}{4\pi} \int_{(\Omega')} \psi(x, \Omega') d\Omega' + S(x)$$

has the representation

$$\psi = \int_{\{\Lambda\}} A(\Lambda) \frac{c}{4\pi} \frac{e^{-\Lambda \cdot x}}{1 - \Lambda \cdot \Omega} d\Lambda$$

where $\{\Lambda\} = \{\Lambda^0\} \cup \{\Lambda^s\} \cup \{\Lambda^e\}$ is the extended spectral set of the transport operator.

We remark that only for reasons of simplicity an isotropic scattering kernel was selected. Now we observe that the exact computational solutions of any realistic problem is the union of such representations over the union of all elementary computational cells. However, to test the accuracy of an approximation operator, it is sufficient to test it on a representative finite subset of rigged normal modes

$$\psi_{\Lambda} = \frac{c}{4\pi} \frac{e^{-\Lambda \cdot x}}{1 - \Lambda \cdot \Omega}$$

The three simple steps to be taken are:

Step 1. For the representative set $\{\Lambda_i\} \subset \{\Lambda\}$ generate benchmark problems over the computational cells.

Step 2. Solve the benchmark problems using the approximated operators.

Step 3. Evaluate the performance of the approximation operators by comparing the results with the exact analytic solutions.

Now observe that

- (1) The entire process can be mechanized.
- (2) The shape of the computational cells is arbitrary, i.e. it may include any type of curved boundaries.
- (3) The benchmark problems are easy to generate and are tailored to specific individual needs.
- (4) They are independent of the coordinate system and the dimension of the problem.
- (5) The method gives a quantitative analysis for a finite domain (as opposed to a qualitative analysis only).
- (6) The entire process is inexpensive, even when the output is tabulated or represented in graphic form for easy reference.
- (7) The results of a cell analysis enables one to select or design an optimum performance code at a given time and for a given purpose.
- (8) Although theoretically complete, the generation of benchmark problems is not restricted to the use of normal modes only.

Indeed, the prototype code developed at Northwestern University permits the use of other test bases such as $x \log x$ - terms, poly-harmonics, and others as seem desirable to analyze a specific response to a specific question. Examples of two- and three-dimensional analysis have been given by Bareiss and Abu-Shumays (1971). However, to simplify this discussion we illustrate the procedure first for one particular set of one-dimensional approximation operators.

Some fifteen years ago the author experimented with various what is now called higher order finite elements for the numerical solution of the one-dimensional transport equation. The results were reported in 1958 in a lecture at the annual SIAM meeting. Among the spacial approximations, the nodes within an element were located to correspond to Gaussian integration. Recently Douglas (1972) introduced the same technique and called it "super convergent". In my numerical experimentation, the results turned out very inferior as compared to the method illustrated below. The reason is that I introduced constraints on the boundaries to force the elements to become conforming. Nonconforming elements in space were considered in violation of the physical realities, although I recommended and used them freely in the angular direction (Bareiss 1958). The recent results obtained by Reed (1973) certainly sparked an interest in nonconforming elements. The star performers however were the Hermite-Birkhoff interpolation methods which resulted in an experimental saving factor of 32 in comparison with RDR4 calculations (Bareiss, Chamot, 1970 Reprint). This method was duplicated and optimized by elementary cell testing and the savings factor could be pushed to an incredible 1000. The reason for the possibility of such an optimization is as follows. There exists an optimum ratio between the "mesh width" in space and the "mesh width" in angle. If one departs from this ratio, no improvement in accuracy is gained, on the contrary, the accuracy may decrease.

Tables 3.2 to 3.5 show the test results of double-Gauss discrete ordinate calculations for four extreme cases of normal mode benchmark problems, with different spacing in angular and spatial direction and for Hermite-Birkhoff interpolation in space of orders 1, 3, and 5. The entries in the upper part of the tables should be read as follows. For

example, take Table 3.2, entry 1st: MESH 8, ANGLE 6. This means: 1st order approximation with mesh width in space of $1/8$ mean free path, and angular approximation equivalent to a double P_3 - approximation. The reading $8^{-4}50$ means: The absolute largest flux error in the numerical solution of the benchmark problem with the exact solution

$\psi = \frac{c}{2} e^{-\lambda x} / (1 - \lambda \mu)$, ($\lambda = .5$, $c = .91$) is $.8 \times 10^{-4}$; and the value of the flux where the maximum error occurred is .50. The entries in the lower part of the tables give the ratios of the maximum errors for successive approximations in units of $1/10$. For example the entry between 4 and 8 under "column" 6 is 35. This means, going from mesh length $1/4$ to $1/8$ of a mean free path reduces the true maximum error in the flux by a factor of 3.5. The entry 85 on "line" 8 between "columns" 4 and 6 means that the maximum error with 4 ordinates in angle is 8.5 as big as the maximum error with 8 discrete ordinates.

By comparing the three tables we see that the smallest maximum errors are located in a small diagonal band, independent of the λ -value of the exact solution. The practical usefulness of such a table is obvious. By consulting such a table, the user of a code not only obtains optimum accuracy in his calculations, but also can cut the computation time appreciably. It is also obvious that:

- (a) such studies cannot be conducted on full scale problems because of prohibitive computing costs,
- (b) the theoretical location of the optimum accuracy band is practically impossible,
- (c) the same phenomena is common to finite element methods and finite difference methods,
- (d) the nuclear engineer does not need a thorough understanding of

Table 3.2

Hermite-Birkhoff - Double Gauss Cell Calculations

MAXIMUM ABSOLUTE ANGULAR FLUX ERROR AND FLUX VALUE
C= .91 LAMBD= .500

ANGLE	1ST								3RD								5TH															
MESH	2	4	6	8	12	16	32	64	2	4	6	8	12	16	32	64	2	4	6	8	12	16	32	64								
1	-1	-2	-2	-2	-2	-2	-2	-2	-1	-3	-4	-4	-4	-4	-4	-4	-1	-3	-4	-6	-6	-6	-6	-6								
2	37	5	46	5	50	5	52	5	53	5	54	5	55	5	55	5	2	36	7	41	3	43	6	33	1	53	1	54	1	55	1	55
4	-1	-2	-2	-2	-2	-2	-2	-2	-1	-3	-4	-4	-4	-4	-4	-4	-1	-3	-4	-6	-6	-6	-6	-6								
8	2	36	1	46	1	50	1	52	1	53	1	54	1	55	1	55	2	36	7	41	2	43	9	52	1	53	1	54	1	55	1	55
16	-1	-3	-3	-3	-3	-3	-3	-3	-1	-3	-4	-6	-6	-7	-7	-7	-1	-3	-4	-6	-9	-9	-10	-10								
32	2	36	8	35	3	50	3	52	3	53	3	54	3	55	3	55	2	36	7	36	2	38	6	39	8	53	8	54	8	55	8	55
64	-1	-3	-4	-4	-4	-4	-4	-4	-1	-3	-4	-6	-8	-8	-8	-8	-1	-3	-4	-6	-9	-12	-12									
128	2	36	7	37	8	50	7	52	8	53	8	54	8	55			2	36	7	39	2	38	6	39	5	53	5	54	5	55		
256	-1	-3	-4	-4	-4	-4	-4	-4	-1	-3	-4	-6	-9	-9	-9	-9	-1	-3	-4	-6	-9	-12	-11									
512	2	36	7	39	3	50	2	52	2	53	2	54	2	55			2	36	7	39	2	39	6	39	5	40	5	39				
	-1	-3	-4	-5	-5	-5	-5	-5	-1	-3	-4	-6	-9	-10			-1	-3	-4	-6	-9	-12										
	2	36	7	39	2	52	5	53	5	54							2	36	7	39	2	39	6	39	5	40	5	39				
	-1	-3	-4	-5	-5	-5	-5	-5	-1	-3	-4	-6	-9	-10			-1	-3	-4	-6	-9	-12										
	2	36	7	39	2	52	5	53	5	54							2	36	7	39	2	39	6	39	5	40	5	39				
	-1	-3	-4	-6	-6	-6	-6	-6	-1	-3	-4	-6	-9	-10			-1	-3	-4	-6	-9	-12										
	 										
	2	36	7																													

Hermite-Brikhoff - Double Gauss Cell Calculations

ANGLE									3RD									5TH								
MESH	2	4	6	8	12	16	32	64	2	4	6	8	12	16	32	64	2	4	6	8	12	16	32	64		
	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-2	-2	-3	-3	-3	-3	-1	-1	-2	-2	-4	-4	-4	-4		
1	8	24	4	43	4	73	5	87	6	22	2	27	5	29	1	25	6	22	2	27	7	15	1	14		
	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-2	-2	-4	-4	-4	-4	-1	-1	-2	-2	-3	-3	-5	-6		
2	6	22	2	26	1	60	1	72	6	22	2	27	5	29	1	30	6	22	2	27	5	29	1	22		
	-1	-1	-2	-2	-2	-2	-2	-2	-1	-1	-2	-2	-4	-5	-5	-5	-1	-1	-2	-2	-4	-4	-8	-8		
4	6	22	2	27	5	29	3	73	6	22	2	27	5	29	1	30	6	22	2	27	5	29	1	30		
	-1	-1	-2	-2	-3	-3	-3	-3	-1	-1	-2	-2	-4	-5	-6	-6	-1	-1	-2	-2	-4	-5	-10	-10		
8	6	22	2	27	5	29	1	28	6	22	2	27	5	29	1	30	6	22	2	27	5	29	1	30		
	-1	-1	-2	-2	-3	-3	-3	-3	-1	-1	-2	-2	-4	-5	-7	-7	-1	-1	-2	-2	-4	-5	-7	-7		
16	6	22	2	27	5	29	1	29	6	22	2	27	5	29	1	30	6	22	2	27	5	29	1	30		
	-1	-1	-2	-2	-4	-4	-4	-4	-1	-1	-2	-2	-4	-5	-5	-5	-1	-1	-2	-2	-4	-5	-5	-5		
32	6	22	2	27	5	29	1	30	6	22	2	27	5	29	1	30	6	22	2	27	5	29	1	30		
	-1	-1	-2	-2	-4	-4	-4	-4	-1	-1	-2	-2	-4	-5	-5	-5	-1	-1	-2	-2	-4	-5	-5	-5		
64	6	22	2	27	5	29	1	30	6	22	2	27	5	29	1	30	6	22	2	27	5	29	1	30		
	-1	-1	-2	-2	-4	-4	-4	-4	-1	-1	-2	-2	-4	-5	-5	-5	-1	-1	-2	-2	-4	-5	-5	-5		
128	6	22	2	27	5	29	1	30	6	22	2	27	5	29	1	30	6	22	2	27	5	29	1	30		
	-1	-1	-2	-2	-4	-4	-4	-4	-1	-1	-2	-2	-4	-5	-5	-5	-1	-1	-2	-2	-4	-5	-5	-5		
256	6	22	2	27	5	29	1	30	6	22	2	27	5	29	1	30	6	22	2	27	5	29	1	30		
	-1	-1	-2	-2	-4	-4	-4	-4	-1	-1	-2	-2	-4	-5	-5	-5	-1	-1	-2	-2	-4	-5	-5	-5		
512	6	22	2	27	5	29	1	30	6	22	2	27	5	29	1	30	6	22	2	27	5	29	1	30		
	-1	-1	-2	-2	-4	-4	-4	-4	-1	-1	-2	-2	-4	-5	-5	-5	-1	-1	-2	-2	-4	-5	-5	-5		
	-1	-1	-2	-2	-4	-4	-4	-4	-1	-1	-2	-2	-4	-5	-5	-5	-1	-1	-2	-2	-4	-5	-5	-5		
	-1	-1	-2	-2	-4	-4	-4	-4	-1	-1	-2	-2	-4	-5	-5	-5	-1	-1	-2	-2	-4	-5	-5	-5		
	-1	-1	-2	-2	-4	-4	-4	-4	-1	-1	-2	-2	-4</													

ANGLE MESH	1ST								3RD								5TH							
	2	4	6	8	12	16	32	64	2	4	6	8	12	16	32	64	2	4	6	8	12	16	32	64
1	21	10	9	8	9	9	10		33	43	43	17	9	9	10		32	28	58	196	39	12	10	
	12	17	35	41	43	43	43	43	10	10	9	9	97	172	165	165	10	10	15	9	7	50	659	389
2	28	21	10	9	9	9	10	41	32	40	42	188	16	9	10		32	40	36	147	284	160	6	
	10	12	20	35	40	41	41		10	10	10	10	10	119	162	162	10	10	10	12	11	1	645	1099
4	32	37	18	10	9	9	10		32	40	42	185	189	12	10		32	40	42	136	18*	556	10	
	10	10	11	25	39	40	40		10	10	10	10	10	10	160		10	10	10	10	14	119	517	
8	32	40	41	16	10	9	40		32	40	42	185	190	189			32	40	42	185	160*	3491		
	10	10	10	10	36	40	40		10	10	10	10	10	10	161		10	10	10	10	10	12	0	
16	32	40	42	54	11	9			32	40	42	185	189	3072			10	10	10	10	10	10		
	10	10	10	10	28	39			32	40	42	184	189				32	40	42	184	189			
32	32	40	42	151	15				10	10	10	10	10				10	10	10	10	10			
	10	10	10	10	12				32	40	42	186					32	40	42	186				
64	32	40	42	186					10	10	10	10					10	10	10	10				
	10	10	10	10					32	40	42						32	40	42					
128	32	40	42						10	10	10	10					10	10	10					
	10	10							32	40	42						32	40	42					
256	32								10	10							10	10						
	10								32								32							
512									10								10							

Table 3.4

Hermite-Birkhoff - Double Gauss Cell Calculations

MAXIMUM ABSOLUTE ANGULAR FLUX ERROR AND FLUX VALUE

C= 1.27 LAMDA= 1.0001.

ANGLE MESH	2	4	6	8	12	16	32	64	2	4	6	8	12	16	32	64	2	4	6	8	12	16	32	64
1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-2	-2	-3	-3	-3	-3	-3	-1	-2	-3	-5	-4	-4	-4	-4
2	1 49	3 39	4 51	4 44	4 46	4 47	4 45	4 46	3 51	4 61	5 59	3 34	5 46	5 47	5 45	5 44	3 51	5 60	5 59	2 58	3 46	3 47	3 59	2 37
4	-1	-2	-1	-1	-1	-1	-1	-1	-1	-2	-3	-4	-4	-4	-4	-4	-1	-2	-3	-4	-6	-6	-6	-5
8	2 49	7 39	1 59	1 58	1 57	1 56	2 56	2 56	3 51	5 60	5 59	3 34	5 46	5 47	5 45	5 44	3 51	5 60	5 59	2 58	3 46	3 47	3 59	2 37
16	-1	-2	-2	-2	-2	-2	-2	-2	-1	-2	-3	-4	-5	-5	-5	-5	-1	-2	-3	-4	-7	-7	-7	-7
32	3 51	3 53	3 59	3 44	3 62	4 62	4 62	4 62	3 51	5 56	5 59	1 58	3 46	3 47	3 45	3 44	3 51	5 56	5 59	2 58	5 62	4 35	1 36	1 35
64	-1	-2	-2	-3	-3	-3	-3	-3	-1	-2	-3	-4	-6	-6	-6	-6	-1	-2	-3	-4	-7	-9	-10	-10
128	3 51	5 53	1 59	7 44	7 46	7 63	9 63		3 51	5 56	5 59	2 58	2 53	2 47	2 45		3 51	5 56	5 59	2 57	4 58	1 56	7 45	
256	-1	-2	-3	-3	-3	-3	-3		-1	-2	-3	-4	-7	-7	-7		-1	-2	-3	-4	-7	-10	-9	
512	3 51	5 56	6 58	2 44	2 44	2 45	2 64		3 51	5 56	5 58	2 57	5 58	1 45	1 47		3 51	5 56	5 58	2 57	4 58	6 58	1 64	
	-1	-2	-3	-4	-4	-4			-1	-2	-3	-4	-7	-9			-1	-2	-3	-4	-7	-10		
	3 51	5 57	5 58	3 34	4 45	4 46			3 51	5 57	5 58	2 58	4 58	8 51			3 51	5 57	5 58	2 58	4 58	6 58		
	-1	-2	-3	-5	-4				-1	-2	-3	-4	-7				-1	-2	-3	-4	-7			
	3 51	5 56	5 58	8 47	1 45				3 51	5 56	5 58	2 58	4 58				3 51	5 56	5 58	2 58	4 58			
	-1	-2	-3	-4					-1	-2	-3	-4	-7				-1	-2	-3	-4	-7			
	3 51	5 56	5 58	1 57					3 51	5 56	5 58	2 58					3 51	5 56	5 58	2 58	4 58			
	-1	-2	-3						-1	-2	-3	-4					-1	-2	-3	-4				
	3 51	5 56							3 51	5 56							3 51	5 56	5 58	2 58				
	-1	-2							-1	-2							-1	-2						
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Table 3.5

Hermite-Birkhoff - Double Gauss Cell Calculations

MAXIMUM ABSOLUTE ANGULAR FLUX ERROR AND FLUX VALUE
 $C = 1.27$ $LAMBDA = 1.0000$

ANGLE MESH	1ST								3RD								5TH							
	2	4	6	8	12	16	32	64	2	4	6	8	12	16	32	64	2	4	6	8	12	16	32	64
1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-2	-3	-3	-3	-3	-3	-3	-1	-2	-3	-5	-4	-4	-4	-4
2	2 25	3 16	3 29	3 21	3 23	3 25	3 27	3 25	2 29	2 44	8 29	6 21	6 23	6 25	6 27	6 26	2 29	3 44	3 49	8 12	1 23	1 6	1 27	3 6
4	-1	-2	-2	-2	-2	-2	-1	-1	-1	-2	-3	-4	-4	-4	-4	-4	-1	-2	-3	-4	-6	-6	-6	-5
8	2 25	7 16	9 29	9 21	9 23	1 32	1 31	1 31	2 29	3 44	3 49	3 21	4 23	4 25	4 27	4 26	2 29	3 44	3 36	1 34	3 2	2 25	2 27	2 3
16	-1	-2	-2	-2	-2	-2	-2	-2	-1	-2	-3	-5	-5	-5	-5	-5	-1	-2	-3	-4	-7	-7	-7	-7
32	2 29	2 28	3 29	2 21	2 23	3 44	3 44	3 44	2 29	3 32	3 38	8 34	3 23	3 25	3 27	3 26	2 29	3 32	3 38	1 40	3 45	5 1	1 2	1 1
64	-1	-2	-3	-3	-3	-3	-3	-3	-1	-2	-3	-4	-6	-6	-6	-6	-1	-2	-3	-4	-7	-10	-10	-10
128	2 29	3 34	8 29	6 21	6 23	6 25	7 49		2 29	3 30	3 44	1 40	2 23	2 25	2 27		2 29	3 38	3 44	1 40	2 42	9 34	6 27	
256	-1	-2	-3	-3	-3	-3	-3	-3	-1	-2	-3	-4	-7	-7	-7	-7	-1	-2	-3	-4	-7	-10	-9	
512	2 29	3 39	4 41	1 21	2 23	2 25	2 52		2 29	3 30	3 41	1 43	3 41	1 25	1 27		2 29	3 38	3 41	1 43	2 42	4 43	1 53	
	-1	-2	-3	-4	-4	-4	-4		-1	-2	-3	-4	-7	-9	-7		-1	-2	-3	-4	-7	-10	-9	
	2 29	3 39	3 41	3 21	4 23	4 25			2 29	3 30	3 41	1 41	2 42	6 25			2 29	3 38	3 41	1 41	2 42	4 43		
	-1	-2	-3	-5	-5	-5			-1	-2	-3	-4	-7				-1	-2	-3	-4	-7			
	2 29	3 38	3 42	7 19	9 23				2 29	3 30	3 41	1 42	2 42				2 29	3 38	3 41	1 42	2 42			
	-1	-2	-3	-5					-1	-2	-3	-4					-1	-2	-3	-4				
	2 29	3 38	3 41	9 40					2 29	3 30	3 41	1 42					-1	-2						
	-1	-2							2 29	3 39							2 29	3 39						
	-1								-1								-1							
	2 29								2 29								2 29							

ERROR RATIO X10 : HORIZ-ANGULAR VERT-SPATIAL

ANGLE MESH	1ST								3RD								5TH								
	2	4	6	8	12	16	32	64	2	4	6	8	12	16	32	64	2	4	6	8	12	16	32	64	
1		6	9	10	10	10	10	10		77	29	14	10	10	10	10		66	100	383	5	10	10	5	
2	11	42	35	35	35	34	31	30		10	8	29	183	153	153	153	153	10	10	11	7	448	620	612	149
4	22	8	10	10	10	9	10		66	102	87	8	10	10	10		65	108	238	352	14	10	1		
8	10	35	36	39	39	38	36	35		10	10	10	39	157	158	159	158	10	10	10	11	103	52	193	1963
16	79	8	11	10	9	9	10		65	107	327	33	10	10	10		65	107	269	3217	7	37	13		
32	9	8	32	40	40	43	42		10	10	10	146	159	159			10	10	10	10	14	5171	2099		
64	69	32	14	10	10	9			63	110	274	576	11	10			63	110	270	4509	2551	15			
128	10	9	21	41	40	40	44		10	10	10	10	58	160	160		10	10	10	10	10	23	5		
256	65	73	27	10	10	9			63	109	272	3401	30	10			63	109	272	4509	5895	3			
512	10	10	13	47	40	40			10	10	10	10	13	154			10	10	10	10	10	10			
	64	98	99	8	10				63	109	272	4630	354				63	109	272	4509	6005				
	10	10	11	44	40				10	10	10	10	10				10	10	10	10					
	63	106	404	7					63	109	272	4509					63	109	272	4509					
	10	10	10	8					10	10	10	10					10	10	10	10					
	63	109	321						63	109	272						63	109	272						
	10	10							10	10							10	10							
	63								63								63								
	10								10								10								
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	63								63								63								
	10								10								10								
	 								

the intricate mathematics underlying this test procedure,

- (e) in practical applications the search for the optimum accuracy band does not require a full table as presented in this illustration.

Figures 3.1 and 3.2 give graphical representations of the flux shapes of the normal modes, used in Tables 3.2 to 3.5 and the error distributions of some examples. Tables 3.6 and 3.7 show the corresponding results for the symmetrized transport operator (Vladimirov's symmetrization). The first table shows the maximum errors associated with the finite difference method, the second the maximum errors in the corresponding variational method with linear finite elements. A complete catalogue of all calculations made so far will be available soon.

Figure 3.1 Flux shapes used in Tables 3.2 to 3.5

1ST ORDER HERMITE-BIRKHOFF METHOD

LEGEND
 SER. NO. = 102103
 C = .6462
 LAMBDA = .8750
 ANGLES = 8
 MESH = 4
 MAX ABS ERR = .51E-02

5TH ORDER HERMITE-BIRKHOFF METHOD

LEGEND
 SER. NO. = 102103
 C = .6462
 LAMBDA = .8750
 ANGLES = 8
 MESH = 4
 MAX ABS ERR = .12E-02

SYMMETRIZED 1D TRANSPORT EQN (FD)

LEGEND
 SER. NO. = 200501311
 C = .6162
 LAMBDA = .8750
 ANGLES = 8
 MESH = 32
 MAX ABS ERR = .51E-03

SYMMETRIZED 1D TRANSPORT EQN (FD)

LEGEND
 SER. NO. = 200501311
 C = .6162
 LAMBDA = .8750
 ANGLES = 8
 MESH = 4
 MAX ABS ERR = .04E-04

Figure 3.2 Error Distribution for Some Benchmark Calculations

Table 3.6.

Vladimirov-Finite Difference Cell Calculations

SYMMETRIZED 1D (FD)
MAX. ABSOLUTE ERROR
(GLOBAL)
C= .910 LAMBDA= .500 MFP= .500

ANGLE	2	4	6	8	12
MESH					
1	-3	-4	-4	-4	
2	-3	-4	-4	-4	
4	-3	-4	-4	-4	
8	-3	-4	-4	-4	
16	-3	-4	-4	-4	
32	-3	-4	-4	-4	
64	-3	-4	-4	-4	
128	-3	-4	-4	-4	

ERROR RATIOS X10

ANGLE	2	4	6	8	12
MESH					
1	43	10	10		
2	8	40	40	40	
4	10	206	10	10	
8	10	40	40	40	
16	10	40	40	40	
32	10	40	40	40	
64	10	40	40	40	
128	10	40	40	40	

SYMMETRIZED 1D (FD)
MAX. ABSOLUTE ERROR
(GLOBAL)
C= .646 LAMBDA= .875 MFP= .500

ANGLE	2	4	6	8	12	16
MESH						
1	-1	-2	-2	-2		
2	-1	-2	-2	-2		
4	-1	-2	-2	-2		
8	-1	-2	-2	-2		
16	-1	-2	-2	-2		
32	-1	-2	-2	-2		
64	-1	-2	-2	-2		
128	-1	-2	-2	-2		

ERROR RATIOS X10

ANGLE	2	4	6	8	12	16
MESH						
1	134	8	9			
2	9	11	28	9	9	
4	10	148	129	42	9	40
8	10	10	16	40	9	40
16	10	10	206	22	9	40
32	10	10	101	42	9	40
64	10	10	215	21	9	40
128	10	10	10	17	40	

SYMMETRIZED 1D (FD)
MAX. ABSOLUTE ERROR
(GLOBAL)
C= 1.273 LAMBDA= 1.000 MFP= .500

ANGLE	2	4	6	8	12
MESH					
1	-2	-2	-2	-2	
2	-2	-2	-2	-2	
4	-2	-2	-2	-2	
8	-2	-2	-2	-2	
16	-2	-2	-2	-2	
32	-2	-2	-2	-2	
64	-2	-2	-2	-2	
128	-2	-2	-2	-2	

ERROR RATIOS X10

ANGLE	2	4	6	8	12
MESH					
1	21	10	10	10	
2	15	41	41	41	41
4	11	55	10	10	10
8	10	11	38	40	40
16	10	10	10	10	10
32	10	10	10	10	10
64	10	10	10	10	10
128	10	10	10	10	10

Table 3.7

Vladimirov-Finite-Element Cell Calculations

SYMMETRIZED 1D (FEM)
MAX. ABSOLUTE ERROR
C= .91 LAMBDA= .500

ANGLE MESH	2	4	8	16	32
1	-2	-2	-3	-3	-3
2	-2	2	-3	-4	-4
4	-2	-2	-3	-4	-4
8	-2	2	-3	-4	-4
16	-2	2	3	7	2
32	-2	2	3	7	

ERROR RATIO X10

ANGLE MESH	2	4	8	16	32
1	4	61	39	11	
2	10	13	11	14	37
4	10	10	11	9	16
8	10	10	11	11	9
16	10	10	10	10	11
32	10	10	10	10	

SYMMETRIZED 1D (FEM)
MAX. ABSOLUTE ERROR
C= .65 LAMBDA= .875

ANGLE MESH	2	4	8	16	32
1	-1	-1	-1	-2	-2
2	-1	-1	-1	-2	-3
4	-1	-1	-1	-2	-3
8	-1	-1	-1	-2	-3
16	-1	-1	-1	-2	
32	-1	-1	-1	-2	

ERROR RATIO X10

ANGLE MESH	2	4	8	16	32
1	2	46	49	15	
2	12	13	12	11	32
4	10	10	11	10	10
8	10	10	11	11	10
16	10	10	10	11	
32	10	10	10	10	

SYMMETRIZED 1D (FEM)
MAX. ABSOLUTE ERROR
C= 1.27 LAMBDA= 1.000

ANGLE MESH	2	4	8	16	32
1	-2	-1	-2	-2	-2
2	-2	-1	-2	-3	-3
4	-2	-1	-2	-3	-4
8	-2	-1	-2	-3	-3
16	-2	-1	-2	-3	
32	-2	-1	-2	-3	

ERROR RATIO X10

ANGLE MESH	2	4	8	16	32
1	6	102	10	9	
2	9	12	6	42	43
4	10	10	10	8	43
8	10	10	10	10	9
16	10	10	10	10	
32	10	10	10	10	

4. The Mathematical Structure of the Solution of the Transport Equation

In order to design effective approximation operators and sensible computational cells, it is imperative to know the analytic behavior of the mathematical solution of the problem. Let us remember that the transport equation is a mathematical model for neutron migration. It is the purpose of a computer code to represent faithfully the mathematical solution of the transport equation. If the model is a good one, it will also represent the actual physical situation. If it does not, it is up to the engineer or physicist to change this model.

We address now the problem of finding the neutron flux distribution in a reactor configuration. Mathematically, the configuration is the union of computational cells, where in each cell the coefficients in the transport equation (i.e. the material coefficients) are constant, but may be different from cell to cell.

We shall restrict ourselves to the discussion of the two-dimensional stationary transport equation

$$\sin \theta \left(\cos \varphi \frac{\partial}{\partial x} + \sin \varphi \frac{\partial}{\partial y} \right) \psi + \sigma \psi = \frac{c}{4\pi} \int_{\varphi'=0}^{2\pi} \int_{\theta'=0}^{\pi} p \psi \sin \theta' d\theta' d\varphi' + S$$

First, let us mention that it is rather easy to prove the existence of a unique solution of the transport equation under very general conditions.

In particular, it can be shown that across interfaces, the flux in direction of the neutron motion is Lipschitz-continuous. While this is a very important piece of information, the numerical analyst wants to know the behavior of $\psi(x,y,\varphi)$ near the interfaces. The answer is obtained in two steps. First, we select a small layer on both sides of the interfaces and by a change of units we change the co-ordinate system in the direction of the interface normal (stretching of the boundary layer). After the

transformation, the transport equation takes the form of a one-dimensional equation, and the problem is reduced to half space problems. It is well known that for the Milne problem, with $\cos \varphi = \mu$, $\mu \ll 1$, the directional flux and the scalar flux Φ respectively behave like

$$\psi(0, \mu) = \frac{c}{2} \left[1 - \frac{c}{2} |\mu| \log |\mu| + O(\mu) \right]$$

$$\Phi(x) = 1 - \frac{c}{2} x \log x + O(x)$$

if the boundary is along the y-axis (i.e. $x = 0$). If there are two different media (1) and (2) then the behavior can be deduced from the two half space problems (1) and (2). The flux is

$$\psi(0, \mu) = \frac{c^{(2)}}{2(1-c^{(2)})} \frac{\lambda_0^{(2)}}{1 + \lambda_0^{(2)} \mu} \frac{\psi^{(1)}(0, \mu)}{\psi^{(2)}(0, \mu)} \quad \mu < 0$$

$$\psi(0, \mu) = \frac{c^{(1)}}{2(1-c^{(1)})} \frac{1 - \lambda_0^{(2)} \mu}{\lambda_0^{(2)}} \frac{(\lambda_0^{(1)})^2}{1 - (\lambda_0^{(1)})^2 \mu^2} \frac{\psi^{(2)}(0, -\mu)}{\psi^{(1)}(0, -\mu)} \quad \mu > 0$$

and therefore exhibits also pathological behavior. There is a discontinuity at $\mu = 0$, namely

$$\psi(0, 0^+) - \psi(0, 0^-) = \frac{1}{2} (c^{(2)} - c^{(1)}) \Phi(0) + s^{(2)} - s^{(1)}$$

While for $\mu \neq 0$, the flux is continuous, its derivative $d\psi/d\mu \sim \log|\mu|$, $\mu \ll 1$, shows a logarithmic behavior. Similarly, the derivative of the scalar flux in the normal direction to the interface is logarithmic, i.e., $d\Phi/dx \sim \log|x|$ for $x \rightarrow 0$. This behavior has implications on the numerical methods used. The first two columns of Table 4.1 show the results of a linear collocation approximation based on the integral transport equation for the Milne problem,

$$\Phi(x) = \frac{c}{2} \int_0^\infty \Phi(x') E_1(|x - x'|) dx', \quad c \leq 1$$

TABLE 4.1

Unnormalized Neutron-density of Milne Problem for $c = 1$
and Linear Collocation Approximation

x	n=18	n=32	n=8 with x log x	Exact
0.0	.0116	.0011	.5789	.5774
0.001		.5812		
0.01	.5784	.5905	.5881	.5882
0.02	.6107	.5940	.5949	.5954
0.04	.5988	.6049	.6062	.6063
0.1	.6450	.6266	.6280	.6279
1.0	.7045	.6992	.6981	.6985
3.0	.7133	.7102	.7098	.7098
20	.7138	.7108	.7104	
∞				.7104

n is the number of mesh points used

TABLE 4.2

Error in Milne Problem at Boundary ($x=0$)

n	Cubic Splines	Cubic Splines with x log x
4	-.0498	-.0394
8	-.0289	-.0105
16	-.0156	-.0022
32	-.0082	-.0006

If no knowledge of the exact solution were assumed, the numerical results would look reasonable at the (free) boundary. The third column shows the results of a similar calculation with an $x \log x$ term added in the first interval. The calculations were repeated with cubic splines and with cubic splines plus an $x \log x$ term added. The results are shown in Table 4.2.

We turn now our attention to the edge effect. Bareiss and Abu-Shumays (1969) applied the integral transformation

$$(1 - v^2) \int \frac{d\Omega(\cdot)}{|\underline{v} - \Omega|^3} \quad (\underline{v} = v\Omega')$$

to the transport equation

$$(\Omega \cdot \nabla \psi + 1) \psi = \frac{c}{4\pi} \int \psi d\Omega + S \quad \psi = \psi(x, \Omega)$$

which lead, to our surprise, to the ultra-hyperbolic partial differential equation of second order

$$(H + K) \chi = C\chi(x, 0) + \hat{S}(x, v)$$

where

$$H = (1 - v^2) \nabla \cdot \nabla_v + 2\underline{v} \cdot \nabla_v \cdot \nabla_v$$

$$K = \underline{v} \cdot \nabla + 2\underline{v} \cdot \nabla_v + 1$$

The quadratic form for the characteristics of H is $\psi^T A \psi$ where the matrix A is

$$A = \begin{bmatrix} 0 & B \\ B & 0 \end{bmatrix}; \quad B = \begin{bmatrix} \frac{1-v^2}{2} + v_1^2 & v_1 v_2 & v_1 v_3 \\ v_1 v_2 & \frac{1-v^2}{2} + v_2^2 & v_2 v_3 \\ v_1 v_3 & v_2 v_3 & \frac{1-v^2}{2} + v_3^2 \end{bmatrix}$$

The index of inertia of A is three, and has the six eigenvalues

$$\omega_1 = \pm \frac{1+v^2}{2}, \quad \omega_2 = \omega_3 = \pm \frac{1-v^2}{2}.$$

Inspection of the characteristic quadratic revealed that every surface in the x -space and every surface in the v -space are basic characteristic surfaces. Now, the inverse transform of the generating function $\chi(x, v\Omega)$ is defined pointwise in x by

$$\psi(\Omega) = \frac{1}{4\pi} (1 + 2v \frac{\partial}{\partial v}) \chi(v\Omega) \Big|_{v=1}$$

Therefore every line on the unit-sphere $|\Omega| = 1$ is a basic characteristic line, while every surface in the x -space is also a basic characteristic surface of the transport operator. The implication is of course that in a multiregion reactor, every edge and corner of a region, radiates and propagates singularities in all directions. In transport problems with spherical, cylindrical or plane geometries this phenomena does not occur. This phenomena is difficult to illustrate in a five dimensional space $E_3 \times \Omega_2$. We therefore illustrate the behavior on a simple two-dimensional transport equation where we have only three independent variables, namely x, y, φ . We assume that we know the exact solution ψ of the transport equation

$$(\cos \varphi \frac{\partial}{\partial x} + \sin \varphi \frac{\partial}{\partial y} + \sigma) \psi = \frac{c}{2\pi} \int_0^{2\pi} \rho \psi d\varphi + S$$

for a particular problem. Looking at this equation as a partial differential equation with a known function on the right side we obtain the differential equation for the basic characteristic lines c_φ from

$$\begin{vmatrix} dx & dy \\ \cos \varphi & \sin \varphi \end{vmatrix} = 0 \text{ or } c_\varphi = x \sin \varphi - y \cos \varphi$$

It is obvious that the partial derivatives of ψ with respect to x and y across a basic characteristic through the vortex of a wedge are generally discontinuous. Without our previous remarks, it is not obvious that the partial derivatives with respect to φ are also discontinuous in general.

We shall prove both cases.

We consider the following representative wedge problem. For the notation we refer to Figure 4.1. Two or more regions with different material coefficients meet at the origin 0 of a Cartesian coordinate system (x,y) . The boundary lines (i.e. interfaces) are indicated by the curves a : $a(x,y) = 0$ and b : $b(x,y) = 0$. The basic characteristic straight line through the origin at angle φ with the x -axis is denoted by

$$c_\varphi : x \sin \varphi - y \cos \varphi = 0 .$$

The angle between a and c_φ at 0 is α , between b and c_φ is β . We denote the known flux $\psi(x,y,\varphi)$ on $a(x,y) = 0$ and $b(x,y) = 0$ by $\psi_a(s,\varphi)$ and $\psi_b(s,\varphi)$ respectively, where s is the positive arc length of a or of b from the origin 0. The values $\psi_a(0,\varphi)$ and $\psi_b(0,\varphi)$ are limit values as $s \rightarrow 0$. We shall investigate the behavior of $\psi(x,y,\varphi)$ in a neighborhood of c_φ . To this end we select an arbitrary but fixed point $P_0 = (x_0, y_0)$ on c_φ . P_0 will also be interpreted as the vector of length

$$r_0 = (x_0^2 + y_0^2)^{\frac{1}{2}}$$

The flux in the wedge W_α bounded by a and c_φ and vortex 0 will be denoted by $\psi_\alpha(x,y,\varphi)$, the flux in the wedge W_β bounded by b and c_φ will be denoted by $\psi_\beta(x,y,\varphi)$.

The method of proving discontinuities over or across c_φ is in all cases as follows.

Step 1. We represent the solutions of our model problem in the form of the collision probability integral.

Step 2. We take the partial derivative of these representations in the (x,y) -plane in direction of the normal n of c_φ , where

$$n = (\sin \varphi, -\cos \varphi) .$$

Step 3. We take the partial derivative of the representations at P_0 with respect to the parameter φ , measured in radians.

The proof of discontinuity is very simple. In each case we derive a linear integral equation for the quantity under investigation which has a unique solution over the domain of existence. Different coefficients (or parameters) in the equations for $\psi_\alpha(P, \varphi)$, $\psi_\beta(P, \varphi)$, or its derivatives indicate different solutions and discontinuity on c_φ . The function spaces to which $\psi_\alpha(x, y, \varphi)$, $\psi_\beta(x, y, \varphi)$ and their derivatives belong can be determined from the respective integral equations by inspection. We note that steps 2 and 3 can be repeated for higher derivations. Based on these remarks, it is sufficient for our purpose to derive the appropriate integral equations. We start with some definitions. The orientation of c_φ is given by the unit vector

$$\omega = (\cos \varphi, \sin \varphi).$$

For any point (x, y) in the wedge W , we define

$$Q(x, y, \varphi) = \frac{c}{2\pi} \int_0^{2\pi} p(\varphi, \varphi') \psi(x, y; \varphi') d\varphi' + S(x, y, \varphi')$$

The notation Q_α (or Q_β) indicates that $Q(x, y, \varphi)$ is the limit value as

$$(x, y) \in W_\alpha \text{ (or } W_\beta) \rightarrow (x, y) \in c_\varphi.$$

Obviously

$$\psi(x, y, \varphi) = \begin{cases} \psi_\alpha(x, y, \varphi) & \text{for } (x, y) \in W_\alpha \\ \psi_\beta(x, y, \varphi) & \text{for } (x, y) \in W_\beta \end{cases}$$

and for $(x, y) \in c_\varphi$, ψ_α and ψ_β are the appropriate limit values.

We begin our investigation with Step 1.

Step 1. Referring to the notation in Figure 4.2 the integral representation for $\psi_\alpha(x_s, y_s, \varphi)$ is

$$\psi_\alpha(P_s, \varphi) = \psi_a(s, \varphi) e^{-\sigma r_s} + \int_0^{r_s} e^{-\sigma r} Q(P_s - rw, \varphi) dr$$

where

$$P_s = (x_s, y_s) \in W_\alpha, \quad rw = (x_s - x, y_s - y)$$

and r_s is the length of r when rw intersects a . Hence, for $s \rightarrow 0$

$$\psi_\alpha(P_0, \varphi) = \psi_a(0, \varphi) e^{-\sigma r_0} + \int_0^{r_0} e^{-\sigma r} Q_\alpha(P_0 - rw, \varphi') d\varphi'$$

and similarly (see Figure 4.3)

$$\psi_\beta(P_0, \varphi) = \psi_b(0, \varphi) e^{-\sigma r_0} + \int_0^{r_0} e^{-\sigma r} Q_\beta(P_0 - rw, \varphi') d\varphi'.$$

We note that continuity of $\psi(x, y, \varphi)$ in the neighborhood of c_φ depends only on the continuity of $\psi_a(s, \varphi)$ and $\psi_b(s, \varphi)$ in the neighborhood of $(0, \varphi)$ and the continuity of p and S in the neighborhood of $\{c_\varphi, \varphi\}$.

However, in many computational problems, the assumption $\psi_a(0, \varphi) = \psi_b(0, \varphi)$ is not true.

Step 2: Referring to Figure 4.2 we have for $P_s \in W_\alpha$

$$ds/dn = 1/\sin \alpha, \quad dr_s/dn = -\cot \alpha$$

Differentiating the integral equation in Step 1 and letting $s \rightarrow 0$, we have

$$\begin{aligned} \frac{\partial}{\partial n} \psi_\alpha(P_0, \varphi) &= \frac{e^{-\sigma r_0}}{\sin \alpha} \left(\frac{\partial}{\partial s} + \sigma \cos \sigma \right) \psi_a(0, \varphi) - \cos \alpha Q_\alpha(0, \varphi) \\ &\quad + \int_0^{r_0} e^{-\sigma r} \frac{\partial}{\partial n} Q_\alpha(P_0 - rw, \varphi) dr. \end{aligned}$$

and similarly for $P_s \in W_\beta$ (Figure 4.3)

$$ds/dn = -1/\sin \beta, \quad dr_s/dn = \cot \beta$$

which yields

$$\begin{aligned} \frac{\partial}{\partial n} \psi_\beta(P_0, \varphi) &= -\frac{e^{-\sigma r_0}}{\sin \beta} \left(\frac{\partial}{\partial s} + \sigma \cos \beta \right) \psi_b(0, \varphi) - \cos \beta Q_\beta(0, \varphi) \\ &\quad + \int_0^{r_0} e^{-\sigma r} \frac{\partial}{\partial n} Q_\beta(P_0 - r\omega, \varphi) dr. \end{aligned}$$

Obviously, even with the assumptions of continuity made in Step 1, $\partial \psi_\alpha / \partial n \neq \partial \psi_\beta / \partial n$, unless $\alpha + \beta = \pi$ and $\partial \psi_a / \partial s = -\partial \psi_b / \partial s$ at 0. Result: In general, the space derivatives of $\psi(P_0, \varphi)$ across C_φ are discontinuous in a wedge problem. Note also, that for $\alpha \rightarrow 0$ ($\beta \rightarrow 0$) the equations become indetermined, since the expressions in brackets $[] \rightarrow 0$ for $\alpha \rightarrow 0$ ($\beta \rightarrow 0$).

Step 3: Referring to Figure 4.4, we deduce in W_α

$$ds/d\varphi = r_0/\sin \alpha, \quad dr_\varphi/d\varphi = -r_0 \cot \alpha, \quad dn/d\varphi = r.$$

Hence, at the point $P_0 \in c_\varphi$, we obtain from the integral equation of Step 1 for $P_s \in W_\alpha$, $P_s \rightarrow P_0$,

$$\begin{aligned} \frac{\partial}{\partial \varphi} \psi_\alpha(P_0, \varphi) &= e^{-\sigma r_0} \left(\frac{\partial}{\partial \varphi} + \frac{r_0}{\sin \alpha} \frac{\partial}{\partial s} + \sigma r_0 \cot \alpha \right) \psi_a(0, \varphi) \\ &\quad - r_0 \cot \alpha e^{-\sigma r_0} Q_\alpha(0, \varphi) + \int_0^{r_0} e^{-\sigma r} \left(r \frac{\partial}{\partial n} + \frac{\partial}{\partial \varphi} \right) Q_\alpha(P_0 - r\omega, \varphi) dr \end{aligned}$$

and similarly in W_β at P_0 ,

$$ds/d\varphi = -r_0/\sin \beta, \quad dr_\varphi/d\varphi = r_0 \cot \beta, \quad dn/dr = r$$

$$\frac{\partial}{\partial \varphi} \psi_{\beta}(P_0, \varphi) = e^{-\sigma r_0} \left(\frac{\partial}{\partial \varphi} - \frac{r_0}{\sin \beta} \frac{\partial}{\partial s} - \sigma r_0 \cot \beta \right) \psi_b(0, \varphi) + r_0 \cot \beta e^{-\sigma r_0} Q_{\beta}(0, \varphi) + \int_0^{r_0} e^{-\sigma r} \left(r \frac{\partial}{\partial n} + \frac{\partial}{\partial \varphi} \right) Q_{\beta}(P_0 - rw, \varphi) dr$$

Result: In general, the angular derivative $\psi(P_0, \varphi)$ is discontinuous if $P_0 \in C_{\varphi}$.

Again, if $\alpha + \beta = \pi$ and ψ_a and $\psi_b \in C^{1,1}(s, \varphi)$ and the terms in Q are elements of $C^{2,1,1}(x, y, \varphi)$, then the discontinuity disappears.

If $\alpha \rightarrow 0$ ($\beta \rightarrow 0$) the equations become indetermined for the same reason as in Step 2.

By varying ψ , the basic characteristics C_{φ} cover the entire interior of a wedge bounded by straight lines a and b . One may conclude that every space point $(x, y) \in W$ is a singular point. This is true. However, if we consider the singularities of $\psi(x, y, \varphi)$ in the (x, y, φ) - space, the discontinuities in ψ are confined to a regular winding surface with the axis of rotation given by $(0, 0, \varphi)$ and φ is limited by the directions of the boundaries of the wedge. Thus in the (x, y, φ) -space, almost every point is a regular point. In Figure 4.5 we illustrate this surface of discontinuities in $\psi(x, y, \varphi)$ for a wedge with vortex angle $\pi/2$ at 0. Only if this "characteristic surface" is penetrated, ψ and/or its derivatives are discontinuous. Thus, in this rather simple problem, the sides a and b of the wedge, the (x, y) plane and the characteristic surface are natural boundaries for a finite element.

Mathematically, the singular behavior is not only propagated in the direction of the neutron motion, as we have tacitly implied in our notation, it can also be traced in the opposite direction. Furthermore,

Figure 4.5 Characteristic Surface of Discontinuities in (x, y, ϕ) -space Induced by Vortex 0 of a Wedge in (x, y) -space

Figure 4.6 Characteristic surface in (x, y, ϕ) -space Over Full Range of ϕ , for Fixed x and y

our arguments can also be extended to wedges with a vortex angle greater than π . Thus, in general, the mathematical "characteristic surface" has the form of the regular winding surface illustrated in Figure 4.6.

The situation becomes worse where many vortices occur such as in actual reactor configurations. Figure 4.7 illustrates two characteristic surfaces caused by the vortices A and B of the near side of a hexagon. As more vortices enter the picture more such surfaces will appear. In addition, according to Step 1, singularities can be transmitted across interfaces, so that the situation for accurate numerical computation becomes rather grave.

So far, we restricted ourselves to the two-dimensional model problem. We turn now to the θ -dependent two-dimensional transport equation as formulated at the beginning of this section. For purposes of geometric visualization, we extend the problem into the three-dimensional Euclidean space. Then the vortex 0 of the wedge W becomes the edge $(0,0,z)$ in Cartesian (x,y,z) -coordinates, (Figure 4.8), i.e. it coincides with the z -axis. We shall retain the notation used in the model problem by identifying the (x,y) -plane with the $(x,y,0)$ -plane in E_3 . Now we impose on all functions F in phase space (x,y,z,Ω) the requirement

$$\frac{\partial F}{\partial z} \equiv 0$$

which is the commonly used definition for a two-dimensional transport problem. Thus, if $P = (x,y,z)$, then, for example, $\psi(P, \Omega) = \psi$

$$\psi(P, \Omega) = \psi(x,y,z, \Omega) = \psi(x,y,0, \Omega) \equiv \psi(x,y, \Omega).$$

The representation of the unit vector Ω in Cartesian coordinates in reference to polar coordinates is

Figure 4.7 Two Characteristic Surfaces of Discontinuities in (x, y, φ) -space Induced by the Vortices A and B of a Hexagon.. Lower Part is Projection on (x, y) -plane

$$\Omega = (\Omega_x, \Omega_y, \Omega_z) = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)$$

and hence

$$\sin \theta \omega = (\Omega_x, \Omega_y, 0) = \sin \theta (\cos \varphi, \sin \varphi, 0).$$

Thus, with our assumptions, the following two formulations of the transport equation are equivalent

$$\begin{aligned} (\Omega \cdot \nabla + \sigma) \psi(P, \Omega) &= Q(P, \Omega) & P &= (x, y, z) \\ (\sin \theta \omega \cdot \nabla + \sigma) \psi(P, \Omega) &= Q(p, \Omega) & P &= (x, y, 0) \end{aligned}$$

where

$$\begin{aligned} Q(P, \Omega) &= \frac{c}{4\pi} \int_{\Omega'} p(\Omega, \Omega') \psi(P, \Omega') d\Omega' + S(P, \Omega) = \\ Q(x, y, \varphi, \theta) &= \frac{c}{4\pi} \int_0^{2\pi} d\varphi \int_0^\pi d\theta \sin \theta p(\varphi, \theta, \varphi', \theta') \psi(x, y, \varphi', \theta') + S(x, y, \varphi, \theta) \end{aligned}$$

Consider the transport equation as a partial differential equation in $(x, y, z, \varphi, \theta, \psi)$ -space. Then the characteristic lines are defined by the following system of ordinary differential equations where the dot ($\dot{\cdot}$) denotes differentiation with respect to a parameter.

$$\dot{x} = \Omega_x, \quad \dot{y} = \Omega_y, \quad \dot{z} = \Omega_z, \quad \dot{\varphi} = 0, \quad \dot{\theta} = 0, \quad \dot{\psi} = -\sigma \psi + Q$$

In the $(x, y, \varphi, \theta, \psi)$ -space formulation we have

$$\dot{x} = \Omega_x, \quad \dot{y} = \Omega_y, \quad \dot{\varphi} = 0, \quad \dot{\theta} = 0, \quad \dot{\psi} = -\sigma \psi + Q.$$

Therefore, the projection of the basic characteristic lines from $(x, y, z, \varphi, \theta)$ -space into (x, y, z) -space represent the neutron paths, and the projection into (x, y) -space yields the identical family of straight lines $\{c_\varphi\}$ as in the model problem. The characteristic surface in (x, y, φ, θ) -space generated by the basic characteristic lines through

$(0,0,\varphi,\theta)$ are given by the regular winding hyper-surface H:

$$\begin{aligned} x &= t \sin \theta \cos \varphi, & \varphi &= \varphi, \\ y &= t \sin \theta \sin \varphi, & \theta &= \theta, \end{aligned}$$

with (t,φ,θ) the parameter space.

To assess the nature of the possible singular behavior of $\psi(x,y,\varphi,\theta)$ in the neighborhood of H, we repeat Steps 1 to 3 of the model problem and add the expressions for $\partial\psi/\partial\theta$ and $\partial\psi/\partial t$ in Steps 4 and 5.

Step 1: Referring to Figure 4.9, the integral equation is

$$\psi_Y(P_0, \Omega) = \psi_g(0, \Omega) e^{-\sigma R_0} + \int_0^{R_0} e^{-\sigma R} Q_Y(P - R\Omega, \Omega) dR$$

or equivalently

$$\psi_Y(P_0, \Omega) = \psi_g(0, \Omega) e^{-\sigma r_0/\sin\theta} + \int_0^{r_0} e^{-\sigma r/\sin\theta} Q_Y(P_0 - r\omega, \Omega) \frac{dr}{\sin\theta}$$

where

$$\gamma = \begin{cases} \alpha \\ \beta \end{cases} \quad g = \begin{cases} a \\ b \end{cases} \quad \text{if } P_0 \leftarrow P_s \in \begin{cases} W_\alpha \\ W_\beta \end{cases}$$

$$P_0 = (x_0, y_0, 0) \in c_\varphi, \quad R_0 = r_0 / \sin \theta$$

Step 2: Referring to Figures 4.9 and 4.3 we have

for W_α :

$$\partial R_0 / \partial n = -\cot \alpha / \sin \theta$$

$$\partial s / \partial n = 1 / \sin \alpha$$

for W_β :

$$\partial R_0 / \partial n = \cot \beta / \sin \theta$$

$$\partial s / \partial n = -1 / \sin \beta$$

$$\begin{aligned} \frac{\partial}{\partial n} \psi_Y(P_0, \Omega) &= e^{-\sigma R_0} \left[\left(\frac{\partial s}{\partial n} \cdot \frac{\partial}{\partial s} - \sigma \frac{\partial R_0}{\partial n} \right) \psi_g(0, \Omega) + \frac{\partial R_0}{\partial n} Q_Y(0, \Omega) \right] \\ &\quad + \int_0^{R_0} e^{-R} \frac{\partial}{\partial n} Q_Y(P - R\Omega, \Omega) dR \end{aligned}$$

Step 3: Referring to Figure 4.10 and 4.3 we have

for W_α :

$$\frac{\partial R_0}{\partial \varphi} = -R_0 \cot \alpha$$

$$\frac{\partial s}{\partial \varphi} = R_0 \frac{\sin \theta}{\sin \alpha}$$

$$\frac{\partial n}{\partial \varphi} = R \sin \theta$$

for W_β :

$$\frac{\partial R_0}{\partial \varphi} = R_0 \cot \beta$$

$$\frac{\partial s}{\partial \varphi} = -R_0 \frac{\sin \theta}{\sin \beta}$$

$$\frac{\partial n}{\partial \varphi} = R \sin \theta$$

$$\begin{aligned} \frac{\partial}{\partial \varphi} \psi_Y(P_0, \Omega) &= e^{-\sigma R_0} \left[\left(\frac{\partial}{\partial \varphi} + \frac{\partial s}{\partial \varphi} \cdot \frac{\partial}{\partial s} - \sigma \frac{\partial R_0}{\partial \varphi} \right) \psi_g(0, \Omega) + \frac{\partial R_0}{\partial \varphi} Q_Y(0, \Omega) \right] \\ &+ \int_0^{R_0} e^{-\sigma R} \left(\frac{\partial n}{\partial \varphi} \frac{\partial}{\partial n} + \frac{\partial}{\partial \varphi} \right) Q_Y(P - R\Omega, \Omega) dR \end{aligned}$$

Step 4: Referring to Figure 4.11 we have

for W_α and W_β : $\partial R_0 / \partial \theta = -R_0 \cot \theta$

$$\begin{aligned} \frac{\partial}{\partial \theta} \psi_Y(P_0, \Omega) &= e^{-\sigma R_0} \left[\left(\frac{\partial}{\partial \theta} + \sigma \frac{\partial R_0}{\partial \theta} \right) \psi_g(0, \Omega) + \frac{\partial R_0}{\partial \theta} Q_Y(0, \Omega) \right] \\ &+ \int_0^{R_0} e^{-\sigma R} \frac{\partial}{\partial \theta} Q_Y(P - R\Omega, \Omega) dR \end{aligned}$$

Step 5: The derivative in direction w yields

$$\begin{aligned} \sin \theta w \cdot \nabla \psi_Y(P_0, \Omega) &= -e^{-\sigma r_0 / \sin \theta} \left[\sigma \psi_g(0, \Omega) - Q_Y(0, \Omega) \right] \\ &+ \int_0^{r_0} e^{-\sigma r / \sin \theta} w \cdot \nabla_{P_0} Q_Y(P_0 - rw, \Omega) dr \end{aligned}$$

which becomes the two-dimensional transport equation as $r_0 \rightarrow 0$.

Reviewing the five equations we see that: (1) Discontinuities will

be propagated in phase-space. (2) The presence of a corner such as the vortex 0 of a wedge W in two-dimensional transport calculations, preserves the continuity of in the flux ψ but causes discontinuities in $\partial\psi/\partial x$, $\partial\psi/\partial y$, and $\partial\psi/\partial\varphi$ at the vortex 0.

The statements made in this section revealed some of the mathematical aspects of transport theory solutions in multiregion problems. They have implications on the general approach to transport theory calculations. It has certainly been demonstrated that transport theory implies weak solutions.

How can these difficulties be overcome? I see three possibilities:

- a) We can restrict the "discrete" directions in a regular configuration so that they pass through as many corners as possible. An example is given in Figure 4.12 which was already published some years ago (Bareiss 1958).
- b) We may have to rely more heavily on nonconforming elements and perhaps rational approximations.
- c) We may apply regularization procedures. In particular, we may have to use the integral form of the transport equation, solve for the scattering integral and then extract ψ . This method seems to me the most promising.

The interface current technique, response matrix method, and collision probability method may best fit into the last proposition. It seems to me highly questionable to invest in high order polynomial approximation methods considering our present state of knowledge. On the other hand, I believe that the variational methods will continue to be useful.

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Figure 4.12 Computation cells of lattice for (a) three-dimensional and (b) two-dimensional calculations

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