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SUMMARY

This progress report is divided into three sections, two of which describe one phase of our effort to develop fast and accurate two dimensional S_N type neutron transport programs. The last section discusses our progress in improving the convergence rate of VARI-QUIR III, an R- θ diffusion theory program.

A substantial decrease in computer time results when S_N type programs are run with really good initial guesses. To attain this end, we have modified our standard diffusion codes to supply a flux guess for DDK, TDC, and DTK. In addition, we have studied the application of the Shanks⁽¹⁾ acceleration technique to the problem of eigenvalue convergence - so far without too much success.

In order to improve the accuracy of S_N calculations, we have developed a method which prevents the occurrence of negative fluxes near control vanes.

We have developed a rigorous, but practical, method for including anisotropic scattering in diffusion theory calculations. This last technique can help provide better flux guesses for transport calculations and can greatly improve diffusion results at interfaces.

Finally, we have discovered the cause of the slow convergence rate of the R- θ version of VARI-QUIR and are making the necessary corrections.

I - CONVERGENCE ACCELERATION

Programming Improvements

During the past year the FLOCOW assembly program has been completed. This replacement for the Los Alamos FLOCO program, coupled with minor program improvements, has halved the running time of S_N programs. This improvement stems mostly from increased input/output efficiency.

Another factor of three reduction in the running time of large two dimensional S_N programs has been attained by modifying the EXTERMINATOR⁽²⁾ diffusion code to supply flux guesses for TDC and DDK. A package of codes, the SINPACK (S_N INPUT PACKAGE) permits automatic editing of EXTERMINATOR (when the output tape is available and DDK fluxes have not been previously obtained), TOPIC⁽³⁾, MIST⁽⁴⁾, and MSPHT⁽⁵⁾ output for input to the appropriate S_N code. This output may be edited to provide input for similar but not necessarily identical reactors; furthermore, S_N output fluxes may be edited for input to similar but non-identical problems.

The Shanks Technique

Introduction

Daniel Shanks⁽¹⁾ has developed a technique for determining the asymptotic value of some slowly convergent sequences. We have attempted to apply his methods to the problem of eigenvalue extrapolation.

Extrapolation technique can be no more accurate than the information contained in already available data. For example, nearly geometric or alternating series converge very slowly; but, when nearly converged, the least

significant digits of each additional term carry much information about the converged value of these series. Shanks method can frequently determine the limit of a sequence from remarkably few terms, and therefore, is highly sensitive to small errors in the least significant digits thereof. We have found that even double precision arithmetic does not prevent occasional wild oscillations of the predicted limits of a sequence and that, despite its great power, the method developed by Shanks is unreliable for use as an automatic extrapolation scheme.

If the random jitter in a machine generated eigenvalue sequence were removed, it is possible that the Shanks technique would be very useful. Unfortunately his formulation does not easily lend itself to smoothing techniques; the following sections contain a reformulation of the method which should permit rapid polynomial smoothing of the predicted limit of a sequence. Although we have not yet attempted a proof, we conjecture that a modified Shanks technique can be shown to be rigorously applicable to a sequence which converges in a numerically useful way.

The Shanks Transforms

Shanks transforms are a family of non-linear sequence-to-sequence transformations which can be powerful aids in determining the limits of slowly converging sequences.

These transforms are generalizations of, or related to, well known algorithms such as the Newton-Raphson method, the Pade Table, Gauss's method

for numerical integration, and Aitken's δ^2 -process. Shanks method is applicable to a rather wide class of problem; however, we shall be concerned only with applying his techniques to finite subsets of (hopefully) convergent sequences.

Motivation

Numerical sequences such as those generated by iterative processes sometimes resemble physical transients. For example figure 1.1 illustrates frequently seen eigenvalue sequences calculated by "under" (fig. 1.1a), "over" (fig. 1.1b), and "critically" (fig. 1.1c) - damped stable iterative processes. Figure 1.1d illustrates a possible eigenvalue sequence from an unstable iterative technique.

Fig. 1.1 Typical Eigenvalue Sequences

Shanks method is designed to remove the "transient", exponential-like, variations from such sequences. Judicious application of this method would almost certainly improve the convergence rate of the sequences pictured in figure (1.1a) and (1.1b), probably would improve that shown in figure (1.1c), and properly applied might induce convergence in the sequence of figure (1.1d).

In general, a function displaying such "transient" behavior may often be written as

$$A(t) = B + \sum_i \alpha_i e^{-\gamma_i t} \quad (1.1)$$

Equations of the type (1.1) are solutions of linear second order differential equations. These equations have the well known property that for repeated roots the solution $A(t)$ should be replaced by

$$A'(t) = B + \sum_i \alpha_i (1+t+t^2+\dots+t^p) e^{-\gamma_i t} \quad (1.2)$$

where p is the order of the degeneracy of γ_i . For simplicity, we shall ignore this complication and merely consider the non-degenerate case.

If the function $A(t)$ converges for large t , the real parts of all γ_i must be positive. It is convenient to demand that no $\gamma_i = 0$, i.e. all constant terms must be absorbed in B ; in this case, B is the limit of $A(t)$ for large t .

$$\lim_{t \rightarrow \infty} A(t) = B, \quad R(\gamma_i) \geq 0 \quad (1.3)$$

$$\gamma_i \neq 0$$

For the moment, let us assume that any finite sequence can be fitted to such a curve. The proof of this assumption, together with the calculation of the limit B , forms that part of the theory of Shanks transformations which we need for our applications. We replace the continuous variable t by a discrete parameter n and write

$$A_n = B + \sum_i \alpha_i e^{\gamma_i n} \quad (1.4)$$

or equivalently,

$$A_n = B + \sum_i \alpha_i q_i^n \quad (1.5)$$

We are willing to accept the following restrictions on q_i :

$$\begin{aligned} q_i &\neq 1 \text{ (no constant terms other than } B), \\ q_i &\neq q_j, i \neq j \text{ (no degeneracies),} \end{aligned} \quad (1.6)$$

and $q_i \neq 0$.

The last restriction is purely for bookkeeping purposes; for example, if A_n is a function of N different exponentials, we may be willing to fit it with $N+1$ exponentials with $\alpha_{N+1} \equiv 0$, $\gamma_{N+1} \neq 0$ but we shall not permit the equivalent fit $\alpha_{N+1} \neq 0$, $\gamma_{N+1} = -\infty$. In practice upon meeting such a case, we simply reduce the number of exponentials used to fit A_n .

Simplified Theory of Shanks Transformations

We shall demonstrate that any finite subset of a sequence is representable by equation (1.5), and that this representation is equivalent to a particular polynomial representation.

Theorem

Any finite sequence with $(2K+1)$ members $A_1, A_2, A_3, \dots, A_{2K+1}$ can be represented by a set of $(2K+1)$ non-degenerate equations such that,

$$A_n = B + \sum_{i=1}^K \alpha_i q_i^n ; \quad q_i \neq q_j, i \neq j, \quad (1.7)$$

with

$$B = \frac{\begin{vmatrix} A_1 & A_2 & \dots & A_{K+1} \\ \Delta A_1 & \Delta A_2 & \dots & \Delta A_{K+1} \\ \Delta A_2 & \Delta A_3 & \dots & \Delta A_{K+2} \\ \vdots & \vdots & \dots & \vdots \\ \Delta A_K & \Delta A_{K+1} & \dots & \Delta A_{2K} \end{vmatrix}}{\begin{vmatrix} 1 & 1 & \dots & 1 \\ \Delta A_1 & \Delta A_2 & \dots & \Delta A_{K+1} \\ \vdots & \vdots & \dots & \vdots \\ \Delta A_K & \Delta A_{K+1} & \dots & \Delta A_{2K} \end{vmatrix}} \quad (1.8)$$

and

$$\Delta A_n = A_{n+1} - A_n . \quad (1.9)$$

Furthermore, this set of equations is unique if we agree to the following restrictions on the q_i .

$$\begin{aligned} q_i &\neq 0 \\ q_i &\neq 1 \end{aligned} \quad (1.10)$$

Remarks

The gist of this theorem is that any finite sequence can be fitted by the solution of a non-degenerate ($q_i \neq q_j$ for $i \neq j$) second order linear differential equation. This fitting is unique if we agree to consolidate all constant terms ($q_i \neq 0$) and to set the coefficients of redundant exponentials to zero ($\alpha_i \equiv 0$, not $q_i \equiv 1$ for $i >$ some maximum value).

The following remarks outline our proof.

The rectangular array (1.7) appears to be a grossly overdetermined set of equations in the $(K+1)$ variables $\{B, q_i\}_{i=1}^K$, although, of course, this is not so. A square array may be formed from the first $(K+1)$ equations and the remaining K equations used to find the quantities $\{\alpha_i\}_{i=1}^K$.

$$\begin{aligned}
 A_1 &= B + \alpha_1 q_1 + \alpha_2 q_2 + \dots + \alpha_K q_K \\
 A_2 &= B + \alpha_1 q_1^2 + \alpha_2 q_2^2 + \dots + \alpha_K q_K^2 \\
 &\vdots \\
 &\vdots \\
 A_j &= B + \alpha_1 q_1^j + \alpha_2 q_2^j + \dots + \alpha_K q_K^j \\
 &\vdots \\
 &\vdots \\
 A_{2K+1} &= B + \alpha_1 q_1^{2K+1} + \alpha_2 q_2^{2K+1} + \dots + \alpha_K q_K^{2K+1}
 \end{aligned} \tag{1.7}$$

It seems easier to work with $(K+1)$ linear equations in $(K+1)$ variables and then to transform the results directly to the form (1.7). The simplest array we can construct which makes direct use of our $(2K+1)$ parameters $\{A_n\}$ is the following:

$$\begin{aligned}
 A_1 &= B + (\Delta A_1) X_1 + (\Delta A_2) X_2 + \dots + (\Delta A_K) X_K \\
 A_2 &= B + (\Delta A_2) X_1 + (\Delta A_3) X_2 + \dots + (\Delta A_{K+1}) X_K \\
 &\vdots \\
 A_j &= B + (\Delta A_j) X_1 + (\Delta A_{j+1}) X_2 + \dots + (\Delta A_{j+K-1}) X_K \\
 &\vdots \\
 A_{K+1} &= B + (\Delta A_{K+1}) X_1 + (\Delta A_{K+2}) X_2 + \dots + (\Delta A_{2K}) X_K
 \end{aligned} \tag{1.11}$$

The solution for B (Equation 1.8) is now obvious, as is the solution for any

x_i . Furthermore, the transformation of equation (1.11) into equations (1.7) is simple. The differences ΔA_i can be found from (1.7),

$$\begin{aligned}
 \Delta A_1 &= \alpha_1 q_1 (q_1-1) + \alpha_2 q_2 (q_2-1) \dots + \alpha_K q_K (q_K-1) \\
 \Delta A_2 &= \alpha_1 q_1^2 (q_1-1) + \alpha_2 q_2^2 (q_2-1) \dots + \alpha_K q_K^2 (q_K-1) \\
 &\vdots \\
 \Delta A_j &= \alpha_1 q_1^j (q_1-1) + \alpha_2 q_2^j (q_2-1) \dots + \alpha_K q_K^j (q_K-1) \\
 &\vdots \\
 \Delta A_{2K} &= \alpha_1 q_1^{2K} (q_1-1) + \alpha_2 q_2^{2K} (q_2-1) \dots + \alpha_K q_K^{2K} (q_K-1)
 \end{aligned} \tag{1.12}$$

substituted into (1.11), and the coefficients of the q_i equated. For example, from (1.11) and (1.12) we obtain

$$\begin{aligned}
 A_j = & B + X_1 \left[\alpha_1 q_1^j (q_1-1) + \dots + \alpha_K q_K^j (q_K-1) \right] \\
 & + X_2 \left[\alpha_1 q_1^{j+1} (q_1-1) + \dots + \alpha_K q_K^{j+1} (q_K-1) \right] \\
 & + \vdots \\
 & + X_K \left[\alpha_1 q_1^{j+K-1} (q_1-1) + \dots + \alpha_K q_K^{j+K-1} (q_K-1) \right]
 \end{aligned} \tag{1.13}$$

$$\begin{aligned}
 = & B + \alpha_1 q_1^j (q_1-1) \left[X_1 + X_2 q_1 + \dots + X_K q_1^{K-1} \right] \\
 & + \alpha_2 q_2^j (q_2-1) \left[X_1 + X_2 q_2 + \dots + X_K q_2^{K-1} \right] \\
 & + \vdots \\
 & + \alpha_i q_i^j (q_i-1) \left[X_1 + X_2 q_i + \dots + X_K q_i^{K-1} \right] \\
 & + \vdots \\
 & + \alpha_K q_K^j (q_K-1) \left[X_1 + X_2 q_K + \dots + X_K q_K^{K-1} \right] .
 \end{aligned}$$

Since we are treating the $\{q_i\}$ as independent variables, we have

$$\alpha_i q_i^j = \alpha_i q_i^j (q_i-1) \left[X_1 + X_2 q_i + \dots + X_K q_i^{K-1} \right] \tag{1.14}$$

as the condition that equations (1.7) represent the sequence $\{A_j\}$. As we shall see, the conditions necessary for the existence of the transformation of (1.11) into (1.7) are precisely the conditions we want to apply a priori.

Proof

A necessary and sufficient condition for the system of equations (1.11) to have a unique solution for the variables $\{B, X_i\}_{i=1}^K$ is for the determinant Δ to be non-vanishing:

$$\Delta = \begin{vmatrix} 1 & \Delta A_1 & \Delta A_2 & \dots & \Delta A_K \\ 1 & \Delta A_2 & \Delta A_3 & \dots & \Delta A_{K+1} \\ \vdots & \vdots & \vdots & & \vdots \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & \Delta A_{K+1} & \Delta A_{K+2} & \dots & \Delta A_{2K} \end{vmatrix} \neq 0 \quad (1.15)$$

This determinant is, of course, identically equal to the denominator of equation (1.8).

Thus, we are left with the task of showing that there exists a unique one-to-one transformation of the system (1.11) into the system (1.7).

Given the "data" $\{A_i\}$ and the condition (1.15), equations (1.11) permit us to find the set $\{B, X_i\}$.

Given the set $\{B, q_i\}$, equations (1.14) also permit us to determine the set $\{B, X_i\}$. Furthermore, we can use (1.14) to prove the existence of the representation (1.7) because the representation (1.11) is guaranteed and (1.14) defines the transformation of (1.11) onto (1.7).

If the set of equations

$$1 = X_1 + X_2 q_i + \dots + X_K q_i^{K-1} \quad (1.16)$$

can be solved for $X_i(q_j)$ or for $q_i(X_j)$, then, with the additional proviso that $q_i \neq 0$, $(q_i - 1) \neq 0$, equations (1.14) permit the transformations (1.11) $\leftrightarrow$ (1.7).

We see that the set $\{q_i\}$ are roots of the equation

$$0 = 1 - \sum_{i=1}^K X_i q^{i-1}. \quad (1.17)$$

It can be shown⁽¹⁾ that in terms of the "data" $\{A_i\}$ the $\{q_i\}$ are the roots of the equation

$$\begin{vmatrix} 1 & \Delta A_1 & \dots & \Delta A_K \\ q & \Delta A_2 & \dots & \Delta A_{K+1} \\ \vdots & \vdots & & \vdots \\ q^K & \Delta A_{K+1} & \dots & \Delta A_{2K} \end{vmatrix} = 0 \quad (1.18)$$

Having obtained the set $\{q_i\}$, we can find the set $\{a_i\}$ from the first K equations of (1.12) as long as $q_i \neq q_j$. This last condition arises from the fact that with $\{q_i\}$ known, the existence of a unique solution of (1.12) depends only on

$$\begin{vmatrix} q_1 (q_1-1) & \dots & q_K (q_K-1) \\ q_1^2 (q_1-1) & \dots & q_K^2 (q_K-1) \\ \vdots & & \vdots \\ q_1^K (q_1-1) & \dots & q_K^K (q_K-1) \end{vmatrix} \neq 0 \quad (1.19)$$

Since $(q_i-1) \neq 0$; the inequality (1.19) reduces to

$$D \equiv \begin{vmatrix} q_1 & q_2 & \dots & q_i & \dots & q_K \\ q_1^2 & q_2^2 & \dots & q_i^2 & \dots & q_K^2 \\ \vdots & \vdots & & \vdots & & \vdots \\ q_1^K & q_2^K & & q_i^K & & q_K^K \end{vmatrix} \neq 0 \quad (1.20)$$

By inspection we can write down the K roots of (1.20) when it is considered to be a K^{th} order polynomial in any q_i (with the other q_j fixed). These roots are $q_i = q_j$ (two columns of the determinant become equal) and $q_i = 0$ (one column vanishes).

To demonstrate the existence of (1.7) we need only solve (1.16) for the $\{X_i\}$ in terms of the $\{q_i\}$ and substitute the results into (1.13). A necessary and sufficient condition for a unique solution of this form is, obviously, that the inequality (1.20) hold.

Summary and Desirable Development

We have shown that Shanks formulation (1.7) is equivalent to a polynomial fitting technique (1.11). In order to make his technique workable with computer generated sequences it will be necessary to study overdetermined polynomial fits and their relationship to a generalization of Shanks formulation.

II - IMPROVING ACCURACY

Anisotropic Scattering in Diffusion Theory

Introduction

In the past, various attempts have been made to include the effects of anisotropic scattering in diffusion calculations. Recently, Pomraning⁽⁶⁾ has published a generalization of the diffusion equation which properly accounts for linearly anisotropic (P1) scattering. His approach, which involves a generalization of Fick's law, leads to the replacement of the diffusion coefficient (which is a vector in energy space) by a diffusion matrix. More accurately speaking, the diagonal diffusion matrix associated with isotropic scattering generalizes to a matrix with non zero off-diagonal elements. Pomraning's results are elegant, but not directly applicable to currently available computer codes.

We have completed an alternative generalization of the diffusion equation which is directly applicable to existing codes. The major difference between our approach and Pomraning's is that he maintains the functional form of Fick's law and thus sacrifices the form of the diffusion equation; our approach is diametrically opposite.

We start with the multigroup approximation to the time independent linear transport equation, and then make the approximation that both neutron fluxes and laboratory scattering cross sections are linearly anisotropic. Straightforward manipulation then leads to our results. Finally, we discuss the question of internal boundaries.

Definitions

$N^g(\underline{x}, \underline{\Omega})$ Neutron angular flux in the direction of a unit vector, $\underline{\Omega}$, (particles/sec-cm²-steradian) with velocities defined by the energy spread of the group g .

$\phi^g(\underline{x}), \vec{j}^g(\underline{x})$ Scalar flux and neutron current, first and second moments of the neutron angular flux respectively.

$\sigma_s^{g' \rightarrow g}(\underline{x}, \underline{\Omega} \cdot \underline{\Omega}')$ Macroscopic laboratory scattering cross section; probability per unit distance of neutron travel that a neutron belonging to group g' undergo a scattering through the angle $\underline{\Omega} \cdot \underline{\Omega}'$ and emerge in group g . Of course, the proper energy-angle relationships are guaranteed by the averaging process which yields the multigroup approximation to the transport equation. We assume non-crystalline scattering.

$\sigma_{so}^{g' \rightarrow g}(\underline{x}), \sigma_{sl}^{g' \rightarrow g}(\underline{x})$ The first and second moments, respectively, of the macroscopic scattering cross section. The first is a scalar flux weighted average of the microscopic isotropic scattering cross section, the second is a current weighted average.

$\sigma_T^g(\underline{x}), \sigma_a^{(g)}(\underline{x})$ Neutron macroscopic cross sections for the energy group g ; respectively, total-, absorption-, removal-, "transport"-cross sections and diffusion coefficient. These are defined as follows:

$\sigma_R^g(\underline{x}), \sigma_{TR}^g(\underline{x})$

$D^g(\underline{x})$

$$\sigma_T^g \equiv \sigma_a^g + \sum_{g'} \sigma_{so}^{g \rightarrow g'}$$

$$\sigma_R^g \equiv \sigma_a^g + \sum_{g' \neq g} \sigma_{so}^{g \rightarrow g'} = \sigma_T^g - \sigma_{so}^{g \rightarrow g}$$

$$\sigma_{TR}^g \equiv \sigma_T^g - \sigma_{sl}^{g \rightarrow g} = \sigma_T^g - \bar{\mu}_0 \sigma_{so}^{g \rightarrow g} \quad (\bar{\mu}_0 - \text{mean cosine of scattering angle})$$

$$D^g \equiv \frac{1}{3\sigma_{TR}^g}$$

$$Q^g(\underline{x}, \underline{\Omega})$$

$$Q_o^g(\underline{x}), \vec{Q}_1^g(\underline{x})$$

Neutron source density at point $\underline{x}$. (neutrons/cm³-sec.) and its first and second moments. $Q^g(\underline{x}, \underline{\Omega})$ includes both fixed and fission sources.

Notation

$$\Omega_i, \Omega_j, \Omega_k$$

Three components of the unit vector $\vec{\Omega}$. In a right-handed spherical polar coordinate system, $\Omega_x = \sin \theta \cos \phi$, $\Omega_y = \sin \theta \sin \phi$, $\Omega_z = \cos \theta$.

$$d\vec{\Omega}$$

An element of solid angle, $d\vec{\Omega} = \sin \theta d\theta d\phi$.

Vectors, matrices

Vectors may be underlined, $\underline{\Omega}$, or arrowed for emphasis, $\vec{\Omega}$. Matrices will always be doubly underscored, $\underline{\underline{A}}$.

Summation
convention

We shall use a notation in which repeated indices are summed. For example, the scalar product

$$\vec{A} \cdot \vec{B} = A_x B_x + A_y B_y + A_z B_z = \sum_{i=1}^3 A_i B_i$$

will be written as

$$\vec{A} \cdot \vec{B} = A_i B_i.$$

Similarly,

$$\vec{\nabla} \cdot \vec{A} = \partial_i A_i \text{ where } \partial_i = \frac{\partial}{\partial x_i}$$

We use a tensorial notation because it permits a very compact representation of those equations in which we are interested. Thus, with the normalization

$$\int d\vec{\Omega} = 4\pi, \tag{2.1}$$

several simple integrals can be written as:

$$\begin{aligned} \int \Omega_i d\vec{\Omega} &= \int \Omega_i \Omega_j \Omega_k d\vec{\Omega} \equiv 0 \\ \int \Omega_i \Omega_j d\vec{\Omega} &= \frac{4\pi}{3} \delta_{ij} \end{aligned} \quad (2.2)$$

where δ_{ij} is the Kronecker symbol. $\left[\begin{array}{l} \delta_{ij} = 0 \text{ (} i \neq j \text{)} \\ \delta_{ij} = 1 \text{ (} i = j \text{)} \end{array} \right]$.

Assumptions

In addition to the usual assumptions leading to the multigroup approximation to the linear transport equation, we assume that the neutron angular flux and macroscopic laboratory scattering cross sections are linearly anisotropic, i.e.,

$$\begin{aligned} N^g(\underline{x}, \underline{\Omega}) &= \frac{1}{4\pi} \left[\phi^g(\underline{x}) + 3 \vec{\Omega} \cdot \vec{J}(\underline{x}) \right] \\ &= \frac{1}{4\pi} \left[\phi^g(\underline{x}) + 3 \Omega_i J_i(\underline{x}) \right] \end{aligned} \quad (2.3)$$

$$\begin{aligned} \sigma_s^{g' \rightarrow g}(\underline{x}, \underline{\Omega} \cdot \underline{\Omega}') &= \frac{1}{4\pi} \left[\sigma_{so}^{g' \rightarrow g}(\underline{x}) + 3 \sigma_{sl}^{g' \rightarrow g}(\underline{x}) \vec{\Omega} \cdot \vec{\Omega}' \right] \\ &= \frac{1}{4\pi} \left[\sigma_{so}^{g' \rightarrow g}(\underline{x}) + 3 \sigma_{sl}^{g' \rightarrow g}(\underline{x}) \Omega_i \Omega'_i \right]. \end{aligned} \quad (2.4)$$

Our starting point is the multigroup approximation to the time independent linear transport equation.

$$\begin{aligned} \vec{\nabla}_x \cdot \vec{\Omega} N^g(\underline{x}, \underline{\Omega}) + \sigma_T^g(\underline{x}) N^g(\underline{x}, \underline{\Omega}) &= Q^g(\underline{x}, \underline{\Omega}) \\ + \sum_{g'} \int d\vec{\Omega}' \sigma_s^{g' \rightarrow g}(\underline{x}, \underline{\Omega} \cdot \underline{\Omega}') N^{g'}(\underline{x}, \underline{\Omega}') \end{aligned} \quad (2.5)$$

This equation is, of course, merely a statement of neutron conservation: All the neutrons in energy group g born in a small volume in space (centered at point $\underline{x}$) in a small range of directions about $\underline{\Omega}$ are either created there (source = Q^g) or scattered there into that group and direction from some group, g' , and direction $\underline{\Omega}'$ (scattering source = $\sum_{g'} \int d\vec{\Omega}' \sigma_s N$). Furthermore these neutrons either die inside ($\sigma_T N$) or flow out of that volume ($\vec{\nabla} \cdot \underline{\Omega} N$).

Reduction of the Transport Equation

Provided that scattering be isotropic (all $\sigma_{s1}^{g' \rightarrow g}(x) \equiv 0$), the ordinary diffusion equation can be obtained from equation (2.5) by substituting from equation (2.3) and (2.4) and then by taking moments (angular averages). The first moment, which is a simple average over all angles, reduces this angular conservation law to a statement of neutron conservation at a point, the continuity equation. The second moment yields Fick's law, which describes neutron flow patterns for any given neutron density distribution. These two equations are then combined to give the diffusion equation. Our derivation follows this same pattern.

The substitution of equations (2.3) and (2.4) into equation (2.5) is straightforward, the scattering term presents the only possible difficulties:

$$\begin{aligned}
& \int d\vec{\Omega} \sigma_s^{g' \rightarrow g}(\underline{x}, \underline{\Omega} \cdot \underline{\Omega}') N^{g'}(\underline{x}, \underline{\Omega}') \\
&= \frac{1}{(4\pi)^2} \int d\vec{\Omega} \left\{ \sigma_{s0}^{g' \rightarrow g}(\underline{x}) \varphi^{g'}(\underline{x}) + 3 \left[\sigma_{s1}^{g' \rightarrow g}(\underline{x}) \underline{\Omega} \cdot \underline{\Omega}' \varphi^{g'}(\underline{x}) \right. \right. \\
&\quad \left. \left. + \sigma_{s0}^{g' \rightarrow g}(\underline{x}) \underline{\Omega}' \cdot \underline{j}^{g'}(\underline{x}) \right] + \sigma_{s1}^{g' \rightarrow g}(\underline{x}) \left[\underline{\Omega}' \cdot \underline{j}^{g'}(\underline{x}) \right] \left[\underline{\Omega} \cdot \underline{\Omega}' \right] \right\} \\
&= \frac{1}{(4\pi)^2} \sigma_{s0}^{g' \rightarrow g}(\underline{x}) \varphi^{g'}(\underline{x}) \int d\vec{\Omega} + \frac{3}{(4\pi)^2} \left[\sigma_{s1}^{g' \rightarrow g}(\underline{x}) \varphi^{g'}(\underline{x}) \Omega_i \right. \\
&\quad \left. + \sigma_{s0}^{g' \rightarrow g}(\underline{x}) j_i^{g'}(\underline{x}) \right] \int \Omega'_i d\vec{\Omega}' + \frac{9}{(4\pi)^2} \sigma_{s1}^{g' \rightarrow g}(\underline{x}) j_i^{g'}(\underline{x}) \Omega_j \\
&\quad \times \int \Omega'_i \Omega'_j d\vec{\Omega}' \\
&= \frac{1}{4\pi} \sigma_{s0}^{g' \rightarrow g}(\underline{x}) \varphi^{g'}(\underline{x}) + \frac{3}{4\pi} \sigma_{s1}^{g' \rightarrow g}(\underline{x}) j_i^{g'}(\underline{x}) \Omega_j \delta_{ij} \\
&= \frac{1}{4\pi} \sigma_{s0}^{g' \rightarrow g}(\underline{x}) \varphi^{g'}(\underline{x}) + \frac{3}{4\pi} \sigma_{s1}^{g' \rightarrow g}(\underline{x}) \vec{\Omega} \cdot \vec{j}^{g'}(\underline{x}) . \tag{2.6}
\end{aligned}$$

Thus substitution gives

$$\begin{aligned}
& \frac{\partial_i \Omega_i}{4\pi} \left[\varphi^{g}(\underline{x}) + 3 \Omega_j j_j^g(\underline{x}) \right] + \frac{\sigma_T^g(\underline{x})}{4\pi} \left[\varphi^{g}(\underline{x}) + 3 \Omega_i j_i^g(\underline{x}) \right] \\
&= \frac{1}{4\pi} \left[Q_0^g(\underline{x}) + 3 \Omega_i Q_{1i}^g(\underline{x}) \right] \\
&\quad + \frac{1}{4\pi} \sum_{g'} \left[\sigma_{s0}^{g' \rightarrow g}(\underline{x}) \varphi^{g'}(\underline{x}) + 3 \sigma_{s1}^{g' \rightarrow g}(\underline{x}) \Omega_i j_i^{g'}(\underline{x}) \right] . \tag{2.7}
\end{aligned}$$

We obtain the continuity equation by integrating (2.7) over all angles; for example, consider the first term in (2.7), we multiply by $d\vec{\Omega}$ and integrate as follows:

$$\begin{aligned}
 & \int d\vec{\Omega} \frac{\partial_i \Omega_i}{4\pi} \left[\phi^g(\underline{x}) + 3 \Omega_j J_j^g(\underline{x}) \right] \\
 &= \frac{\partial_i}{4\pi} \phi^g(\underline{x}) \int d\vec{\Omega} \Omega_i + \frac{3}{4\pi} \partial_i J_j^g(\underline{x}) \int d\vec{\Omega} \Omega_i \Omega_j \\
 &= 0 + \partial_i J_j^g(\underline{x}) \delta_{ij} \\
 &= \partial_i J_i^g(\underline{x}) \\
 &= \vec{\nabla}_x \cdot \vec{J}(\underline{x}) .
 \end{aligned}$$

Integrating term by term leads to

$$\partial_i J_i^g(\underline{x}) + \sigma_T^g(\underline{x}) \phi^g(\underline{x}) = Q_0^g(\underline{x}) + \sum_{g'} \sigma_{so}^{g' \rightarrow g}(\underline{x}) \phi^{g'}(\underline{x}) . \quad (2.8)$$

Similarly we obtain a generalized form of Fick's law by multiplying (2.7) by an arbitrary Ω_K and then averaging over all angles:

$$\frac{\partial_K}{3} \phi^g(\underline{x}) + \sigma_T^g(\underline{x}) J_K^g(\underline{x}) = \left\{ Q_{1K}^g(\underline{x}) + \sum_{g'} \sigma_{s1}^{g' \rightarrow g}(\underline{x}) J_K^{g'}(\underline{x}) \right\} . \quad (2.9)$$

Equations (2.8) and (2.9) may be recast in the usual vector notation

$$\begin{aligned}
 & \vec{\nabla} \cdot \vec{J}^g(\underline{x}) + \sigma_T^g(\underline{x}) \phi^g(\underline{x}) = Q_0^g(\underline{x}) + \sum_{g'} \sigma_{so}^{g' \rightarrow g}(\underline{x}) \phi^{g'}(\underline{x}) \\
 & \frac{1}{3} \vec{\nabla} \phi^g(\underline{x}) + \sigma_T^g(\underline{x}) \vec{J}^g(\underline{x}) = \left\{ \vec{Q}_1^g(\underline{x}) + \sum_{g'} \sigma_{s1}^{g' \rightarrow g}(\underline{x}) \vec{J}^{g'}(\underline{x}) \right\} . \quad (2.10)
 \end{aligned}$$

The bracketed terms in (2.9) and (2.10) represent the difference between the starting point for ordinary diffusion theory and our generalization thereof. As discussed earlier, there are two ways to treat these terms. Let us digress for a moment and examine Fick's law; for simplicity, let $\vec{Q}_1^g(\underline{x}) = 0$. In simple diffusion theory we assume that the Pl transfer matrices vanish,

$$\sigma_{s1}^{g' \rightarrow g}(\underline{x}) \equiv 0, (\text{all } g, g'), \quad (2.11)$$

and equation (2.9) becomes

$$\vec{J}^g(\underline{x}) = - \frac{1}{3\sigma_T^g(\underline{x})} \vec{\nabla} \phi^g(\underline{x}) \quad (2.12)$$

The coefficient $\frac{1}{3\sigma_T^g(\underline{x})}$ is identified as the diffusion coefficient.

If we assume the Pl transfer matrices vanish for group-to-group transfer, but not for in-group transfer; we have one of the more common "transport approximations":

$$\sigma_{s1}^{g' \rightarrow g}(\underline{x}) = 0 \quad , \quad (g' \neq g).$$

Because of energy and momentum conservation, this is generally quite a good approximation for a few-group scheme and is, in fact, rigorous for the one-group approximation. Fick's law then becomes

$$\vec{J}_{s1}^g(\underline{x}) = - \frac{1}{3[\sigma_T^g(\underline{x}) - \sigma_{s1}^{g \rightarrow g}(\underline{x})]} \vec{\nabla} \phi^g(\underline{x}) = - D^g(\underline{x}) \vec{\nabla} \phi^g(\underline{x}) \quad , \quad (2.13)$$

and (2.13) differs from (2.12) only in the definition of the diffusion coefficient.

If we desire to include the full effects of linearly anisotropic transfer, we may, with Pomraning, decide to maintain the functional form of Fick's law and write:

$$\vec{j}^g(\underline{x}) = - D^{gg'} \vec{\nabla} \phi^g(\underline{x}). \quad (2.14)$$

In the finite dimensional space of energy groups, this amounts to replacing the diagonal diffusion matrix D^g by a full matrix $D^{gg'}$

$$\begin{aligned} \underline{\underline{D}}^{-1} = 3 & \begin{bmatrix} \sigma_T^1 & & 0 \\ & \sigma_T^2 & \\ 0 & & \ddots \end{bmatrix} - 3 \begin{bmatrix} \sigma_{s1}^{1 \rightarrow 1} & & 0 \\ & \sigma_{s1}^{2 \rightarrow 2} & \\ 0 & & \ddots \end{bmatrix} \\ \Rightarrow 3 & \begin{bmatrix} \sigma_T^1 & & 0 \\ & \sigma_T^2 & \\ 0 & & \ddots \end{bmatrix} - 3 \begin{bmatrix} \sigma_{s1}^{1 \rightarrow 1} & \sigma_{s1}^{1 \rightarrow 2} & \dots \\ \sigma_{s1}^{2 \rightarrow 1} & \sigma_{s1}^{2 \rightarrow 2} & \dots \\ \vdots & \vdots & \ddots \end{bmatrix} \end{aligned} \quad (2.15)$$

This process leads to an unwieldy diffusion equation; instead we may give up an elegant formulation of Fick's law in an attempt to salvage the functional form of the diffusion equation. We now show how this is done.

For simplicity, let us assume that Q_1^g and all σ 's are piecewise constant; then differentiation of (2.9), followed by suppression of the explicit spatial dependence, gives

$$\frac{1}{3} \nabla_x^2 \phi^g + \sigma_T^g \nabla_x \cdot \underline{j}^g = \sum_{g'} \sigma_{s1}^{g' \rightarrow g} \nabla_x \cdot \underline{j}^{g'}. \quad (2.16)$$

Note that the vector source term vanishes in equation (2.16); a spatially constant vector source contributes no net neutrons to any volume element.

We want to follow the derivation of the ordinary diffusion equation as closely as possible; therefore, let us rearrange equations (2.8) and (2.16),

$$\nabla_x \cdot \underline{j}^g + \sigma_R^g \phi^g = Q_O^g + \sum_{\substack{g' \\ g' \neq g}} \sigma_{s0}^{g' \rightarrow g} \phi^{g'} \quad (2.17)$$

$$\frac{1}{3} \nabla_x^2 \phi^g + \sigma_{TR}^g \nabla_x \cdot \underline{j}^g = \sum_{\substack{g' \\ g' \neq g}} \sigma_{s1}^{g' \rightarrow g} \nabla_x \cdot \underline{j}^{g'}, \quad (2.18)$$

and substitute (2.17) into (2.18) to obtain

$$\frac{1}{3} \nabla_x^2 \phi^g + \sigma_{TR}^g \left[Q_O^g + \sum_{\substack{g' \\ g' \neq g}} \sigma_{s0}^{g' \rightarrow g} \phi^{g'} - \sigma_R^g \phi^g \right] = \sum_{\substack{g' \\ g' \neq g}} \sigma_{s1}^{g' \rightarrow g} \nabla_x \cdot \underline{j}^{g'} \quad (2.19)$$

or

$$-D^g \nabla_x^2 \phi^g + \sigma_R^g \phi^g - \left[Q_O^g + \sum_{\substack{g' \\ g' \neq g}} \sigma_{s0}^{g' \rightarrow g} \phi^{g'} \right] = - \sum_{\substack{g' \\ g' \neq g}} \frac{\sigma_{s1}^{g' \rightarrow g}}{\sigma_{TR}^g} \nabla_x \cdot \underline{j}^{g'}. \quad (2.20)$$

The left-hand side of (2.20) is the ordinary diffusion equation, the right-hand side contains the full effect of anisotropic group-to-group transfer. By substituting equation (2.17) in equation (2.20) we obtain

$$\begin{aligned}
 & D^g \nabla_x^2 \phi^g + \sigma_R^g \phi^g - \left[Q_o^g + \sum_{\substack{g' \\ g' \neq g}} \sigma_{so}^{g' \rightarrow g} \phi^{g'} \right] \\
 &= - \sum_{\substack{g' \\ g' \neq g}} \frac{\sigma_{sl}^{g' \rightarrow g}}{\sigma_{TR}^g} \left[-\sigma_R^{g'} \phi^{g'} + Q_o^{g'} + \sum_{\substack{g'' \\ g'' \neq g'}} \sigma_{so}^{g'' \rightarrow g'} \phi^{g''} \right] \\
 &= - \sum_{\substack{g' \\ g' \neq g}} \frac{\sigma_{sl}^{g' \rightarrow g}}{\sigma_{TR}^g} \left[\sigma_{so}^{g' \rightarrow g} \phi^g + Q_o^{g'} - \sigma_T^{g'} \phi^{g'} + \sum_{\substack{g'' \\ g'' \neq g}} \sigma_{so}^{g'' \rightarrow g'} \phi^{g''} \right].
 \end{aligned} \tag{2.21}$$

Now note that in the right-hand side of (2.21) both g' and g'' are dummy indices. We may interchange the order of summation and relabel quantities to obtain

$$\begin{aligned}
 & -D^g \nabla_x^2 \phi^g + \left[\sigma_R^g + \sum_{\substack{g' \\ g' \neq g}} \frac{\sigma_{sl}^{g' \rightarrow g} \sigma_{so}^{g \rightarrow g'}}{\sigma_{TR}^g} \right] \phi^g \\
 &= \left[Q_o^g - \sum_{\substack{g' \\ g' \neq g}} \frac{\sigma_{sl}^{g' \rightarrow g}}{\sigma_{TR}^g} Q_o^{g'} \right] \\
 &+ \sum_{\substack{g' \\ g' \neq g}} \left[\sigma_{so}^{g' \rightarrow g} + \sigma_{sl}^{g' \rightarrow g} \frac{\sigma_T^{g'}}{\sigma_{TR}^g} - \sum_{\substack{g'' \\ g'' \neq g}} \frac{\sigma_{so}^{g'' \rightarrow g} \sigma_{sl}^{g' \rightarrow g''}}{\sigma_{TR}^g} \right] \phi^{g'}.
 \end{aligned} \tag{2.22}$$

If we define effective removal and scattering cross sections and an effective source, we find that the form of the diffusion equation remains unchanged:

$$\begin{aligned}
 -D^2 \nabla_x^2 \phi^g + \hat{\sigma}_R^g \phi^g &= \hat{Q}_O^g + \sum_{\substack{g' \\ g' \neq g}} \hat{\sigma}_{so}^{g' \rightarrow g} \phi^{g'} \\
 \hat{\sigma}_R^g &= \sigma_R^g + \sum_{\substack{g' \\ g' \neq g}} \frac{\sigma_{sl}^{g' \rightarrow g} \sigma_{so}^{g \rightarrow g'}}{\sigma_{TR}^g} \\
 \hat{\sigma}_{so}^{g' \rightarrow g} &= \sigma_{so}^{g' \rightarrow g} + \frac{\sigma_T^{g'} \sigma_{sl}^{g' \rightarrow g}}{\sigma_{TR}^g} - \sum_{\substack{g'' \\ g'' \neq g}} \frac{\sigma_{so}^{g'' \rightarrow g} \sigma_{sl}^{g' \rightarrow g''}}{\sigma_{TR}^g}, \quad (g \neq g') \\
 \hat{Q}_O^g &= Q_O^g - \sum_{\substack{g' \\ g' \neq g}} \frac{\sigma_{sl}^{g' \rightarrow g}}{\sigma_{TR}^g} Q_O^{g'}. \quad (2.23)
 \end{aligned}$$

Fission Sources

The source term, $Q_O^g(\underline{x})$, includes a fission source, $F^g(\underline{x})$, which must be replaced by an effective fission source, $\hat{F}^g(\underline{x})$,

$$\begin{aligned}
 \hat{F}^g(\underline{x}) &= F^g(\underline{x}) - \sum_{\substack{g'' \\ g'' \neq g}} \frac{\sigma_{sl}^{g'' \rightarrow g}(\underline{x})}{\sigma_{TR}^g(\underline{x})} F^{g''}(\underline{x}) \\
 &= \frac{1}{K} \sum_{g'} [\nu \sigma_f(\underline{x})]^{g' \rightarrow g} \phi^{g'}(\underline{x}) - \frac{1}{K} \sum_{\substack{g'' \\ g'' \neq g}} \frac{\sigma_{sl}^{g'' \rightarrow g}(\underline{x})}{\sigma_{TR}^g(\underline{x})} \times \\
 &\quad \sum_{g'} [\nu \sigma_f(\underline{x})]^{g' \rightarrow g''} \phi^{g'}(\underline{x}) \quad (2.24) \\
 &= \frac{1}{K} \sum_{g'} \left\{ [\nu \sigma_f(\underline{x})]^{g' \rightarrow g} - \sum_{\substack{g'' \\ g'' \neq g}} \frac{\sigma_{sl}^{g'' \rightarrow g}(\underline{x})}{\sigma_{TR}^g(\underline{x})} [\nu \sigma_f(\underline{x})]^{g' \rightarrow g''} \right\} \phi^{g'}(\underline{x}).
 \end{aligned}$$

Equivalently, we have

$$\left[\nu \hat{\sigma}_f(\underline{x}) \right]^{g' \rightarrow g} = \left[\nu \sigma_f(\underline{x}) \right]^{g' \rightarrow g} - \sum_{\substack{g'' \\ g'' \neq g}} \frac{\sigma_{sl}^{g'' \rightarrow g}(\underline{x})}{\sigma_{TR}^g(\underline{x})} \left[\nu \sigma_f(\underline{x}) \right]^{g' \rightarrow g''}. \quad (2.25)$$

It is usually assumed that the fission spectrum is independent of the initial neutron energy, and then equation (2.25) reduces to

$$\left[\nu \hat{\sigma}_f(\underline{x}) \right]^{g' \rightarrow g} = X^g \left[\nu \sigma_f(\underline{x}) \right]^{g'} - \sum_{\substack{g'' \\ g'' \neq g}} \frac{\sigma_{sl}^{g'' \rightarrow g}(\underline{x})}{\sigma_{TR}^g(\underline{x})} \left[\nu \sigma_f(\underline{x}) \right]^{g'} X^{g''}. \quad (2.26)$$

The practical application of this last formula depends on the computer program being used; with those few codes which permit spatially dependent spectra

$\left[X^g = X^g(\underline{x}) \right]$, there is no difficulty at all. We may write

$$\left[\nu \hat{\sigma}_f(\underline{x}) \right]^{g' \rightarrow g} = \left\{ X^g(\underline{x}) - \sum_{\substack{g'' \\ g'' \neq g}} \frac{\sigma_{sl}^{g'' \rightarrow g}(\underline{x})}{\sigma_{TR}^g(\underline{x})} X^{g''}(\underline{x}) \right\} \left[\nu \sigma_f(\underline{x}) \right]^{g'} \quad (2.27)$$

or

$$\hat{X}_g(\underline{x}) = X^g(\underline{x}) - \sum_{\substack{g'' \\ g'' \neq g}} \frac{\sigma_{sl}^{g'' \rightarrow g}(\underline{x})}{\sigma_{TR}^g(\underline{x})} X^{g''}(\underline{x}). \quad (2.28)$$

We leave the question of fission normalization to the next section; the normalization implied by equation (2.28) is not necessarily the best one for direct comparison of an anisotropic with an isotropic calculation.

Even with computer programs which do not permit spatially dependent neutron spectra, the difficulties in obtaining effective fission cross sections and neutron fission spectra are more apparent than real. In a few group scheme most $\chi^{g''}$ and $\sigma_{s1}^{g'' \rightarrow g}$ vanish, and it is frequently possible to partition $[\nu\sigma_f(\underline{x})]^{g' \rightarrow g}$ into two terms, of which one ($\hat{\chi}^g$) contains the entire dependence on the parameter g .

For fixed source or constant reactivity problems there is no need to partition the effective fission cross section; the extra term may be distributed between the scattering source and removal terms. Finally, when absolutely necessary, it is simpler to reprogram a diffusion theory code to accept spatially dependent neutron spectra than it is to handle a non-diagonal diffusion matrix. The former change cannot disturb convergence accelerating techniques, whereas the latter can have a profound effect on the convergence of numerical procedures.

Physical Interpretation

The physical interpretation of the redefined cross sections is fairly simple: these new quantities merely include the effects of anisotropic group-to-group transfer. Most difficulty arises in understanding the negative sign associated with the cross section corrections. However, consider the effects of in-group anisotropic scattering: by adding to the forward scattering (without increasing absorption) anisotropic in-group scattering effectively increases the diffusion length. Group to-group anisotropic transfer has a similar effect.

For example, consider the source term

$$Q_0^g(\underline{x}) \rightarrow \hat{Q}^g(\underline{x}) = Q_0^g(\underline{x}) - \sum_{\substack{g' \\ g' \neq g}} \frac{\sigma_{sl}^{g' \rightarrow g}(\underline{x})}{\sigma_{TR}^g(\underline{x})} Q_0^{g'}(\underline{x}) . \quad (2.29)$$

The crucial point is that anisotropic transfer appears in Fick's law (2.18) and not in the continuity equation (2.17); thus the right-hand term of (2.29) does not directly represent an addition from another energy region to the neutron birth rate at point $\underline{x}$. In order to maintain neutron conservation, rather, it is necessary to reduce the source rate at which neutrons are anisotropically transferred into any element of phase space.

From the preceding discussion, it can be seen that the best fission normalization for direct comparison of an isotropic problem and its associated anisotropic case is that for which $\sum_g \hat{X}^g(\underline{x}) = \sum_g X^g(\underline{x})$; i.e.,

$$\hat{X}^g(\underline{x}) = \frac{\sum_g X^g(\underline{x})}{\sum_g \left[X^g(\underline{x}) - \sum_{\substack{g' \\ g' \neq g}} \frac{\sigma_{sl}^{g' \rightarrow g}(\underline{x})}{\sigma_{TR}^g(\underline{x})} X^{g'} \right]} \left\{ X^g(\underline{x}) - \sum_{\substack{g' \\ g' \neq g}} \frac{\sigma_{sl}^{g' \rightarrow g}(\underline{x})}{\sigma_{TR}^g(\underline{x})} X^{g'} \right\} . \quad (2.30)$$

Internal Boundaries

One question remains to be resolved: does the preceding prescription properly treat material discontinuities within a reactor? Despite such discontinuities, it is reasonable to insist that the angular flux at any energy be continuous across internal boundaries. The diffusion equation deals with

only the first two moments of the angular flux and therefore any internal boundary condition applied thereto is more or less inaccurate. For physical reasons, it is usual to demand that the neutron current be continuous everywhere within a reactor. This condition is consistent with the continuity equation provided that no point or surface sources exist within the reactor and provided that the flux is everywhere finite. Furthermore Fick's law ($\vec{J} = -D\vec{\nabla}\phi$) then implies the continuity of $D\vec{\nabla}\phi$, and it is this latter condition which is actually used with the diffusion equation. We shall now show that the continuity of $D^g\vec{\nabla}\phi^g$ is still desirable in the presence of anisotropic transfer and, therefore, that standard diffusion codes can be used with our new technique.

We start with the diffusion equation and make the usual assumptions that the neutron flux is everywhere finite and that we have no isotropic point or surface sources. The material description of the reactor is assumed to be piecewise constant and we consider an internal boundary as illustrated below. Let $\vec{s}$ be a unit normal to the boundary and let $(\vec{J}_s)_\pm$ be the currents immediately to the left and right of this surface.

Fig. 2.1 An Internal Boundary

The diffusion equation can be written as

$$D^g(\underline{x}) \nabla_x^2 \phi^g(\underline{x}) = -\sigma_R \phi^g(\underline{x}) + \text{Source}^g(\underline{x}). \quad (2.31)$$

By integrating over the volume element dV and by making use of the divergence theorem we obtain

$$\begin{aligned} & \int_{\Delta V} D^g(\underline{x}) \nabla_x^2 \phi^g(\underline{x}) \, d\mathbf{s} dS \\ &= \oint D^g(\underline{x}) \vec{\nabla}_x \phi^g(\underline{x}) \cdot \vec{dS} \\ &= \int d\mathbf{s} dS \left[-\sigma_R^g \phi^g(\underline{x}) + \text{Source}^g(\underline{x}) \right]. \end{aligned} \quad (2.32)$$

In the limit as $\Delta s \rightarrow 0$, this reduces to

$$\left| \left(D^g \frac{\partial \phi^g}{\partial \vec{s}} \right)_+ - \left(D^g \frac{\partial \phi^g}{\partial \vec{s}} \right)_- \right| \leq (\Delta s) \times \text{Constant}. \quad (2.33)$$

Therefore, when the ordinary physical arguments are applied directly to the diffusion equation, we obtain the ordinary continuity conditions. Examining Fick's Law, we find that the component of the neutron current which arises from anisotropic group-to-group transfer is no longer continuous across internal boundaries,

$$(J_s^g)_+ - (J_s^g)_- = \sum_{\substack{g' \\ g' \neq g}} \left[\left(\frac{\sigma_{sl}^{g' \rightarrow g}}{\sigma_{TR}^g} J_s^{g'} \right)_+ - \left(\frac{\sigma_{sl}^{g' \rightarrow g}}{\sigma_{TR}^g} J_s^{g'} \right)_- \right]. \quad (2.34)$$

That is to say, the effects of anisotropic group-to-group transfer require the introduction of fictitious anisotropic surface sources at internal boundaries. A few moments reflection will show this to be perfectly reasonable; for example, see the discussion following equation (2.16)*.

Sample Case

As an example of an extreme case, a two group, two region, thermal, one dimensional slab problem was posed. The two regions differed only in their group-to-group anisotropic transfer; for one region the transfer was down only, for the other up only. The slab was chosen thick enough for diffusion theory to be an excellent approximation when group-to-group anisotropic transfer was omitted. (Comparison with a high order transport calculation being the criterion.) When the anisotropic transfer was included, diffusion theory still agreed remarkably well with transport calculations (to considerably better than 1% in reactivity and flux distribution). Since the object of this investigation was to demonstrate the applicability of this technique to existing computer codes, no attempt was made to find an analytic solution.

*Anisotropic slowing down is handled in precisely this fashion by the PLMG computer program.

Negative Fluxes in DDK

Negative fluxes frequently occur in DDK clustered in the reentrant portion of highly absorbing control drums. The cross hatched area in figure 2.2 illustrates a typical example.

Fig. 2.2 Occurrence of Negative Fluxes in DDK

These control surfaces are essentially surface absorbers, and we have found that the resulting self-shielding effects are easily compensated. By redefining the total and absorption cross sections such that the minimum vane thickness is $2\frac{1}{2}$ to 3 mean free paths, we have removed the negative fluxes. This procedure

gives improper flux gradients at the vane surface and distorts the energy deposition distribution with the vanes, but it does give correct total energy deposition within the vanes. Also, the distorted flux distribution, with positive fluxes, is preferable to the larger inaccuracies which propagate from points of negative flux. For example, the anomolous scalloping previously found at the core-reflector interface is reduced.

III - INTEGRATION SCHEME FOR VARI-QUIR III

Difficulty in obtaining converged results from R- θ VARI-QUIR⁽⁷⁾ problems involving angularly narrow regions has been found to be caused by the order of integration. The radial variation of fast group fluxes should resemble a Bessel function when an annular ring of thermal absorber is included in the reactor, but heretofore, these fluxes were not even monotonically decreasing functions of radial position.

The integration scheme formerly used in VARI-QUIR III was derived from the successful schemes of the slab and R-Z versions of this program and integrates first radially and then tangentially. Since the EXTERMINATOR⁽²⁾ program is known to require integration in the direction of minimum buckling and since the order of integration in EXTERMINATOR is under input control, it was decided to run identical R- θ VARI-QUIR and EXTERMINATOR problems to partial convergence. It was observed that the eigenvalue change was the same for 15°, 30°, 60°, and 360° periodic problems when integrating in the θ direction, but was quite different for the same problems when integrating in the R direction. After 16 iterations all of the θ -direction problems were approaching the converged eigenvalue (0.90133), but in the R-direction problems only the 360° problem was approaching the converged value. The other R-direction problems (15°, 30°, and 60°) were oscillating around 0.8750. Figure 3.1 below is a graph of eigenvalue vs. iteration.

Fig. 3.1 EXTERMINATOR RUNS

VARI-QUIR III has now been modified to integrate first tangentially and then radially, and the convergence rate improved by a factor of fifteen.

Possibly because the coupling of tangentially adjacent points is weak for angularly narrow regions, the improvement in VARI-QUIR is not as great as for EXTERMINATOR. We are now investigating different possible point orderings for generally tangential integration schemes.

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