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TRANSPORT THEORY

THE METHOD OF DISCRETE ORDINATES

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THE METHOD OF DISCRETE ORDINATES

by

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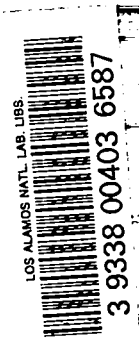

Abstract

Methods, based on the principles of neutron transport physics, are described for formulating and solving discrete ordinates representations of the general linear Boltzmann transport equation. In a first approach, the transport equation is formulated directly in terms of discrete variables, while in a second approach discrete ordinates equations are formulated that are equivalent to generalized moment representations of the analytic transport equation. Both formulations include general specifications of the collision and fission sources. Selection of discrete ordinates angular quadrature coefficients is described, and simplifications of the transport equation (including diffusion theory) are outlined. Solution techniques are described that combine the principles of neutron conservation, flow attenuation, and flux positivity with accuracy and calculational simplicity. A sample problem is used to illustrate the techniques discussed.

PREFACE

This report is a first draft of Chapter III of "The Application of Digital Computers to Problems in Reactor Physics," a book edited by H. Greenspan, C. Kelber, and D. Okrent and to be published by the Addison-Wesley Publishing Company. The book is intended for use by advanced graduate students in nuclear engineering, and the authors of this chapter welcome suggestions for improvement.

The material of this report includes and augments that of Los Alamos Report LA-2996. On some topics it supercedes the material in that report.

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CHAPTER III

TRANSPORT THEORY - THE METHOD OF DISCRETE ORDINATES

B. G. Carlson - K. D. Lathrop

Discrete ordinates equations for numerical solution of the equations describing neutron ensembles can be formulated in many ways. This chapter describes methods, based on the principles of neutron transport physics, for formulating and solving discrete ordinates equations. Physical principles are used not only to insure correspondence between mathematical and physical descriptions of neutron transport, but to insure and accelerate convergence of the numerical solution. That solutions converge to the true solutions of the problems posed is a conjecture, but for the methods discussed below the conjecture is supported by the pragmatic test of numerical computing. That is to say, in a wide variety of test problems, numerical results obtained with these methods have agreed with exact solutions (when available); with other types of numerical solutions; and, allowing for cross section uncertainties, with experiment. We begin describing discrete ordinates methods by defining terms and stating assumptions.

The goal of neutron transport theory is to determine a distribution function $\psi(\underset{\sim}{r}, v\underset{\sim}{\Omega}, t)$. In the most general situations ψ is a function of three position variables denoted by $\underset{\sim}{r}$, two angular variables denoted by $\underset{\sim}{\Omega}$, the neutron speed, v, and the time, t. In these terms ψ/v is the neutron density distribution, the number of neutrons per unit volume per unit velocity ($v\underset{\sim}{\Omega}$) at time t. With several fundamental assumptions,

conservation of neutrons is expressed, in terms of ψ, by the linear Boltzmann transport equation. Briefly, it is assumed a) that neutrons flow without change of direction or speed until they either interact with atomic nuclei in the domain of $\underset{\sim}{r}$ or escape from the domain, b) that the number of neutrons considered is large enough that statistical fluctuations can be neglected and small enough that neutron-neutron interactions can be ignored, c) that neutrons do not appreciably alter the medium with which they interact within the time intervals considered, and d) that quantum mechanical effects are unimportant. In what follows these assumptions are made. However, the methods of this chapter may be applied even when some of the above assumptions do not hold.[1,2]

3.1 Formulation of Discrete Ordinates Equations in Terms of Discrete Variables

Discrete ordinates equations can be written by applying difference methods directly to the analytic form of the Boltzmann neutron transport equation, but this approach has several disadvantages. The resulting equations may conserve neutrons only in the limit of small intervals, they may prove to be numerically unstable, or they may result in complex and unrealistic couplings among the various components of ψ. Here, using averages of ψ over $\underset{\sim}{r}$, v, $\underset{\sim}{\Omega}$, and t, the Boltzmann transport equation is derived for finite cells in phase space. By constantly insisting on neutron conservation and by following the physical neutron flow, simple, general, numerically stable difference equations are obtained. The

averages of ψ, which are denoted by subscripted quantities N, are frequently of direct use in applications; and the detailed connection between N and ψ is usually not explored. However, the approach here described permits the orderly formulation of difference equations beginning from representations of ψ.

3.1.1 Coordinate Systems

The domain of $\underset{\sim}{r}$ is defined by a set of non-overlapping mesh cells. The volume of these cells is designated by $V_{i+\frac{1}{2}, j+\frac{1}{2}, k+\frac{1}{2}}$ where the centered subscripts locate the center of the cell, and i, j, and k indicate the position of the cell as measured in the coordinate system defined by the components of $\underset{\sim}{r}$. The areas of the cell surfaces are indicated by quantities with non-centered subscripts. For instance, the surface of the cell that is a distance from the origin, and perpendicular to the direction, indicated by i is written as $A_{i, j+\frac{1}{2}, k+\frac{1}{2}}$.

Although not necessary, it is frequently convenient to adopt orthogonal coordinate systems in which mesh cells are defined by the intersection of the orthogonal surfaces of the geometry. For instance, in rectangular (x, y, z) geometry the mesh cells are rectangular parallelpipeds. A typical such cell is shown in Fig. III-1.

Fig. III-1

The volume of the above cell is $V_{i+\frac{1}{2}, j+\frac{1}{2}, k+\frac{1}{2}} = (x_{i+1} - x_i)\ (y_{j+1} - y_j)\ (z_{k+1} - z_k) = \Delta x \cdot \Delta y \cdot \Delta z$. The area of the cell face perpendicular to the x direction at $x = x_i$ is $A_{i, j+\frac{1}{2}, k+\frac{1}{2}} = \Delta y \cdot \Delta z$. The area of the parallel face at $x = x_{i+1}$, $A_{i+1, j+\frac{1}{2}, k+\frac{1}{2}}$, is the same. The areas of the two faces

perpendicular to the y axis, $B_{i+\frac{1}{2},j,k+\frac{1}{2}}$ and $B_{i+\frac{1}{2},j+1,k+\frac{1}{2}}$, are $\Delta x \cdot \Delta z$; and the areas of the remaining faces, $C_{i+\frac{1}{2},j+\frac{1}{2},k}$ and $C_{i+\frac{1}{2},j+\frac{1}{2},k+1}$ are $\Delta x \cdot \Delta y$. Areas and volume elements for orthogonal rectangular, cylindrical, and spherical geometries of varying dimensionality are given in Table III-1.

Table III-1

Note that although all three subscripts are used in the areas A, B, C, the actual areas are not, in general, functions of all subscripts. The range of subscripts is i = 0 to IM, j = 0 to JM, k = 0 to KM with the (0,0,0) triplet locating the origin. In this notation there are IM + 1 coordinate surfaces and IM intervals in the i direction. In the discussions that follow, only the coordinate systems of Table III-1 are considered.

When orthogonal geometric coordinate systems are used, the angular variables can be measured in a rectangular coordinate system (μ, n, ξ) locally aligned with the unit vectors of the geometric system. Typical such alignments are shown in Fig. III-2.

Fig. III-2

For a discrete direction Ω_m the components of Ω_m along the μ, n, and ξ axes are μ_m, n_m, and ξ_m; and these coordinates are the direction cosines of Ω_m. Consequently $\mu_m^2 + n_m^2 + \xi_m^2 = 1$. The direction Ω_m can be pictured as a point on the surface of a unit sphere with which a surface area, w_m, is associated. The w_m can then be assigned the role of angular quadrature weights with the obvious requirement that the weights sum to the surface area of the unit sphere. In the convention here adopted, M directions

are chosen, and angular areas are measured in units of 4π so that $\sum_{m=1}^{M} w_m = 1$. In the ensuing derivation of discrete ordinates equations additional restrictions on the components of $\underset{\sim}{\Omega}_m$ and on the w_m arise. A discussion of the selection of angular quadrature sets is deferred until these restrictions are obtained.

To complete the discrete representation of coordinates, speeds in the range $v_{g-\frac{1}{2}}$ to $v_{g+\frac{1}{2}}$ are referred to as v_g, $g = 1,2,\ldots,G$, and times in the range $t = t_s$ to t_{s+1} are given the subscript $s + \frac{1}{2}$, $s = 0,1,\ldots,S$. While the smallest values of s refer to smallest times, the smallest values of g represent the largest neutron speeds.

3.1.2 Local Averages of the Distribution Function ψ

The first average of ψ that is needed is the average of ψ in the speed range $v_{g-\frac{1}{2}}$ to $v_{g+\frac{1}{2}}$, $\psi_g(\underset{\sim}{r},\underset{\sim}{\Omega},t)$. That is, the multigroup approximation is made. For convenience in handling integrations over speed, the number of neutrons in the speed range, defined by $N_g(\underset{\sim}{r},\underset{\sim}{\Omega},t) = \psi_g(\underset{\sim}{r},\underset{\sim}{\Omega},t)(v_{g-\frac{1}{2}} - v_{g+\frac{1}{2}})$, is used. That is, all the neutrons in the speed range are treated as a unit. However, if it is necessary to treat the detailed speed variation (as in an age theory approximation), then the number per unit speed, ψ_g, would be used. The multigroup approximation requires weighted speed averages of cross sections, for which many recipes are available. Here, the averaging process is indicated by affixing the subscript g to cross sections.

In addition to the speed average of ψ, several averages of N_g over all but one of the remaining independent variables are needed. These

averages are denoted by a subscripting convention in which the non-centered subscripts indicate which variable is not included in the averaging process. For example, the average of N_g over the volume of a mesh cell, $V_{i+\frac{1}{2}, j+\frac{1}{2}, k+\frac{1}{2}}$, and over the area on the unit directional sphere, w_m, at $t = t_s$ is written $N_{g,s,m,i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}$. In this notation, $i+\frac{1}{2}$, $j+\frac{1}{2}, k+\frac{1}{2}$, m, and g are centered subscripts but s is not; and the average N has the dimensions of neutron flux per unit volume per unit direction. Similarly, in rectangular geometry, the average of N_g over the cell face at $x = x_i$, over the direction range w_m, and the time range $\Delta t = t_{s+1} - t_s$, is written $N_{g,s+\frac{1}{2},m,i,j+\frac{1}{2},k+\frac{1}{2}}$ where i is the only non-centered subscript and N has the dimensions of neutron flux per unit area, per unit direction, per unit time. Rectangular geometry requires six averages of N over cell faces, directions, and time; one average of N over the cell volume, directions, and time; and two averages over volume and directions at fixed times. Curved geometries require additional averages of N_g, over time and volume at the "edges" of a direction cell.* All these averages are unknown functions in the discrete form of the transport equation, and difference relations are required to balance the number of unknowns with the number of equations to be solved.

*The meaning of a direction cell "edge" is clarified below in the treatment of neutron angular redistribution.

3.1.3 The Neutron Transport Equation in Three-Dimensional Rectangular Geometry

Within the cell of Fig. III-1 the rate of change of the number of neutrons is the difference between the population increase, due to flows from adjoining cells and sources, and the decrease, due to flows to adjoining cells and collisions (direction, number, or speed altering) in the cell. The difference between the number of neutrons in the cell, in the direction range denoted by m, at times t_s and t_{s+1}, is, in terms of averages defined above,

$$w_m\left(N_{g,s+1,m,i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}} - N_{g,s,m,i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}\right)V_{i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}/v_g \qquad (3\text{-}1)$$

The number of neutrons crossing a cell face in the direction range m in time Δt is the product of the average flux at the cell surface, the cosine of the angle between the surface normal and the neutron direction, the angular area, the cell surface area, and the time interval. In rectangular geometry the orientation of the angular coordinate system is such that the cosines of the angles between surface normals and the neutron direction are just the direction cosines of the angular coordinate system. Picking, for convenience, a direction Ω_m such that μ_m, η_m, and ξ_m are positive, the flow of neutrons <u>into</u> the cell of Fig. III-1 is

$$w_m \mu_m A_{i,\, j+\frac{1}{2},\, k+\frac{1}{2}} N_{g,\, s+\frac{1}{2},\, m,\, i,\, j+\frac{1}{2},\, k+\frac{1}{2}} \Delta t +$$

$$+ w_m \eta_m B_{i+\frac{1}{2},\, j,\, k+\frac{1}{2}} N_{g,\, s+\frac{1}{2},\, m,\, i+\frac{1}{2},\, j,\, k+\frac{1}{2}} \Delta t + \qquad (3\text{-}2)$$

$$+ w_m \xi_m C_{i+\frac{1}{2},\, j+\frac{1}{2},\, k} N_{g,\, s+\frac{1}{2},\, m,\, i+\frac{1}{2},\, j+\frac{1}{2},\, k} \Delta t$$

For the same direction the flow of neutrons <u>out of</u> the cell is

$$w_m \mu_m A_{i+1,\, j+\frac{1}{2},\, k+\frac{1}{2}} N_{g,\, s+\frac{1}{2},\, m,\, i+1,\, j+\frac{1}{2},\, k+\frac{1}{2}} \Delta t +$$

$$+ w_m \eta_m B_{i+\frac{1}{2},\, j+1,\, k+\frac{1}{2}} N_{g,\, s+\frac{1}{2},\, m,\, i+\frac{1}{2},\, j+1,\, k+\frac{1}{2}} \Delta t + \qquad (3\text{-}3)$$

$$+ w_m \xi_m C_{i+\frac{1}{2},\, j+\frac{1}{2},\, k+1} N_{g,\, s+\frac{1}{2},\, m,\, i+\frac{1}{2},\, j+\frac{1}{2},\, k+1} \Delta t$$

With the number of source neutrons produced in the cell per unit volume, per unit direction, per unit time indicated by the average $S_{g,\, s+\frac{1}{2},\, m,\, i+\frac{1}{2},\, j+\frac{1}{2},\, k+\frac{1}{2}}$, the number of source neutrons released in the cell is

$$w_m S_{g,\, s+\frac{1}{2},\, m,\, i+\frac{1}{2},\, j+\frac{1}{2},\, k+\frac{1}{2}} V_{i+\frac{1}{2},\, j+\frac{1}{2},\, k+\frac{1}{2}} \Delta t \qquad (3\text{-}4)$$

The above source is taken to include the collision source, that is, those neutrons that arrive in the direction and speed ranges considered as a result of collisions in other speed and direction ranges.* The detailed treatment of the source term is discussed in Section 3.1.5 below.

---

*The concept can be generalized to include neutrons emitted at earlier time intervals which arrive in the time range considered, i.e., delayed neutrons.

The number of neutrons removed from the cell by collisions is the product of the total macroscopic cross section, the average flux in the cell, the angular area, the cell volume, and the time inverval:

$$w_m \sigma_{g,\, s+\frac{1}{2},\, i+\frac{1}{2},\, j+\frac{1}{2},\, k+\frac{1}{2}} \; N_{g,\, s+\frac{1}{2},\, m,\, i+\frac{1}{2},\, j+\frac{1}{2},\, k+\frac{1}{2}} \; V_{i+\frac{1}{2},\, j+\frac{1}{2},\, k+\frac{1}{2}} \Delta t \qquad (3\text{-}5)$$

Equating the change of the cell neutron number, Eq. (3-1), to gains, Eqs. (3-2) and (3-4), minus losses, Eqs. (3-3) and (3-5), gives a conservation relation for a finite cell:

$$(N_{s+1} - N_s)V/v\Delta t = \mu(A_i N_i - A_{i+1} N_{i+1}) + \eta(B_j N_j - B_{j+1} N_{j+1}) + \\ + \xi(C_k N_k - C_{k+1} N_{k+1}) + SV - \sigma N V \qquad (3\text{-}6)$$

In equation (3-6) each term was divided by $w_m \Delta t$. Also, only the non-centered subscripts are indicated, a convention which is henceforth adopted except when a particular coordinate dependence is emphasized. However, it is to be understood that, in general, the quantities of Eq. (3-6) depend upon the full range of subscripts as indicated in Eqs. (3-1) to (3-5).

Equation (3-6) is an exact statement of neutron conservation for a finite cell with each term having a well-defined physical interpretation. With the definitions of the area and volume elements in rectangular geometry, Eq. (3-6) can be written

$$\frac{N_{s+1} - N_s}{v\Delta t} + \frac{\mu(N_{i+1} - N_i)}{\Delta x} + \frac{\eta(N_{j+1} - N_j)}{\Delta y} + \frac{\xi(N_{k+1} - N_k)}{\Delta z} + \sigma N = S \qquad (3\text{-}7)$$

or, in the limit of vanishingly small coordinate intervals,

$$\frac{1}{v}\frac{\partial N}{\partial t} + \frac{\mu \partial N}{\partial x} + \frac{\eta \partial N}{\partial y} + \frac{\xi \partial N}{\partial z} + \sigma N = S \qquad (3\text{-}8)$$

which is the analytic form of the neutron transport equation in the multigroup approximation.

3.1.4 The Neutron Transport Equation in Curved Geometries

In a sense, Cartesian geometry is anomalous because it is not curved. In curved geometries the orientation of the angular coordinate system changes with geometrical position. Thus, as a neutron travels through the system, the magnitude of its angular coordinates is constantly changing even though the neutron does not physically change direction. In effect, the neutron is being transferred from direction to direction in the process of streaming, and some provision must be made for this transfer. In the analytic form of the neutron transport equation, the angular derivatives account for directional transfers, and direct differencing of these derivatives can be used to form difference equations. However, such a procedure can destroy the neutron conservation so carefully preserved in Eq. (3-6). Moreover, direct differencing can produce strong directional coupling - physically improbable - and may lead to tedious iterative solution. For example, Eq. (3-6) involves the unknown N for a single direction subscript m, but treatment of directional transfer may introduce unknowns depending upon several values of m (cf. Section 3.2.2). An artifice which main-

tains neutron conservation and permits minimal directional coupling is the following. Equation (3-6) is written in the stationary case, when cross sections and external sources are time independent, for a geometry curved in one direction, say cylindrical, giving

$$\mu(A_{i+1}N_{i+1} - A_iN_i) + \eta(B_{j+1}N_{j+1} - B_jN_j) + \xi(C_{k+1}N_{k+1} - C_kN_k) + \\ + (\alpha_{m+\frac{1}{2}}N_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}}N_{m-\frac{1}{2}})/w_m + V\sigma N = VS \qquad (3\text{-}9)$$

In this equation the terms in α are introduced as flow terms from the "edges" or "surfaces" of the directional cell. That is, in general, $N_{m-\frac{1}{2}}$ is the average of the neutron flux in the cell volume in the time interval Δt but in the direction $m-\frac{1}{2}$, where the directions $m\pm\frac{1}{2}$ define the "edges" of the angular range denoted by w_m. Then, $\alpha_{m-\frac{1}{2}}N_{m-\frac{1}{2}}\Delta t$ is the flow, due to angular redistribution, into the angular range being considered and is directly analogous to flow through the geometric surface of the cell. Division by $w_m\Delta t$ produces the terms of Eq. (3-9).

The coefficients α are determined by examining the case of everywhere uniform flow when $V\sigma N = VS$. Then, all N's are identical, and with the geometry curved in only one direction $B_{j+1} = B_j$ and $C_{k+1} = C_k$. The non-vanishing terms of Eq. (3-9) give a recursion relation for the α:

$$\alpha_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}} = -w_m\mu_m(A_{i+1} - A_i) \qquad (3\text{-}10)$$

In order that the angular redistribution process be conservative, the α terms must neither create nor destroy neutrons. That is, when (3-9) is

multiplied by w_m and summed over m ("integrated" over directions) the sum of the α terms

$$\sum_{m=1}^{M} (\alpha_{m+\frac{1}{2}} N_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}} N_{m-\frac{1}{2}}) = \alpha_{M+\frac{1}{2}} N_{M+\frac{1}{2}} - \alpha_{\frac{1}{2}} N_{\frac{1}{2}} \qquad (3\text{-}11)$$

must vanish. By ordering directions so that neutrons only flow out of the first directional cell ($\alpha_{\frac{1}{2}} = 0$) and only flow into the last cell ($\alpha_{M+\frac{1}{2}} = 0$), Eq. (3-11) vanishes for any N, and neutron conservation is maintained.

With positive w_m, $A_{i+1} > A_i$, and direction sets ordered so that the μ_m increases uniformly on the interval [-1,1], the α coefficients have the desirable property of being non-negative so that terms in Eq. (3-9) can actually be interpreted as directional flows. With $\alpha_{\frac{1}{2}} = \alpha_{M+\frac{1}{2}} = 0$ the m sum of the left side of Eq. (3-10) vanishes. For consistency, then, the right side m sum must vanish, or

$$\sum_{m=1}^{M} w_m \mu_m = 0 \qquad (3\text{-}12)$$

which represents an additional constraint on the angular quadrature coefficients. However, Eq. (3-12) is satisfied by any direction set symmetric with respect to the midpoint of the μ range, and unsymmetric sets are undesirable because computational results are not invariant under geometrical inversion. Symmetric sets also guarantee that if $\alpha_{\frac{1}{2}} = 0$, then $\alpha_{M+\frac{1}{2}}$ is identically zero.

In the limit of small intervals the above procedure reproduces the angular derivatives of the analytic transport equation. For example, in a one-dimensional, spherically symmetric system Eq. (3-9) can be written

$$\frac{\mu(A_{i+1}N_{i+1} - A_iN_i)}{V} + \frac{(\alpha_{m+\frac{1}{2}}N_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}}N_{m-\frac{1}{2}})}{Vw_m} + \sigma N = S \tag{3-13}$$

The first term is (see Table III-1)

$$\frac{3\mu(r_{i+1}^2N_{i+1} - r_i^2N_i)}{(r_{i+1}^2 + r_ir_{i+1} + r_i^2)(r_{i+1} - r_i)} \tag{3-14}$$

which is $\frac{\mu}{r^2}\frac{\partial(r^2N)}{\partial r}$ in the limit of small intervals. The second term suggests the derivative of the quantity αN with respect to direction, here designated by μ. From Eq. (3-10)

$$\frac{\alpha_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}}}{Vw_m} = -\frac{\mu_m(A_{i+1} - A_i)}{V} = -\frac{3\mu(r_{i+1} + r_i)}{r_{i+1}^2 + r_ir_{i+1} + r_i^2} \tag{3-15}$$

In the limit this term gives $\partial\alpha/\partial\mu = -2\mu/r$, or, by integrating, $\alpha = -\mu^2/r + \text{constant}$. But α, in the limit, vanishes at both ends of the μ range $[\alpha_{\frac{1}{2}} = \alpha_{M+\frac{1}{2}} = 0]$, that is, at $\mu = \pm 1$. Thus, $\alpha = (1 - \mu^2)/r$. Equation (3-13) is then

$$\frac{\mu}{r^2}\frac{\partial(r^2N)}{\partial r} + \frac{1}{r}\frac{\partial[(1-\mu^2)N]}{\partial\mu} + \sigma N = S \tag{3-16}$$

which is the conservation form of the Boltzmann equation in a one-dimensional spherical geometry.

The point of the above procedure for determining α coefficients is that the resulting expressions guarantee neutron conservation for finite intervals, while a direct approach, say writing the angular derivative of (3.16) as

$$\frac{(1 - \mu^2_{m+\frac{1}{2}})N_{m+\frac{1}{2}} - (1 - \mu^2_{m-\frac{1}{2}})N_{m-\frac{1}{2}}}{rw_m} \tag{3-17}$$

is unnecessarily restrictive because when the above equation is multiplied by w_m and summed over all m it vanishes only when $\mu^2_{M+\frac{1}{2}} = \mu^2_{\frac{1}{2}} = 1$.

In more general situations, direct differencing approaches may be more complicated as well as restrictive, but coefficients similar to the α can easily be determined. For example, if the geometry is curved in two directions so that $B_{j+1} \neq B_j$, in addition to the α, coefficients β defined by

$$\beta_{m+\frac{1}{2}} - \beta_{m-\frac{1}{2}} = - w_m \eta_m (B_{j+1} - B_j) \tag{3-18}$$

(with $\beta_{\frac{1}{2}} = \beta_{M+\frac{1}{2}} = 0$) readily permit neutron conserving treatment of direction to direction transfer.

3.1.5 Definition of the Source Term

The source term of Eq. (3-6) includes external sources, sources due to fission, and the scattering collision source.

The external sources are here denoted by $Q_{g,s+\frac{1}{2},m,i+\frac{1}{2},j+\frac{1}{2},k+\frac{1}{2}}$ with dimensions of neutrons per unit time, per unit direction, per unit volume, but not per unit speed, consistent with the definition of the group flux. Experience has shown that external shell sources can be represented by narrow distributed sources, so that the main computational problem in handling external sources is finding storage space for what may be a seven-dimensional array.

The fission source is assumed to result from a process which distributes neutrons isotropically in direction but with a spectrum of energies. Because the process is isotropic the number (density) of fission neutrons produced in the g^{th} group is

$$F_g = (\nu\sigma^f)_g \bar{N}_g \tag{3-19}$$

where $(\nu\sigma^f)_g$ is the fission cross section times the mean number of neutrons per fission in group g and $\bar{N}_g$ is the average group flux

$$\bar{N}_g = \sum_{m=1}^{M} w_m N_{gm} \tag{3-20}$$

or, what is the same thing, the zeroth (or isotropic) Legendre component of the angular flux in terms of a discrete ordinates quadrature. The total number of fission neutrons released is the sum of F_g over all groups, and the number released per group can be represented as the product of this sum and a fission spectrum, χ_g,

$$(\text{FISSION SOURCE})_g = \chi_g \sum_{h=1}^{G} F_h = \chi_g \sum_{h=1}^{G} \nu\sigma_h^f \bar{N}_h \qquad (3\text{-}21)$$

In the above context χ_g is simply the fraction of the total number of fission neutrons which enter the g^{th} group. A more general representation of the fission source can be made by assuming that the fission spectrum is a function of the group in which the fission occurred. Then,

$$(\text{FISSION SOURCE})_g = \sum_{h=1}^{G} \chi_{gh} \nu\sigma_h^f \bar{N}_h \qquad (3\text{-}22)$$

in which χ_{gh} is the fraction of neutrons produced in the g^{th} group due to fission in group h. Further generalizations in which the fission spectrum is material, and hence spatially, dependent are possible, but seldom are needed in practice.

The scattering collision source is the sum, over all directions and groups, of the product of the angular flux in group h in direction m' times the scattering cross section for transferring neutrons from direction m', group h, to direction m, group g,

$$(\text{COLLISION SOURCE})_{gm} = \sum_{h=1}^{G} \sum_{m'=1}^{M} w_{m'} \sigma^s_{ghmm'} N_{hm'} \qquad (3\text{-}23)$$

In anayltic terms, the above equation represents a double integral, over all initial directions and speeds, of the product of a transfer kernel and the angular flux. In discrete terms, the angular integration is denoted by the m' sum with weight $w_{m'}$ while the speed integration is indicated

simply by the h sum, the speed "weight" being included in the definition of N. Equation (3-23) is a very general treatment of anisotropic scattering, but is one which has several computational disadvantages. The transfer cross section $\sigma^s_{ghmm'}$ is at least a four-dimensional array which may also be a function of position. Equation (3-23) also requires that the angular flux for all positions, groups, and directions be available. Together these two arrays pose a storage and manipulation problem. In addition, the complete transfer cross section is seldom available and in many cases is not needed. If the order of the truncated Legendre expansion, L, needed to represent the scattering function

$$\sigma^s(v'\underset{\sim}{\Omega}' \rightarrow v\underset{\sim}{\Omega}) = \sum_{\ell=0}^{L} \frac{2\ell+1}{4\pi} \sigma^s_\ell \quad (v' \rightarrow v) P_\ell(\underset{\sim}{\Omega}' \cdot \underset{\sim}{\Omega}) \tag{3-24}$$

is less than M, as it usually is, the collision source can be conveniently represented by a Spherical Harmonics expansion evaluated at the discrete directions of the quadrature scheme used. In these terms*

$$\text{(COLLISION SOURCE)}_{gm} = \sum_{\ell=0}^{L} 2\ell+1 \left\{ \sum_{h=1}^{G} \sigma^s_{\ell gh} P_\ell(\xi_m) \left[\sum_{m'=1}^{M} w_{m'} P_\ell(\xi_{m'}) N_{hm'} + \right.\right.$$
$$\left.\left. + 2 \sum_{r=1}^{\ell} \frac{(\ell-r)!}{(\ell+r)!} P^r_\ell(\xi_m) \sum_{m'=1}^{M} w_m P^r_\ell(\xi_{m'}) \cos(\varphi_m - \varphi_{m'}) N_{hm'} \right] \right\} \tag{3-25}$$

where 4π is included in w_m. $\sigma^s_{\ell gh}$ represents the appropriate averages of $\sigma^s_\ell(v' \rightarrow v)$ of Eq. (3-24), and the remaining terms are from the expansion of $P_\ell(\underset{\sim}{\Omega}' \cdot \underset{\sim}{\Omega})$ in Legendre and associated Legendre polynomials and

*For rectangular and cylindrical geometry. For spherical geometry. $\xi_m \rightarrow \mu_m$, $\mu_m \rightarrow \eta_m$, $\eta_m \rightarrow \xi_m$. (See Fig. III-2).

angular integrations. φ is an angle such that

$$\mu_m = (1 - \xi_m^2)^{\frac{1}{2}} \cos \varphi_m, \quad \text{and} \quad \eta_m = (1 - \xi_m^2)^{\frac{1}{2}} \sin \varphi_m$$

Certain terms of Eq. (3-25) are not needed if the system considered possesses symmetries. For instance, in one-dimensional cylindrical or in two-dimensional x-y geometry the angular flux is even in ξ, and the integrations of the flux and polynomials odd in ξ are not required. Equation (3-25) is relatively simple provided L is not large. When $\ell = 0$ the isotropic portion of Eq. (3-25) is just

$$\sum_{h=1}^{G} \sigma_{ogh}^{s} \sum_{m'=1}^{M} w_{m'} N_{hm'} = \sum_{h=1}^{G} \sigma_{ogh}^{s} \bar{N}_h \tag{3-26}$$

and, with some manipulation the $\ell = 1$ term can be shown to be

$$\sum_{h=1}^{G} 3\sigma_{1gh}^{s} (\mu_m I_h + \eta_m J_h + \xi_m K_h) \tag{3-27}$$

where I, J, and K are the currents

$$\begin{aligned} I_h &= \sum_{m=1}^{M} w_m \mu_m N_{hm} \\ J_h &= \sum_{m=1}^{M} w_m \eta_m N_{hm} \\ K_h &= \sum_{m=1}^{M} w_m \xi_m N_{hm} \end{aligned} \tag{3-28}$$

Higher order terms have no such simple expressions.

With the above definitions and linearly anisotropic scattering, S of Eq. (3-4) is

$$S_{gm} = Q_{gm} + \chi_g \sum_{h=1}^{G} \nu\sigma_h^f \bar{N}_h + \sum_{h=1}^{G} \sigma_{ogh}^s \bar{N}_h + \qquad (3\text{-}29)$$

$$+ 3 \sum_{h=1}^{G} \sigma_{1gh}^s (\mu_m I_h + \eta_m J_h + \xi_m K_h)$$

In the solution of the transport equation in the gth group, external sources are known, the fission source is assumed known, either from previous calculation of all $\bar{N}_h$ or from an initial guess, but portions of the collision source depend upon the flux which is to be calculated. That is, in group g, the average flux and currents for other groups can be assumed known, but the average flux and currents for group g are determined after the calculation of the angular flux in group g. This implies an iterative solution process, in which the source is calculated from the best previous information, the equation solved, and the source recomputed. The control of this iterative process, described in detail below, is facilitated by the fact that σ_{ogg}^s appears as part of the total cross section of Eq. (3-6) and as part of the source term.

3.2 Formulation of Discrete Ordinates Equations Directly From the Analytic Form of the Neutron Transport Equation

Although the preceding discrete ordinates equations are quite general, it is useful to examine formulations made directly from analytic representations of the transport equation. For this purpose a generalized moment representation, including spherical harmonics as a subcase, is considered; and the conditions necessary for equivalence of a moments and a discrete ordinates representation are derived. By establishing this equivalence valuable insights are obtained about the structure of the equations derived in the previous section, and guidance is provided in the selection of discrete ordinates quadrature sets. All essential points are made by considering the stationary, monoenergetic, transport equation in one-dimensional spherical geometry.

3.2.1 A Generalized Moment Representation of the Transport Equation

The analytic neutron transport equation in spherical geometry can be written in conservation form as

$$\frac{1}{r^2}\frac{\partial(r^2\mu\psi)}{\partial r} + \frac{1}{r}\frac{\partial[(1-\mu^2)\psi]}{\partial\mu} + \sigma\psi(r,\mu) = S(r,\mu) \qquad (3\text{-}30)$$

For convenience, the source is limited to an isotropic external source, S_f, isotropic fission, and a linearly anisotropic scattering source so that

$$S(r,\mu) = S_f(r) + \frac{\nu\sigma_f + \sigma_o^s}{2}\int_{-1}^{1}\psi(r,\mu')d\mu' + \frac{3\sigma_1^s\mu}{2}\int_{-1}^{1}\mu'\psi(r,\mu')d\mu' \equiv$$

$$\equiv S_o(r) + 3\mu S_1(r) \tag{3-31}$$

Defining a moment operator

$$\tilde{M}_m = \frac{1}{2}\int_{-1}^{1}\mu^m \cdot d\mu \tag{3-32}$$

such that $\tilde{M}_m\psi = \psi_m$ and applying $\tilde{M}_m$ to Eq. (3-30) gives the moment equations, $m = 0,1,\ldots,$

$$\frac{1}{r^2}\frac{d(r^2\psi_{m+1})}{dr} + \frac{m}{r}(\psi_{m+1} - \psi_{m-1}) + \sigma\psi_m =$$

$$= \begin{cases} S_o/(m+1), & m \text{ even} \\ 3S_1/(m+2), & m \text{ odd} \end{cases} \tag{3-33}$$

The first n of the above equations, $m = 0,1,\ldots,n-1$, can be solved for the moments ψ_m by analytic or numerical methods. First, however, the ψ_n moment must be eliminated from the equation for $m = n-1$ to obtain an equal number of equations and unknowns. This elimination is made using a terminating condition obtained by assuming a representation for $\psi(r,\mu)$ as a function of μ. Letting ψ be represented in terms of n arbitrary coefficients which may be functions of r and operating on the representation with $\tilde{M}_m$, $m = 0$ to n, gives n+1 relations which can be used to express ψ_n in terms of the other ψ_m, $m < n$. With this relation solution of the

moment equations is possible; and the angular flux can be reconstructed from the moments; i.e., the arbitrary coefficients in the assumed representation can be determined. As a simple example of this procedure consider the case of a homogeneous medium with an isotropic scattering and fission source. Then $S_1 = 0$ and $S_o = (\nu\sigma^f + \sigma_o^s)\psi_o$. With r measured in mean free paths, the first two equations of (3-33) are

$$\frac{1}{r^2}\frac{d}{dr}(r^2\psi_1) + \psi_o = c\psi_o$$

$$\frac{1}{r^2}\frac{d}{dr}(r^2\psi_2) + \frac{1}{r}(\psi_2 - \psi_o) + \psi_1 = 0 \qquad (3\text{-}34)$$

where $c = (\nu\sigma^f + \sigma_o^s)/\sigma$. ψ_2 is eliminated by representing $\psi(r,\mu)$ as a polynomial with two undetermined coefficients

$$\psi(r,\mu) = a_0(r) + a_1(r)\mu \qquad (3\text{-}35)$$

When $\tilde{M}_m$ is applied to ψ for m = 0, 1, and 2 to obtain the relations

$$\begin{aligned} \psi_0 &= a_0(r) \\ 3\psi_1 &= a_1(r) \\ 3\psi_2 &= a_0(r) \end{aligned} \qquad (3\text{-}36)$$

it is seen that the last equation is satisfied if $\psi_2 = \psi_0/3$. Using this equation in Eq. (3-34) and eliminating ψ_1 gives

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\psi_o}{dr}\right) + 3(c - 1)\psi_o = 0 \qquad (3\text{-}37)$$

the familiar diffusion theory or P_1 spherical harmonics equation. The application of boundary conditions now permits ψ_0 and ψ_1 to be determined (say for the sphere critical radius). The first two of the Eqs. (3-36) then give a_0 and a_1 and hence the angular flux in Eq. (3-35).

The above procedure is quite general, particularly in the choice of representations of ψ. Three choices which readily permit coefficients to be expressed in terms of ψ_m are (a) a single polynomial of degree n-1 over the μ interval $[-1,1]$: $\psi(r,\mu) = \sum_{m=0}^{n-1} a_m(r)\mu^m$; (b) two separate polynomials, each of degree $n/2 - 1$, one on the range $[-1,0]$, the other on the range $[0,1]$; and (c) a sequence of step functions with n different amplitudes over the interval $[-1,1]$. Representation (a) is that of Spherical Harmonics (cf. the example with n=2 above), while (b) is similar but not equivalent to Yvon's (the double Legendre) method and applies to curved as well as rectangular geometries. In addition to the n amplitudes of representation (c) the partitioning of the μ interval gives extra degrees of freedom which are, in effect, an implicit weight function for the moment operator Eq. (3-32).

For a boundary condition of no incoming flux, Marshak boundary conditions are most suitable, being expressible as moments of ψ. The Marshak conditions are, for odd m,

$$\int_{-1}^{0} d\mu\mu^m\psi(r,\mu) = 0, \qquad r \text{ on the boundary} \qquad (3\text{-}38)$$

The first of these is the condition of no inward current, while the higher order conditions can be interpreted by associating partial currents with each even order moment ψ_m. For the representation of Eq. (3-35), the Marshak condition is $-a_0(r)/2 + a_1(r)/3 = 0$ or $2\psi_1(r) = \psi_0(r)$ for r on the sphere boundary.

The moments equations above may be made more general by including a weight function, with or without adjustable parameters, in the definition of $\tilde{M}_m$. However, only with a unit weight function is the m=0 moment equation the neutron balance equation. Also, without a unit weight function the Eqs. (3-33) become dependent upon the coefficients of the ψ representation. A detailed description of general moments equations for the three representations of ψ and for three one-dimensional geometries is given in Reference 3.

3.2.2 Discrete Ordinate Equations Equivalent to Moments Representations

Let Eq. (3-30) be evaluated at n discrete values of $\mu = \mu_k$ $k = -n/2, \ldots, 0, \ldots, n/2$ and be written as

$$\frac{1}{r^2}\frac{d}{dr}(r^2\mu_k\phi_k) + \frac{1}{r}\sum_{\ell=-n/2}^{n/2}\beta_{k\ell}\phi_\ell + \sigma\phi_k = S_o + 3\mu_k S_1 \qquad (3\text{-}39)$$

where $\phi_k(r) = \psi(r,\mu_k)$ and the sum involving $\beta_{k\ell}$ represents the μ differentiation of ψ with coefficients to be determined. A reasonable condition for equivalence between the moments equations and the discrete representation, Eq. (3-39), is that the terminating condition be satisfied.

For the three representations of $\psi(r,\mu)$ discussed above, the terminating condition can be written, for even n, as

$$\sum_{m=0}^{n/2} c_{2m}\psi_{2m}(r) = 0 \tag{3-40}$$

But in terms of a discrete ordinates quadrature the moment ψ_m is

$$\psi_m(r) = \sum_{k=-n/2}^{n/2} w_k \mu_k^m \phi_k(r) \tag{3-41}$$

so that Eq. (3-30) becomes, interchanging the order of the finite sums,

$$\sum_{k=-n/2}^{n/2} w_k \phi_k \left(\sum_{m=0}^{n/2} c_{2m}\mu_k^{2m} \right) = 0 \tag{3-42}$$

Equation (3-42) is satisfied if the μ_k are the ($\pm$ paired) roots of the polynomial $\sum_{m=0}^{n/2} c_{2m}\mu_k^{2m} = 0$. If a single polynomial representation of $\psi(r,\mu)$ is used, these roots are the roots of the Legendre polynomials $P_n(\mu)$.

Another condition for equivalence is that the moment equations (3-33) should be obtainable by the application of the discrete moment operator

$$M_m = \sum_{k=-n/2}^{n/2} w_k \mu_k^m \tag{3-43}$$

to Eq. (3-39) with moments ψ_m defined as in Eq. (3-41). After operation with M_m, the right side of Eq. (3-38) is equivalent to the right side of

Eqs. (3-33) if

$$\sum_{k=-n/2}^{n/2} w_k \mu_k^{2m} = 1/(2m + 1), \qquad m = 0, 1, \ldots, n/2 \tag{3-44}$$

and the left sides are identical if

$$m(\psi_{m+1} - \psi_{m-1}) = \sum_{k=-n/2}^{n/2} w_k \mu_k^m \sum_{\ell=-n/2}^{n/2} \beta_{k\ell} \phi_\ell \tag{3-45}$$

or, rewriting both sides, if

$$m \sum_k \phi_k \left[w_k \mu_k^{m-1} (\mu_k^2 - 1) \right] = \sum_\ell \phi_\ell \sum_k w_k \mu_k^m \beta_{k\ell} \tag{3-46}$$

that is, if for all ℓ,

$$\sum_k w_k \mu_k^m \beta_{k\ell} = -m w_\ell \mu_\ell^{m-1} (1 - \mu_\ell^2) \tag{3-47}$$

with $m = 0, 1, \ldots, n-1$. If Eqs. (3-42), (3-44), and (3-47) are satisfied, discrete ordinates quadrature coefficients are determined, and the discrete ordinates equations are equivalent to the moments equations. For the representations of $\psi(r, \mu)$ considered above and even n, Eq. (3-42) determines the μ_k which are symmetric with respect to $\mu = 0$, Eq. (3-44) determines all the weights (equal weights to symmetric directions), and

Eq. (3-46) determines the curvature coefficients.* For spherical harmonics moment equations the β matrix is full. This is an example of the detailed directional coupling of flux equations that can occur in discrete ordinates representations (cf. Section 3.1.4). Note, too, that even if spherical harmonics weights and directions are used in Eq. (3-9) the formulation is not the same (because of the treatment of the curvature term) unless $N_{m+\frac{1}{2}}$ and $N_{m-\frac{1}{2}}$ are specially defined. In geometries without curvature the two treatments are the same (assuming the same application of the boundary conditions).

The manipulations leading to Eq. (3-47) above point the way to extending the treatment of the curvature term developed in Section 3.1.4. That is, the angular coupling there introduced can be made more complicated without, however, going to the extreme of introducing a complete coupling matrix.

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* It should be noted that moments equations can also be formulated without using the vehicle of polynomial representation. If an arbitrary (but symmetric) quadrature set is selected and angular moments defined as in Eq. (3-41), the first n/2 of the "even" equations [m = 0,2,...,n-2 in Eq. (3-41)] can be solved for $(\phi_k + \phi_{-k})$ in terms of ψ_m and the results used in the m = n equation to obtain the coefficients, c_{2m}, of the terminating condition, Eq. (3-40). At a bare boundary (where $\phi_{-k} = 0$), Eq. (3-41) can be solved for ϕ_k in terms of ψ_m, m even, and these results used in the odd m equations to obtain the Marshak boundary conditions. From this point the procedures discussed in the text are followed.

Given a moments representation, the procedure of the text produces equivalent discrete ordinates equations. The point of this note is that "moments" representations which are equivalent to arbitrary discrete ordinates quadrature can also be constructed. Whether direct solution of such moments equations is practicable has not been examined.

When the above analysis is extended to one-dimensional cylindrical geometries by generalizing the moment operator to include two angular variables, it is found that in order to satisfy all terminating conditions, interesting restrictions are imposed on the quadrature coefficients.[3] Although these restrictions have not been fully explored they seem akin to symmetry restrictions which are discussed next.

3.3 Selection of Discrete Ordinates Angular Quadrature Coefficients

Up to this point, directions have been indicated simply by the vector $\underset{\sim}{\Omega}_m$ with components (μ_m, η_m, ξ_m). The weights associated with the directions $\underset{\sim}{\Omega}_m$ sum to unity provided the surface area on the unit directional sphere is measured in units of 4π. As also has been seen, in curved geometries, some or all of the conditions

$$\sum_{m=1}^{M} w_m \mu_m = 0, \quad \sum_{m=1}^{M} w_m \eta_m = 0, \quad \sum_{m=1}^{M} w_m \xi_m = 0 \tag{3-48}$$

may be necessary to guarantee neutron conservation. Insuring that physical symmetries are satisfied imposes additional conditions. For example, computations in a heterogeneous plane slab should give results which are invariant under geometrics orientations of the slab. If the slab consists of two regions, say a moderator and an absorber region, and the slab is oriented with the absorber on the right, a coarse spatial mesh might be used in the moderator region and a fine mesh in the absorber. If then the absorber and moderator regions are interchanged, without

changing the spatial mesh, it is unlikely that the same computational result would be obtained. Such a difference would not have been possible if a uniform spatial mesh had been used. While common sense dictates that the spatial mesh should be rearranged if the system components are interchanged, it is usually not possible or feasible to make a similar rearrangement of the direction mesh. That is, while it is customary to allow great freedom in the specification of the spatial mesh, it is also customary to use the same direction mesh in all groups and space cells.* Thus, to preserve computational invariance of solutions under geometric transformations, the direction mesh itself must be made invariant under geometric transformations.

To apply the above considerations in the general case of three-dimensional geometry consider a homogeneous cube. A 90° rotation of the cube about the z axis is equivalent to a 90° spatial coordinate rotation which also rotates the μ axis into the η axis. For the flux coordinate representation to remain the same, the positive μ_m must be the same as the positive η_m. A second rotation of 90° about the z axis shows that the positive μ_m should be the same in magnitude as the negative μ_m; i.e., the μ_m must be symmetric with respect to $\mu = 0$. Other rotations show that the ξ_m must also be chosen from the same direction set as the μ_m.

*It is, of course, possible to allow the direction set to be a function of group and position. The simplest variant is to allow a group dependence of the order, n, of the angular quadrature.

Thus, to preserve physical symmetry, quadrature sets for angular integration in a cube must be chosen so that the μ_m, η_m, and ξ_m are the same and symmetrically located with respect to the origin. Hence, all of Eqs. (3-48) are satisfied. If the geometric dimensionality is reduced, some symmetry restrictions can be relaxed. For example, in two-dimensional x-y geometry, one set must be used for both μ_m and η_m while a different set may be used for ξ_m.

With the same distribution of cosines on each axis, the directional points on the surface of the unit sphere lie on latitudes, which leads to a decided computational convenience. For, except in one-dimensional slabs and spheres, two independent variables are required for angular quadrature, and latitudinal point arrangement permits a two-dimensional quadrature to be accomplished as simply as a one-dimensional integration. A typical, completely symmetric, latitudinal arrangement is shown in Fig. III-3 where, along ξ latitudes, only μ and η change, and since $\mu^2 + \xi^2 + \eta^2 = 1$ only one variable is independent.

Fig. III-3

In the arrangement of Fig. III-3 there are $n(n + 2)$ points, $n = 2, 4, 6\ldots,$ on the surface of the unit sphere. This n is the subscript of the commonly used S_n discrete ordinates scheme. As described here n refers to a symmetry preserving point arrangement and not to a specific quadrature set. Although such sets satisfy constraining conditions, degrees of freedom remain, and particular additional conditions may be imposed for special purposes.

If full symmetry is not required the latitudinal point arrangement can be relaxed as well. However, the direct sum evaluation of a two-dimensional angular integral can still be retained. For example, in one-dimensional cylindrical geometry, points can be arranged on ξ latitudes, but not on μ and η latitudes. In such geometry the point arrangement of Fig. III-4 might be used in lieu of the symmetric arrangement of Fig. III-3.

Fig. III-4

If the geometry is not three-dimensional, all the points on the unit sphere are not needed even if full symmetry is retained. For instance, in two-dimensional x-y geometry, the flux is symmetric in ξ; and only half the ξ range is needed, say the upper hemisphere. In one-dimensional cylindrical geometry the flux is symmetric in ξ and η, so that only a quadrant, containing the entire range of μ, is needed. In general, the number of points required in a completely symmetric arrangement is

$$M = 2^d n(n + 2)/8 \tag{3-49}$$

where d is the geometric dimensionality. In one-dimensional slabs and spheres the flux is independent of ξ or η, and then only M = n values of μ are needed.

With full symmetry, latitudinal point arrangement, and n direction cosines, the requirement that

$$\mu_m^2 + \eta_m^2 + \xi_m^2 = 1 \tag{3-50}$$

becomes

$$\mu_i^2 + \mu_j^2 + \mu_{n/2-2-i-j}^2 = 1 \tag{3-51}$$

Here, the subscripts refer to the coordinates of $\underset{\sim}{\Omega}_m$ with $i = 1,2,3,\ldots,n/2$, $j = 1,2,3,\ldots,n/2-i+1$. The correlation between the i and j subscripts (ordering cosines on an axis) and the subscript m (numbering points on the unit sphere) may be made in any convenient manner. For example, when $n = 8$ (Fig. III-3) the point $m = 1$ might be taken to have coordinates $\mu = \mu_1$, $\eta = \mu_1$, and $\xi = \mu_4$. Equation (3-51) is then $2\mu_1^2 + \mu_4^2 = 1$. In general, Eq. (3-51) is solved by

$$\begin{aligned} \mu_i^2 &= \mu_1^2 + (i-1)\Delta, \qquad i = 1,2,\ldots,n/2 \\ \Delta &= 2(1 - 3\mu_1^2)/(n-2) \end{aligned} \tag{3-52}$$

as may be verified by direct substitution. Equation (3-52) shows how strong the restraint of complete symmetry is, since only one direction cosine remains independent. Selection of μ_1 determines the spread of direction cosines along the axes. For small μ_1^2 cosines are clustered along the ends of the interval [0,1]. For larger $\mu_1^2 \leq 1/3$ the cosines are clustered nearer the middle of the interval.

Symmetry also imposes conditions upon the number of independent point weights, for the weights as well as directions must be invariant

under geometric transformations. For n = 2 each point has the same weight. That is, there are eight directions, one through the midpoint of each sphere octant; and by requiring that weights be invariant under 90° degree rotations of the (μ,η,ξ) coordinate system it is easily seen that each weight must be the same. For n = 4 again all weights are equal, and for $2 < n \leq 12$ there are $n/2 - 1$ independent point weights. For $n > 12$ the number of different point weights grows rapidly. In any case the freedom of Gaussian quadrature sets is not present. That is, it is not possible to correctly integrate the first 2n powers of μ, but for $n \leq 12$ only n such moment conditions can be satisfied (the odd powers of μ are correctly integrated because the μ_m are symmetrically located on [-1,1]). However, it can be shown[4] that quadrature sets satisfying Eq. (3-52) with the number of independent point weights restricted to $n/2 - 1$, all n, also satisfy the relation

$$\sum_{m=1}^{M} w_m \mu_m^2 = \frac{1}{3} \tag{3-53}$$

Symmetric sets which integrate as many even powers of μ as possible are given in Reference 5. For $n > 22$ negative weights, which are computationally undesirable, occur; but such large values of n are seldom required.

When complete symmetry is not required, many of the above restraints can be removed.[5] In particular, in one-dimensional slabs and spheres, the integration reduces to quadrature on the interval [-1,1] for which

Gaussian quadrature sets may be used. In these cases the flux is independent of η and ξ so that for a given μ the point weights can be accumulated to produce "level" weights, the normal weights for integration on a line. Gauss-Legendre quadrature on [-1,1] is the familiar P_{n-1} discrete ordinates system of quadrature.* Separate Gauss-Legendre quadrature on [-1,0] and [0,1] is known as the double Legendre, $DP_{n/2-1}$, system. For integration in one-dimensional cylinders or in two-dimensional x-y geometry, P or DP quadrature for ξ integration can be combined with Tschebyscheff coefficients in the μ-η directions.

It should be emphasized that there is no optimum type of quadrature for all situations. Even in the simple case of a plane homogeneous slab, $DP_{n/2-1}$ quadrature, while very accurate in thin slabs, is less accurate than P_{n-1} quadrature in very thick slabs. This being the case, the moment matching completely symmetric sets are preferred because of their generality, and special sets are reserved for the special situations where they are most accurate. Moment matching is particularly important if anisotropic scattering is approximated by a Legendre polynomial expansion so that the polynomials can be integrated correctly. That is, if the flux should be isotropic, all the Legendre moments except the zeroth should vanish, and sets which integrate polynomials guarantee this.

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*Remember, however, that the discrete ordinates formulation of Section 3.1.4 is not equivalent, in curved geometries, to the spherical harmonics formulation of Section 3.2.2 unless the same quadrature coefficients are used and the curvature fluxes as especially defined.

Regardless of the quadrature set selected a problem solution should be tested, just as in the evaluation of an integral, for dependence upon the order of quadrature. However, solutions of the transport equation are more complicated because spatial as well as angular quadrature is involved. Experience has shown that errors involved in spatial and angular quadrature are interdependent. Qualitatively, the error surface is like a valley between two ridges. If error is plotted against order of angular quadrature along one axis and order of spatial quadrature along an orthogonal axis, the ridges of the surface lie above these axes. Hence, if a calculation gives a result in the error valley, both quadratures must be refined to remain in this error valley. On the other hand, for a given spatial mesh, refining the angular quadrature may actually increase the error, and conversely.

3.4 Approximations and Simplifications

In particular problems, or parts of problems, the entire panoply of Eq. (3-6) or Eq. (3-9) may not be needed. Some methods that can be used to reduce complexity and computational effort are here described.

3.4.1 The Diffusion Theory Approximation

A diffusion theory representation of neutron transport is obtained by letting n = 2 in Eq. (3-6) and assuming that N_m is linear in the direction cosines

$$N_m = \bar{N} + 3\mu_m I + 3\eta_m J + 3\xi_m K \qquad (3\text{-}54)$$

When n = 2, there are eight directions corresponding to two values of each of the direction cosines. When Eq. (3-54) is multiplied by w_m and summed over m, the left side is $\bar{N}$ by the definition of Eq. (3-26). The right side is $\bar{N}$ only if each weight is equal to 1/8 and only if the two values of each direction cosine are equal and opposite in sign. When Eq. (3-54) is multiplied by $w_m\mu_m$ and summed the left side is I by the definition of Eq. (3-28), but the right side gives I only if $\mu^2 = 1/3$. That is, Eq. (3-53), sometimes called the diffusion theory condition, must be satisfied. Similarly, η^2 and ξ^2 must be equal to 1/3. All these conditions are met by the completely symmetric direction set for n = 2 in which all weights are equal and $\mu^2 = \eta^2 = \xi^2 = 1/3$ (cf. Eq. (3-50)).

Reduction of Eq. (3-6) to a set of diffusion theory equations is accomplished by procedures analogous to those of analytic theory. The treatment of curvature terms, however, requires additional assumptions. These not very restrictive assumptions are illustrated by beginning with Eq. (3-6) written for a geometry curved in the i direction.

$$(N_{s+1} - N_s)V/v\Delta t + \mu(A_{i+1}N_{i+1} - A_iN_i) + \eta(B_{j+1}N_{j+1} - B_jN_j) +$$

$$+ \xi(C_{k+1}N_{k+1} - C_kN_k) + (\alpha_{m+\frac{1}{2}}N_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}}N_{m-\frac{1}{2}})/w_m + \sigma NV = SV \qquad (3\text{-}55)$$

Multiplying the above equation by w_m and summing over m gives, as for any n, the neutron balance equation

$$(\bar{N}_{s+1} - \bar{N}_s)V/v\Delta t + A_{i+1}I_{i+1} - A_iI_i + B_{j+1}J_{j+1} - B_jJ_j +$$

$$+ C_{k+1}K_{k+1} - C_kK_k + \sigma\bar{N}V = \bar{S}V \qquad (3\text{-}56)$$

Where $\bar{S}$ is the isotropic component of the source, $\bar{S} = \Sigma\, w_m S_m$. The next step in the reduction is to obtain a current equation in the i direction by multiplying Eq. (3-55) by $w_m\mu_m$ and summing. The procedure is made clearer by explicity defining the eight directions, letting

$$\begin{aligned}
N_1 &= \bar{N} - \sqrt{3}I - \sqrt{3}J - \sqrt{3}K \\
N_2 &= \bar{N} + \sqrt{3}I - \sqrt{3}J - \sqrt{3}K \\
N_3 &= \bar{N} - \sqrt{3}I + \sqrt{3}J - \sqrt{3}K \\
N_4 &= \bar{N} + \sqrt{3}I + \sqrt{3}J - \sqrt{3}K \\
N_5 &= \bar{N} - \sqrt{3}I - \sqrt{3}J + \sqrt{3}K \\
N_6 &= \bar{N} + \sqrt{3}I - \sqrt{3}J + \sqrt{3}K \\
N_7 &= \bar{N} - \sqrt{3}I + \sqrt{3}J + \sqrt{3}K \\
N_8 &= \bar{N} + \sqrt{3}I + \sqrt{3}J + \sqrt{3}K
\end{aligned} \qquad (3\text{-}57)$$

Then, the sum of $w_m\mu_m$ times the first terms of Eq. (3-55) yields a time difference of the current I. Because each $\mu^2 = 1/3$, the sum of the terms involving μ gives a spatial difference of the average flux, while the terms containing η and ξ vanish as may be seen by inspecting the ordering of signs of Eq. (3-57). The resulting current equation is then

$$(I_{s+1} - I_s)V/v\Delta t + (A_{i+1}\bar{N}_{i+1} - A_i\bar{N}_i)/3 + \sum_{1}^{8} \mu_m(\alpha_{m+\frac{1}{2}}N_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}}N_{m-\frac{1}{2}}) +$$

$$+ \sigma IV = S_I V \qquad (3\text{-}58)$$

where $S_I = \Sigma\, w_m\mu_m S_m$. From the ordering of μ values in Eq. (3-57) and the definition of α, Eq. (3-10), the only non-vanishing α's are for $m = 1, 3, 5,$ and 7. At each of these values of m, μ_m is the same, and hence all the non-vanishing α's are equal. Then

$$\sum_{1}^{8} \mu_m(\alpha_{m+\frac{1}{2}}N_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}}N_{m-\frac{1}{2}}) = \frac{A_i - A_{i+1}}{3} \sum_{1,3,5,7} 2w_m N_{m+\frac{1}{2}} \qquad (3\text{-}59)$$

But because of the linear assumption, Eq. (3-54), $N_{m+\frac{1}{2}} = (N_{m+3/2} + N_{m-\frac{1}{2}})/2$, or what is the same thing $2N_{m+\frac{1}{2}} = (N_{m-\frac{1}{2}} + N_{m+\frac{1}{2}})/2 + (N_{m+\frac{1}{2}} + N_{m+3/2})/2$ so that

$$\sum_{1,3,5,7} w_m 2N_{m+\frac{1}{2}} = \sum_{m=1}^{8} w_m(N_{m-\frac{1}{2}} + N_{m+\frac{1}{2}})/2 \qquad (3\text{-}60)$$

Now, if the coefficients of the terms on the right of Eq. (3-54) are continuous, the average of the angular flux is equal the average of the spatial flux, i.e., $(N_{i+1} + N_i)/2 = (N_{m-\frac{1}{2}} + N_{m+\frac{1}{2}})/2$. With this assumption Eq. (3-60) becomes $\frac{1}{2}(\bar{N}_{i+1} + \bar{N}_i)$. When multiplied by $(A_i - A_{i+1})/3$ this term can be combined with the similar term in Eq. (3-58) to give the current equation

$$(I_{s+1} - I_s)V/v\Delta t + A(\bar{N}_{i+1} - \bar{N}_i)/6 + \sigma IV = S_I V \qquad (3\text{-}61)$$

where $A = A_{i+1} + A_i$. If there is no curvature Eq. (3-58) does not contain the α term sum, but the absence of curvature implies $A_i = A_{i+1}$ so that Eqs. (3-58) and (3-61) are then consistent. Two additional current equations, obtained by multiplying by $w_m\eta_m$ or $w_m\xi_m$ and summing, are given by

$$\begin{aligned}(J_{s+1} - J_s)V/v\Delta t + B(\bar{N}_{j+1} - N_j)/6 + \sigma JV &= S_J V \\ (K_{s+1} - K_s)V/v\Delta t + C(\bar{N}_{k+1} - N_k)/6 + \sigma KV &= S_K V\end{aligned} \tag{3-62}$$

Above, $B = B_{j+1} + B_j$ and $C = C_{k+1} + C_k$ to include the possibility of curvatures in these directions.

Equations (3-56), (3-61), and (3-62) are discrete analogs of the consistent P-1 approximation; and, in the limit of small intervals, the analytic forms are easily obtained.

It is worth noting that only four linear combinations of the eight S_2 equations were needed to form the above equations. For geometric dimensionality d, the diffusion approximation converts 2^d S_2 equations into d + 1 equations. Thus, for $d > 1$, the accuracy of the diffusion approximation is possibly less than that of the S_2 equations. Numerical results for d = 2 tend to confirm this hypothesis; and the difference between the two results is much like the diffusion theory error itself, decreasing as the flux becomes more nearly isotropic. However, since it is possible to cancel the within group scattering cross section from both sides of Eq. (3-56), iterative procedures in diffusion theory are simpler. With

the neglect of higher order angular resolution of the source term, a requisite for the use of diffusion theory, the diffusion approximation can be made selectively by groups.

3.4.2 Reduction of Dimensionality

Equation (3-6) can be reduced to a sequence of steady-state problems by the simple assumption, requiring only that ψ be a continuous function of time, that $N_{s+\frac{1}{2}} = (N_{s+1} + N_s)/2$. Using this relationship to remove N_{s+1} from Eq. (3-6) gives

$$\mu(A_{i+1}N_{i+1} - A_iN_i) \cdots (\sigma + 2/v\Delta t)NV = SV + 2N_sV/v\Delta t \qquad (3\text{-}63)$$

$2N_sV/v\Delta t$ is then the source of neutrons transmitted into the time interval from the previous time step. With known values of N_s, either from initial data or from calculation in a previous time interval, Eq. (3-63) can be solved for $N_{s+\frac{1}{2}}$. Then, $N_{s+1} = 2N_{s+\frac{1}{2}} - N_s$ is the input for the next time interval.

If the time dependence of all fluxes and sources is such that they can be approximated by $N = \tilde{N}f(t)$, $S = \tilde{S}f(t)$, with $\tilde{N}$ and $\tilde{S}$ time independent, then time dependence can be eliminated entirely. In the limit of small Δt

$$(N_{s+1} - N_s)/v\Delta t \rightarrow \frac{\tilde{N}}{v}\frac{df}{dt} = \frac{\tilde{N}f}{v}\frac{d(\ell nf)}{dt} \qquad (3\text{-}64)$$

If $f = e^{\lambda t}$, Eq. (3-6) becomes, dividing all terms by f,

$$\mu(A_{i+1}\tilde{N}_{i+1} - A_i\tilde{N}_i) \ldots (\sigma + \frac{\lambda}{v})\,\tilde{N}V = \tilde{S}V \tag{3-65}$$

The quantity λ/v, the time absorption, appears as a correction to σ and is frequently the object of an implicit eigenvalue search.

Total elimination of spatial variables is also possible. For instance, in rectangular geometry, suppose that the y dependence of the flux is such that a diffusion theory shape is adequate. Set $N = \hat{N}\cos(\pi y/2b)$, assuming that N is time independent and that the flux vanishes at $y = \pm b$. Considering, for convenience, a time independent problem with an isotropic source, Eq. (3-62) can be used to determine J

$$J = -B(\bar{N}_{j+1} - \bar{N}_j)/6V\sigma = -(\bar{N}_{j+1} - \bar{N}_j)/3\sigma\Delta y =$$

$$= -\hat{N}\{\cos[\pi(y + \Delta y)/2b] - \cos(\pi y/2b)\}/3\sigma\Delta y \quad \text{or, in the limit of small } \Delta y, \tag{3-66}$$

$$J = \hat{N}\pi\sin(\pi y/2b)/6\sigma b$$

This relationship can be used to eliminate J from the balance equation, Eq. (3-56), since

$$\lim_{\Delta y \to 0} \frac{B_{j+1}J_{j+1} - B_jJ_j}{V} = \hat{N}\sigma(\pi/2b\sigma)^2\cos(\pi y/2b)/3 \tag{3-67}$$

Finally, if there are no external sources, or if all sources are assumed to be given by $S = \hat{S}\cos(\pi y/2b)$, Eq. (3-56) becomes

$$A_{i+1}\hat{I}_{i+1} - A_i\hat{I}_i \ldots \sigma[1 + \frac{1}{3}(\frac{\pi}{2b\sigma})^2]\hat{N}V = \hat{S}V \qquad (3\text{-}68)$$

and the Δy of A, C, and V cancel. That is, the two-dimensional area and volume elements can be used. Equation (3-68) is then a two-dimensional equation with a buckling absorption correction to the total cross section to approximate the effects of y direction leakage. The same correction can be made to the x-z dependent form of Eq. (3-6). The same type of correction can also be used to remove x dependence as well, and the correction is additive. If the x thickness is 2a the effective total cross section becomes

$$\sigma[1 + (\pi/2b\sigma)^2/3 + (\pi/2a\sigma)^2/3] \qquad (3\text{-}69)$$

The above correction can be made assuming either that b is an actual dimension or that b is an extrapolated half-width related to the actual half-width t by $b = t + \delta$. To the order of approximation made above $\delta = 2/3\sigma$, but in Eq. (3-6) $\delta = 0.71045\lambda_{tr}/c$ can be used. Here, λ_{tr} is the transport mean free path and c is the local secondaries ratio $c = (\nu\sigma_g^f + \sigma_{ogg}^s)/\sigma_g$.

The cancellation of the assumed y shape from all terms of the equation was fortuitous. Had the shape $N = \hat{N}[1 - (y/b)^2]$ been used the derivatives of Eqs. (3-66) and (3-67) would have given $2\hat{N}/3\sigma b^2$ which does not contain N as a factor. In this situation a y average can be used. The average of the correction is divided by the average of N. In other words, Eq. (3-56) is integrated over y and divided by the y integral of N. For the quadratic shape $N = \hat{N}[1 - (y/b)^2]$ this process gives

$$\int_{-b}^{b} (2\hat{N}/3\sigma b^2)dy / \int_{-b}^{b} \hat{N}[1 - (y/b)^2]dy = 1/\sigma b^2 \qquad (3\text{-}70)$$

and the corrected total cross section is $\sigma[1 + 1/(\sigma b)^2]$.

3.4.3 Source Simplifications

Practically all source simplifications involve additional approximations. Computationally the most profitable are those simplifications which reduce the complexity of anisotropic scattering. Frequently, Eq. (3-25) is simply truncated after the L = 0 term to give Eq. (3-26). Some anisotropic scattering effects can be included within the framework of isotropic scattering by making the transport approximation. For within group scattering this approximation subtracts σ^s_{1gg} from σ_g and σ^s_{0gg}, while for group-to-group scattering a variety of recipes are available.[6] By including all scattering effects in isotropic cross sections, all the sums of Eq. (3-25) and the time consuming computation of Legendre flux moments are eliminated.

To insure iterative stability or to accelerate convergence it is sometimes useful to transpose terms to the source side of the equation. In the buckling correction made above the cross section correction is a true absorption which belongs on the loss side of the equation. But if a more complicated flux shape had been assumed, or if a pointwise correction had been made, the correction might have been negative. Then the negative correction, say σ^*NV, could have been transposed to the

source side of the equation. When terms are transposed to the source side of the equation the angular dependence of the flux is approximated by $N \sim \overline{N} + 3\mu I + 3\eta J + 3\xi K$ or higher orders of anisotropy if desired. This device can be used to define a modified transport theory by subtracting $V\sigma^{s}_{ogg}N$ from the left hand side of Eq. (3-9), thus changing the term $V\sigma N$ to $V\sigma^{a}N$, and subtracting $V\sigma^{s}_{ogg}(\overline{N} + 3\mu I + 3\eta J + 3\xi K)$ from the right hand side. This approximation removes from the source term side of Eq. (3-9) the isotropic component $V\sigma^{s}_{ogg}\overline{N}_g$ of in-group scattering (see Eq. (3-29)), which has certain advantages in numerical solutions as will become apparent later.

Inverse transpositions are also possible. If, say, the time absorption is very large, a portion of the source term might be moved to the left side of the equation to reduce the size of the collision term.

Finally, if the average velocity change per collision is small compared to group width, an age theory type assumption can be made, letting collision contributions to S come only from groups $g + 1$ and $g - 1$. Under these conditions, N_g should be redefined to be the number of neutrons per unit speed to allow within-group structure, i.e., derivatives with respect to speed.

3.5 Solution of Discrete Ordinates Equations

Equation (3-6), when written for curved geometry, is a very general statement of the neutron transport equation and can be used to describe very complicated problems. Because complicated problems can be

computationally time consuming, methods of solution must be efficient as well as sure and accurate. Thus, while some of the methods described below are based on mathematical and physical principles, other methods are selected on the pragmatic basis that they are the simplest rather than the most accurate. If it is felt that such considerations are in some sense a lowering of standards, it should be remembered that, as of early 1965, no general solution of the three space dimensioned transport equation has been attempted, and two-dimensional, time independent problems typically require a few hours on the fastest computing machines.*

The curved geometry form of Eq. (3-6) contains eleven fluxes

$$(N_{s+1} - N_s)V/v\Delta t + \mu(A_{i+1}N_{i+1} - A_iN_i) + \eta(B_{j+1}N_{j+1} - B_jN_j) + \\ + \xi(C_{k+1}N_{k+1} - C_kN_k) + (\alpha_{m+\frac{1}{2}}N_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}}N_{m-\frac{1}{2}})/w_m + \sigma NV = SV \qquad (3\text{-}55)$$

only five of which can be assumed known from calculations in adjoining cells, previous directions, or previous time steps. The additional flux equations which are necessary in order to solve Eq. (3-55) are provided by difference relationships.

3.5.1 Elementary Difference Methods

The "diamond" difference equations provide a particularly simple set of flux relationships. Requiring only continuity of $N_g(\underset{\sim}{r},\underset{\sim}{\Omega})$ for

*Even a very complex one-dimensional problem requires only a few minutes for solution.

application, these relations are

$$N_{s+1} + N_s = N_{i+1} + N_i = N_{j+1} + N_j = N_{k+1} + N_k = N_{m+\frac{1}{2}} + N_{m-\frac{1}{2}} = 2N \qquad (3\text{-}71)$$

and state simply that the arithmetic average of the cell "surface" averages is the average of N_g over the entire cell. These equations lead to a simple recursion relation for N and generally provide good accuracy relative to the computational effort involved.

If it is assumed that N_i, N_j, N_k, N_s, and $N_{m-\frac{1}{2}}$ are known, that is, if the calculation is proceeding in the direction of positive cosines, increasing time, and increasing direction index, then Eq. (3-71) is used to eliminate N_{i+1}, N_{j+1}, N_{k+1}, N_{s+1}, and $N_{m+\frac{1}{2}}$ from Eq. (3-55), which is then solved for N in terms of the known fluxes. Simple substitutions give

$$N = \frac{\mu A N_i + \eta B N_j + \xi C N_k + \alpha N_{m-\frac{1}{2}}/w + \tilde{\sigma} V N_s + SV}{2\mu A_{i+1} + 2\eta B_{j+1} + 2\xi C_{k+1} + 2\alpha_{m+\frac{1}{2}}/w + \tilde{\sigma} V + \sigma V} \qquad (3\text{-}72)$$

where $A = A_{i+1} + A_i$, $B = B_{j+1} + B_j$, $C = C_{k+1} + C_k$, $\alpha = \alpha_{m+\frac{1}{2}} + \alpha_{m-\frac{1}{2}}$, and $\tilde{\sigma} = 2/v\Delta t$. Since there is no curvature in the j and k directions $2B_{j+1} = B$ and $2C_{k+1} = C$. The curvature equation, Eq. (3-10), can be used to write

$$2\alpha_{m+\frac{1}{2}}/w = (\alpha_{m+\frac{1}{2}} + \alpha_{m-\frac{1}{2}})/w - \mu(A_{i+1} - A_i) \qquad (3\text{-}73)$$

which allows Eq. (3-72) to be expressed as

$$N = \frac{\mu A N_i + \eta B N_j + \xi C N_k + C N_{m-\frac{1}{2}}/w + \tilde{\sigma} V N_s + S V}{\mu A + \eta B + \xi C + \alpha/w + \tilde{\sigma} V + \sigma V} \qquad (3\text{-}74)$$

In the above form, N, the average flux in the cell, is the weighted average of all the flux sources in the cell.

Equation (3-74) is completely general except that additional curvature terms may be needed. Such terms can be added by inspection. The specialization of Eq. (3-74) for systems of reduced dimensionality is accomplished by removing terms. For example, the form applicable to time independent problems is obtained by letting $\tilde{\sigma} = 0$. Computationally, the relation of Eq. (3-74) is advantageous because many of the same coefficients appear twice and portions of these can be precomputed. Further simplification is obtained by dividing each term of the numerator and denominator by V, remembering that α is proportional to area elements in the i direction.

Once N is determined from Eq. (3-74), the remaining unknowns are found from Eq. (3-71). These fluxes are then used as inputs for the next time-space-direction cell, and solution proceeds recursively. Iterative solution is required only because S depends on N. For accuracy in calculation, the ordering of the progression from cell to cell must be such that no cancellation occurs in the denominator of Eq. (3-74). The strategy employed to avoid cancellation is described in Section 3.6 below.

If evaluation of fluxes is proceeding in the negative ξ direction the appropriate recursion equation for N is obtained by replacing ξ by $-\xi$ and N_k by N_{k+1}. Similarly if η is negative η is replaced by $-\eta$ and N_{j+1} by N_j; while if both directions are negative, both replacements are made, and so forth for all combinations of direction cosines. These replacements are simply the result of using Eq. (3-71) in Eq. (3-55) to solve for N. In contrast to spatial directional evaluation, progression on the m index can be ordered so that $N_{m-\frac{1}{2}}$ always appears in the recursion relation, while time evaluation naturally proceeds in the direction of increasing time. Thus, actual calculations can be performed with a single recursion relation, using magnitudes of direction cosines and entering the formula with appropriate fluxes.

While initial values of the spatially dependent fluxes are given by boundary conditions and initial conditions supply the first values of the time dependent flux, some initial values of $N_{m-\frac{1}{2}}$ are needed when the geometry is curved. These values are found by examining Eq. (3-55) in directions in which there is no angular redistribution. In one-dimensional spherical geometry, as can be seen from Eq. (3-30), $\mu = -1$ is a direction in which the angular derivative vanishes and is also a direction suitable for initiating a recursive solution beginning at the outer boundary of a sphere. In the other curved geometries described in Table III-1 several starting directions are needed. With the angular orientations of Fig. III-2, these directions correspond to $\eta = 0$, $\tilde{\mu}_i = (1 - \xi_i^2)^{\frac{1}{2}}$; $i = 1,2,\ldots,n/2$. In order that these special directions not affect

symmetries of a quadrature set, they are assigned zero weight. For these directions, then, $N_{m+\frac{1}{2}} = N_{m-\frac{1}{2}}$; and from the diamond difference relations, $N_{m+\frac{1}{2}} = (N_i + N_{i+1})/2$. Also for these directions, $\alpha_{m-\frac{1}{2}} = 0$; and as w_m approaches zero, Eq. (3-10) gives

$$\alpha_{m+\frac{1}{2}}/w_m = -\mu_m(A_{i+1} - A_i) \tag{3-75}$$

Thus, for these special directions, the curvature term is

$$(\alpha_{m+\frac{1}{2}}N_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}}N_{m-\frac{1}{2}})/w_m = \mu_m(A_i - A_{i+1})(N_{i+1} + N_i)/2 \tag{3-76}$$

which, when combined with the similar term in Eq. (3-55), gives

$$\begin{aligned}(N_{s+1} - N_s)\, V/v\Delta t + \mu A(N_{i+1} - N_i)/2 + \eta(B_{j+1}N_{j+1} - B_jN_j) + \\ + \xi(C_{k+1}N_{k+1} - C_kN_k) + \sigma NV = SV\end{aligned} \tag{3-77}$$

A recursion relation for N obtained from this equation differs from Eq. (3-74) only in the absence of the α terms. Hence, in practice, Eq. (3-74) is used in all cases, with zero α for the special directions.

The special initial recursion relation can be eliminated by employing less accurate difference relations. The relatively crude "step function" relations assume that N is constant over the mesh cell. That is, the unknown boundary N's are assumed to equal the average flux in the cell. For μ, η, and ξ positive these relations are

$$N = N_{i+1} = N_{j+1} = N_{k+1} = N_{s+1} = N_{m+\frac{1}{2}} \tag{3-78}$$

Substituting these in Eq. (3-55) gives

$$N_{i+1} = \frac{\mu A_i N_i + \eta B_j N_j + \xi C_k N_k + \alpha_{m-\frac{1}{2}} N_{m-\frac{1}{2}}/w_m + VN_s/v\Delta t + VS}{\mu A_{i+1} + \eta B_{j+1} + \xi C_{k+1} + \alpha_{m+\frac{1}{2}}/w_m + V/v\Delta t + V\sigma} \qquad (3\text{-}79)$$

Since for the special directions in curved geometries $\alpha_{m-\frac{1}{2}} = 0$, the above recursion relation is applicable for all geometries. As in the case of diamond model difference scheme, proper directional evaluation of Eq. (3-79) insures that the terms of the numerator and denominator remain positive and hence that unfortunate cancellations do not occur.*

Both Eq. (3-74) and Eq. (3-79) have the property that individual terms correspond to quantities which, physically, are positive. If the diamond difference scheme is solved for a recursion for N_{i+1}, as was originally done, this valuable property is lost. With some negative terms in the numerator, the relation occasionally led to flux oscillations and an incorrect estimate of the worth of the diamond difference method. However, Eq. (3-74) has been found to be both reliable and accurate. In general, its accuracy and simplicity have warranted its use in preference to the step function recursion relation.

*The special directions and associated evaluations can also be avoided by determining $N_{m+\frac{1}{2}, i+\frac{1}{2}}$, when no $N_{m-\frac{1}{2}, i+\frac{1}{2}}$ is available, from $N_{m, i+\frac{1}{2}}$ and $\bar{N}_{i+\frac{1}{2}}$ by linear interpolation. This procedure has so far only been explored in the case of modified transport theory and n = 2 which in one space dimension is equivalent to diffusion theory. See Section 3.5.4.

3.5.2 More General Difference Relations

It is possible to make various ad hoc combinations of step and diamond difference schemes or to use weighted diamond relationships such as $aN_{i+1} + (1-a)N_i = N$. However, a more fruitful, albeit only partially explored, possibility is to use functional relationships for the flux $\psi(\underline{r}, \underline{\Omega}, t)$ and obtain difference relations by applying the definitions of cell averages. Suppose that $\psi = \psi(x, \mu)$ only and that, in the cell shown in Fig. III-5, ψ is represented by, including

Fig. III-5

centered subscripts,

$$\psi(x,\mu) = \psi_{m,i+\frac{1}{2}} + (\psi_{m,i+\frac{1}{2}} - \psi_{m,i})(x-\bar{x})/(\bar{x}-x_i) + \tag{3-80}$$

$$+ \frac{(\psi_{m,i+\frac{1}{2}} - \psi_{m-\frac{1}{2},i+\frac{1}{2}})(\mu - \bar{\mu})}{(\bar{\mu} - \mu_{m-\frac{1}{2}})} \left[1 - \frac{3(\mu_{m+\frac{1}{2}} + \mu_{m-\frac{1}{2}} - 2\bar{\mu})(\mu - \mu_{m-\frac{1}{2}})}{(2\mu_{m+\frac{1}{2}} + \mu_{m-\frac{1}{2}} - 3\bar{\mu})(\mu_{m+\frac{1}{2}} - \mu_{m-\frac{1}{2}})}\right]$$

The above is an expression, linear in x and quadratic in μ, that assumes the value $\psi_{m,i}$ at $x = x_i$, $\mu = \bar{\mu}$; the value $\psi_{m-\frac{1}{2},i+\frac{1}{2}}$ at $x = \bar{x}$, $\mu = \mu_{m-\frac{1}{2}}$; and the value $\psi_{m,i+\frac{1}{2}}$ at $x = \bar{x}$, $\mu = \bar{\mu}$. Further, if $\bar{x} = (x_{i+1} + x_i)/2$ the x and μ averages of Eq. (3-80), as defined in Section 3.1.2, are given simply by $N_{m,i+\frac{1}{2}} = \psi_{m,i+\frac{1}{2}}$, $N_{m,i} = \psi_{m,i}$, and $N_{m-\frac{1}{2},i+\frac{1}{2}} = \psi_{m-\frac{1}{2},i+\frac{1}{2}}$. For example, $N_{m,i+\frac{1}{2}}$ is defined by

$$N_{m,i+\frac{1}{2}} = \int_{x_i}^{x_{i+1}} \int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} \psi(x,\mu)\,d\mu\,dx \Big/ \int_{x_i}^{x_{i+1}} \int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} d\mu\,dx \tag{3-81}$$

and the result of this average of Eq. (3-80) is $\psi_{m,i+\frac{1}{2}}$. Now with $\psi(x,\mu)$ given by Eq. (3-80) the μ average of $\psi(x_{i+1},\mu)$, which by definition is $N_{m,i+1}$ gives $N_{m,i+1} = 2\psi_{m,i+\frac{1}{2}} - \psi_{m,i}$ or $N_{m,i+1} + N_{m,i} = 2N_{m,i+\frac{1}{2}}$, which is a diamond difference relation. However, the x average of $\psi(x,\mu_{m+\frac{1}{2}})$, $N_{m+\frac{1}{2},i+\frac{1}{2}}$, gives $N_{m+\frac{1}{2},i+\frac{1}{2}} + \alpha N_{m-\frac{1}{2},i+\frac{1}{2}} = (1+\alpha)N_{m,i+\frac{1}{2}}$ where

$$\alpha = \frac{(\mu_{m+\frac{1}{2}} - \bar{\mu})(\mu_{m+\frac{1}{2}} + 2\mu_{m-\frac{1}{2}} - 3\bar{\mu})}{(\mu_{m-\frac{1}{2}} - \bar{\mu})(2\mu_{m+\frac{1}{2}} + \mu_{m-\frac{1}{2}} - 3\bar{\mu})} \tag{3-82}$$

Equation (3-82) is a weighted diamond difference relation. If $\bar{\mu}$ is taken to be $(\mu_{m+\frac{1}{2}} + a\mu_{m-\frac{1}{2}})/(a+1)$, α is $a(2-a)/(2a-1)$, and the weighting choice is dependent upon the selection of an average cosine. This cosine may be selected arbitrarily, or alternatively, it may be determined by substituting Eq. (3-80) in the applicable analytic transport equation and requiring, say, that the μ average of the equation is satisfied at some point in the cell.

Clearly, ψ representations more complicated than Eq. (3-80) can be used and more conditions satisfied. For instance, a flux form matching known fluxes at the three corners of the cell could be used to find expressions for the cell average and remaining corner fluxes. Higher polynomial relations can be assumed so that, in addition to boundary fluxes, other conditions are matched. However, the resulting difference and recursion relations quickly become more complicated than

the diamond scheme, and such methods have not been tested. There is undoubtedly a balance point at which benefits due to increased accuracy are offset by increased computational effort. Even with the diamond difference assumption, choice of spatial mesh size is frequently dictated by the requirement of resolving spatial detail rather than by the requirement of accuracy.

3.5.3 Simplifications in One Space Dimension

As mentioned above, iterative solution of the recursion relation of Eq. (3-74) is required because S depends upon N. In one-dimensional problems Eq. (3-9) becomes

$$\mu(A_{i+1}N_{i+1} - A_iN_i) + (\alpha_{m+\frac{1}{2}}N_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}}N_{m-\frac{1}{2}})/w + \sigma NV = SV \qquad (3\text{-}83)$$

with subscripts i and m only. It is possible to transform Eq. (3-83) to a set of equations which, at each space point, may be solved, once and for all, for N_m by a form of matrix inversion.[7,8] The transformation is necessary to insure numerical stability and is similar to the one described below for solution of the diffusion equations. Whether or not this special form of solution involves fewer numerical operations than direct iteration is an unexplored question.

In diffusion theory approximations the in-group flux terms of the source can be subtracted from similar terms on the loss side of the equation so that no in-group iteration is needed. In one space dimension the resulting equations are, from Eqs. (3-56) and (3-61),

$$A_{i+1}I_{i+1} - A_iI_i + (\sigma - \sigma^s_{ogg})NV = (\bar{S} - \sigma^s_{ogg}\bar{N})V$$

$$A(\bar{N}_{i+1} - \bar{N}_i)/6 + (\sigma - \sigma^s_{1gg})IV = (S_I - \sigma^s_{1gg}I)V \qquad (3\text{-}84)$$

where the source terms no longer contain $\bar{N}$ or I for the group (except for the possibility of isotropic fission, $\nu\sigma^f\bar{N}$, which is handled as a separate, outer, iteration). By using the diamond difference equations $2\bar{N} = \bar{N}_{i+1} + \bar{N}_i$ and $2I = I_{i+1} + I_i$ it is possible to write recursion relations for $\bar{N}$ and I. Unfortunately, these equations are not numerically stable with respect to round-off error. However, rewriting equations in terms of two unknowns p and q such that

$$I_\ell = p_\ell\bar{N}_\ell - q_\ell, \qquad \ell = i \text{ or } i+1 \qquad (3\text{-}85)$$

leads to stable recursion relations for p and q. These relations are found by substituting Eq. (3-85), $\ell = i+1$, into Eq. (3-84) in which I and $\bar{N}$ are replaced by their diamond difference equivalents. Then, eliminating $\bar{N}_{i+1}$ from the two resulting equations gives an equation of the form $I_i = fN_i - g$. Equating f and g to p and q of Eq. (3-85) gives

$$p_i = [p_{i+1}(AA_{i+1} + \sigma_o\sigma_1) + 2A\sigma_o]/(p_{i+1}A\sigma_1 + AA_i + \sigma_1\sigma_o)$$

$$q_i = [q_{i+1}(AA_{i+1} - \sigma_o\sigma_1) + S_o(A + \sigma_1p_{i+1}) - S_1(A_{i+1}p_{i+1} + \sigma_o)]/ \qquad (3\text{-}86)$$

$$/(p_{i+1}A\sigma_1 + AA_i + \sigma_1\sigma_o)$$

where the abbreviations

$$\sigma_o = (\sigma - \sigma^s_{ogg})V/2, \qquad \sigma_1 = 3(\sigma - \sigma^s_{1gg})V$$
$$S_o = (\bar{S} - \sigma^s_{ogg}\bar{N})V, \qquad S_1 = 6(S_I - \sigma^s_{1gg}I)V \tag{3-87}$$

are used. The numerically stable recursion relations of Eq. (3-86) are applied by starting at an outer boundary where q_{i+1} and p_{i+1} are given by boundary conditions. Computation proceeds recursively until the inner boundary is reached. At the inner boundary $\bar{N}_i$ is determined by boundary conditions and then computed for increasing i from the relation

$$\bar{N}_{i+1} = [(A_i p_{i+1} - \sigma_o)\bar{N}_i + A_{i+1}q_{i+1} - A_i q_i + S_o]/(A_{i+1}p_{i+1} + \sigma_o) \tag{3-88}$$

which is obtained from the first equation of (3-84) by using Eq. (3-85) to eliminate I_i and I_{i+1}. At the same time $\bar{N}$ is computed I is calculated from Eq. (3-85).

In terms of an albedo, $0 \leq r \leq 1$, and the ratio $\beta = (1-r)/(1+r)\sqrt{3}$, the inner boundary condition is $I = -\beta N$ and the outer boundary condition is $I = \beta N$ where I, N, and β are evaluated at the appropriate boundary. From Eq. (3-85), boundary conditions become

$$p = \beta \quad q = 0, \qquad \text{outer boundary}$$
$$\bar{N} = q/(p + \beta), \qquad \text{inner boundary} \tag{3-89}$$

The transformation of Eq. (3-85) is a reflection principle, similar to that introduced in the technique of invariant imbedding, which is used to establish a relationship between the incoming and outgoing neutron flow. By its application, solution of the diffusion equations is reduced to a two-pass traverse of the system, an incoming pass to find p and q and an outgoing pass to find I and $\overline{N}$. If the principle is applied directly to the discrete ordinates form of the transport equation,[8] Eq. (3-85) becomes a vector-matrix relationship; and, as mentioned above, the question of matrix inversion time arises. Unfortunately, no way has been found to apply the principle to multi-dimensional problems. However, in two dimensions, say, the three diffusion equations (one flux and two current equations) can be treated as two pairs of one-dimensional equations. First the J currents can be assumed known while the flux and I current equations are solved as above. Then, using the latest values of $\overline{N}$ and I, the flux and J current equations can be solved as a separate one-dimensional pair, etc. This process, in effect a detailed buckling iteration, was examined for efficiency in several simple two-dimensional problems. Compared to solutions of the second order differential diffusion equations it was found to be considerably faster; however, the method was only comparable in speed to iteration of the S_2 transport equations which, as mentioned in Section 3.4.1, contain more information and are presumably more accurate.

3.5.4 Diffusion Theory Solutions Within the Framework of Transport Theory

One argument for using diffusion theory solutions is that diffusion theory gives accurate results in energy groups where transport theory solutions are slowly converging. To overcome this slow convergence, diffusion theory solutions are often used selectively, by energy group, or in the early phases of a computation. A method of diffusion theory solution that is applicable to all geometrical dimensionalities and that fits within the framework of the transport theory solutions previously described is the following. For notational clarity the discrete ordinates equation, Eq. (3-55), is written for one-dimensional spherical geometry assuming a single incoming and a single outgoing direction. Letting $\mu = 1/\sqrt{3}$ and letting $\bar{N}$ denote the incoming directional flux the incoming flux equation is

$$-\mu A_{i+1}\bar{N}_{i+1} + \mu A_i \bar{N}_i + \mu(A_{i+1} - A_i)N + \sigma^r \bar{N} V = \\ = V(\bar{Q} + F + 3\mu\tilde{\sigma}J) \tag{3-90}$$

The average flux N and the current J are defined, in terms of $\bar{N}$ and the outgoing flux, N^+, by

$$N = (N^+ + \bar{N})/2 \quad J = \mu(N^+ - \bar{N})/2 \tag{3-91}$$

and hence

$$N = \bar{N} + 3\mu J \tag{3-92}$$

This last equation was used to transpose $\sigma^s_{ogg}\bar{N}V$ ($\sigma^r + \sigma^s_{ogg} = \sigma$) from the left to the right side of the equation so that $\tilde{\sigma} = \sigma^s_{ogg} - \sigma^s_{lgg}$. $\bar{Q}$ is the incoming component of external sources, here including sources external to the group. The curvature term is represented in the same approximation as in the derivation of diffusion theory. Using Eq. (3-92) and the diamond relation $2\bar{N} = \bar{N}_i + \bar{N}_{i+1}$ in Eq. (3-90) gives the recursion for the incoming flux

$$\bar{N} = \frac{\mu A \bar{N}_{i+1} - (A_{i+1} - A_i)J^o + V(\bar{Q} + F + 3\mu\tilde{\sigma}J^o)}{\mu A + \sigma^r V} \qquad (3\text{-}93)$$

Above, J is given a superscript to indicate that previous information is needed to compute the current and that iteration is necessary. For the outgoing flux

$$\mu A_{i+1}N^+_{i+1} - \mu A_i N^+_{i+1} - \mu(A_{i+1} - A_i)N + \sigma^r V N^+ = V(Q^+ + F - 3\mu\tilde{\sigma}J) \qquad (3\text{-}94)$$

The same substitutions as for the incoming flux give

$$N^+ = \frac{\mu A N^+_i + (A_{i+1} - A_i)(\mu\bar{N} + J^o) + V(Q^+ + F - 3\mu\tilde{\sigma}J^o)}{2\mu A_{i+1} + \sigma^r V} \qquad (3\text{-}95)$$

Iteration solution of Eqs. (3-93) and (3-95) is begun by assuming a value of J^o, traversing inward to compute $\bar{N}$ and outward to compute N^+. From these values, the current is recomputed to repeat the calculations.

The recursion relations above are very similar to Eq. (3-74) and can easily be imbedded within that transport theory formula so that selective diffusion theory solution is feasible. The sum of Eqs. (3-94) and (3-90) give the neutron balance equation despite the fact that J^{o} depends upon previous information. Because Eq. (3-92) was used to form each recursion, the solutions also satisfy neutron balance, and no extra effort is needed to guarantee that balance is maintained* (cf. the subject of scaling, Section 3.7.1).

3.6 Principles of Solution Evaluation

Once a set of recursion relations is decided upon, every effort is used to insure that they are accurately evaluated. The desirability of obtaining relations with positive numerator and denominator terms has already been emphasized. Two other aids to accurate computation are the use of negative flux fix-ups and the application of the principle of directional evaluation.

3.6.1 Directional Evaluation - Following the Neutron Flow

Accuracy is generally improved if the coupling among fluxes is relatively weak, that is, if the recursion relation represents an attenuation relation. The idea here is that if effects of far distant fluxes (fluxes separated by many indices) are important, they must be

*Had $N = N^{+} - 3\mu J$ been used to form the recursion for N^{+} symmetrical formulae would have been obtained but neutron balance would have been sacrificed.

passed, by many successive calculations, to the point of interest, decreasing accuracy. Physically, attenuation relations are obtained by following neutron flows. Spatially, the neutron flux is attenuated most in those directions of most nearly directly inward or outward flow. Hence, it is advisable to begin calculation in the most inward (to begin with outer boundary conditions) direction and then to proceed smoothly to the next most inward direction. By proceeding in this fashion an inward spatial traverse is made for all incoming directions before inner boundary conditions are imposed and the outward traverse is begun. In several dimensions the procedure is more complicated, but the principle is the same. For illustration consider a cube in the first octant of a rectangular coordinate system with the back bottom left corner at the origin. Here calculation is begun at the front top right corner with μ, η, and ξ negative. Then, beginning with the most negative μ, η, and ξ an inward x traverse is made along the front top edge. With fixed η and ξ, inward traverses are made along this edge until all negative μ are covered, and then outward traverses are made for each positive μ. Next, with an inward and outward series of traverses for negative and positive μ on each z level, a downward traverse is made along the front face successively following all negative ξ flow. In turn an upward z traverse is made, again traversing inward and outward directions. Finally the inward-outward y traverse is begun with x and z traverses in each plane parallel to the front surface. Such a procedure entails eight major sweeps through the directional mesh, one sweep for each octant of directions.

As implied by the above, directional evaluation along uniformly changing values of direction cosines is also important. In one-dimensional plane geometry for instance, each direction is independent of the other and the order of directional solution is conceptually immaterial. In practice, however, the flux at $\mu = -1$ can be very different than the flux at $\mu = 0$, say; and by proceeding $\mu = -1, 0, -0.9\ldots$ rather than in the order $\mu = -1, -0.9\ldots 0, \ldots$ flux oscillations can be introduced.

In energy also, solution is guided by neutron flow. Since slowing down neutron flows are most frequent, calculations are customarily begun at the highest neutron speeds. Then, a maximum amount of fresh information is passed from group-to-group, and the effects of absorption attenuation enhance accuracy.

3.6.2 Flux and Source Fix-ups

Even if all the terms of Eq. (3-74) are positive, insuring a successful calculation of N, the use of the difference equations (3-71) to extrapolate across a mesh cell may produce negative fluxes. These values used as input to adjoining cells may then result in catastrophic oscillations in or negative values of the scalar flux. In practice these situations usually arise when cross sections are large or inadequate spatial resolution is used (too many mean free paths per cell width), but sometimes occur in the early stages of calculations when the flux is grossly in error. To prevent the propagation of these

negative values, flux fix-up routines are used. On the physical grounds that fluxes are always non-negative and that a negative N_{i+1}, N_{j+1}, N_{k+1}, N_{s+1}, $N_{m+\frac{1}{2}}$ is merely the result of an over-enthusiastic extrapolation, the offending flux is set equal to zero. Then a new recursion relation, obtained from Eq. (3-55) by equating the previously negative flux to zero,* is used to recompute the remaining fluxes. These are again tested for positivity and corrected, if necessary. If more than one flux is at first negative, only one negative flux is set to zero before recomputing, hoping that recomputation will improve all remaining fluxes. This procedure is continued until all fluxes are either positive or zero. This method, which requires several different recursion relations to cover all possibilities, has successfully prevented negative fluxes in situations where previous, simpler recipes have failed. In addition, the method has been tested in a consistent manner. In a plane slab critical calculation a normal computation produced no negative fluxes and gave a known result. When the direction cosines were re-ordered, negative fluxes occurred, but these were corrected by fix-up routines to give the same known answer.

Although all the terms of Eq. (3-74) are normally positive, situations arise when either the source or total cross section may be negative. Cross sections may be negative due to time absorption or buckling corrections, (n,2n) reactions treated as negative absorption, or whimsical

*This procedure ensures that neutron conservation is maintained.

use of cross section recipes. Sources may be negative due to anisotropic scattering approximations. For instance, if the source is represented by a linear anisotropic expansion, $S = S_o + 3\mu S_1$, S_1 may be large enough to force S negative for some values of μ. While a negative source may sometimes be tolerated because it may be overwhelmed by the remaining terms of the numerator of Eq. (3-74), the negative cross section is more dangerous. Both negative sources and cross sections are eliminated by transpositions of the type discussed in Section 3.4.3.

3.7 Iteration Cycles and Convergence Criteria

3.7.1 Inner Iterations

The cycle of calculations in a given group in which the within group (self-scattering) collision source is successively recomputed is termed inner iteration. Based on the best available information, the within group source is computed and then a complete traverse, through all directions and space cells, is made to compute the angular flux. This process is, by definition, one inner iteration.

The iterative process is terminated when two successive self-scattering sources differ, by some established criterion, by less than a prescribed amount. Convergence is accelerated and system wide neutron conservation is insured by a process known as scaling. The neutron balance equation, obtained by multiplying Eq. (3-55) by w_m and summing over m, is

$$A_{i+1}I_{i+1} - A_iI_i + B_{j+1}J_{j+1} - B_jJ_j + C_{k+1}K_{k+1} - C_kK_k +$$

$$+ (\sigma^r + \sigma^s_{ogg})\bar{N}V = (S' + \sigma^s_{ogg}\bar{N}^p)V \qquad (3\text{-}96)$$

Above, $\sigma^r + \sigma^s_{ogg} = \sigma$ and $S = S' + \sigma^s_{ogg}\bar{N}^p$. On the right $\bar{N}^p$ indicates that this flux is a previous value; and were it not for this fact, Eq. (3-96) would be an exact statement of neutron balance. The difference between the actual collision source and the correct collision source represents an error in the form of a false source. By introducing a scale factor f as a parameter, the flux level over the whole system can be adjusted so that, over the system, the false source is zero. Multiplying Eq. (3-96) by f and rearranging the source terms gives

$$f[A_{i+1}I_{i+1} - A_iI_i + B_{j+1}J_{j+1} - B_jJ_j + C_{k+1}K_{k+1} - C_kK_k + (\sigma^r + \sigma^s_{ogg})NV] =$$

$$= f\,\sigma^s_{ogg}\bar{N}V + VS' + f\sigma^s_{ogg}(\bar{N}^p - \bar{N})V + (f-1)S'V \qquad (3\text{-}97)$$

If the only terms on the right of this equation were $f\sigma^s_{ogg}\bar{N}V + S'V$, then the equation would be an exact statement of balance for a flux level fN and the correct fixed source VS'. Thus, if f is chosen so that the remaining terms vanish, neutron conservation is assured. However, with a single constant f, the best that can be done is to satisfy one condition, say to make the system average of the additional source terms vanish, i.e., let

$$\sum_R [f\,\sigma^s_{ogg}(\bar{N}^p - \bar{N}) + (f-1)S']V = 0 \qquad (3\text{-}98)$$

or, choose f according to

$$f = \sum_R S'V / \sum_R [\sigma^s_{ogg}(\bar{N}^p - \bar{N}) + S']V \qquad (3\text{-}99)$$

where R denotes summation over all cells. The scale factor of Eq. (3-99) is used to adjust all fluxes before beginning another inner iteration. As $\sum_R \sigma^s_{ogg}\bar{N}V$ approaches $\sum_R \sigma^s_{ogg}\bar{N}^pV$, f approaches unity. At the expense of more complicated equation solving, additional scaling unknowns could be introduced to guarantee neutron conservation within system subdivisions. Generalizations of the scaling process have not been widely explored.

Based on the scaling process a possible convergence criterion is that iteration be terminated when the false source is small, i.e., when

$$\left|\sum_R \sigma^s_{ogg}(\bar{N} - \bar{N}^p)V\right| < \epsilon S^p_{avg} \qquad (3\text{-}100)$$

where S^p_{avg} is the average non-collision source per group, determined by dividing the total system source (based on previous information) by the number of groups, and ϵ is a specified convergence precision. A related test is to require that

$$\sum_{R=1}^{H} \sigma^s_{ogg}\,|\bar{N} - \bar{N}^p|V < \epsilon\sqrt{HS^p_{avg}} \qquad (3\text{-}101)$$

where the more stringent condition on the left is balanced by the statistical relaxation on the right, H being the total number of space cells. Both of the above tests are volume weighted averages of errors and tend to emphasize errors in large cells and neglect errors in small cells. Generally this emphasis is the one of interest; but occasionally the detailed behavior of the flux is important, and then the very stringent test

$$\underset{\text{over R}}{\text{Max}} \quad |1 - \bar{N}/\bar{N}^{p}| < \epsilon \tag{3-102}$$

should be used.

3.7.2 Outer Iterations

Once inner convergence is obtained in the first group, the calculation proceeds to the second group. The cycle of calculation which obtains converged inner solutions for all groups, beginning with group one and ending with group G, is termed an outer iteration. In this cycle of iteration collision and fission sources are recomputed. The down scattering source can be computed for all lower energy groups as soon as an inner iteration is finished, but upscattering collision sources and the fission source cannot be computed until an outer iteration is finished. If there is no upscatter or fission source (implying that an external source must exist in at least the first group) one outer iteration concludes the calculation. If, however, fission or

upscattering sources are present, the total source must be recomputed after an outer iteration, and the outer iterative process must be continued until sources stabilize.

The upscattering source is an implicit source analogous to the in-group scattering source of inner iteration, and a similar scaling procedure can be used to accelerate convergence and insure neutron conservation in the mean. A scaling condition is obtained from the balance equation for the whole system, i.e., from Eq. (3-96) summed over all groups

$$\sum_g (L_{g,R} + \sigma_g \bar{N}_g V) = \sum_g VS_g \tag{3-103}$$

For brevity all the current terms are symbolized by L, for leakage. Now from the definition of the source term, Eq. (3-29),

$$\sum_{g=1}^{G} VS_g = \sum_{g=1}^{G} V\left(Q_g + \chi_g \sum_{h=1}^{G} \nu\sigma_h^f \bar{N}_h + \sum_{h=1}^{G} \sigma_{ogh}^s \bar{N}_h\right) \tag{3-104}$$

where the anisotropic collision terms vanish in the m sum made to form Eq. (3-96) and Q_g is the isotropic component of the external source. From the definition of differential scattering cross sections

$$\begin{aligned} \sigma_g &= \sigma_g^a + \sum_{h=1}^{G} \sigma_{ohg}^s = \\ &= \sigma_g^a + \sum_{h<g} \sigma_{ohg}^s + \sigma_{ogg}^s + \sum_{h>g} \sigma_{ohg}^s \equiv \\ &\equiv \sigma_g^a + \sigma_g^d + \sigma_{ogg}^s + \sigma_g^u \end{aligned} \tag{3-105}$$

where the superscripts d and u refer to down and up scattering. With these definitions Eq. (3-103) becomes

$$\sum_{g=1}^{G} [L_{g,R} + (\sigma_g^u + \sigma_g^d + \sigma_{ogg}^s + \sigma_g^u)\bar{N}_g V] = \tag{3-106}$$

$$= \sum_{g=1}^{G} V(Q_g + \chi_g F^p) + \sum_{h=1}^{G} V(\sigma_h^d \bar{N}_h + \sigma_{ohh}^s \bar{N}_h + \sigma^u \bar{N}_h^p)$$

where, again, p indicates that fission and upscatter sources depend on previous information. Now if Eq. (3-106) is summed over all cells, the self-scatter terms cancel since the volume average of the self scatter terms was made equal by inner iteration. The down scatter terms also vanish because the same $\bar{N}$ is used to compute each. Then, except for upscatter imbalance, Eq. (3-106) states that the system leakage and absorption equals the system source:

$$\sum_{g,R} [L_{g,R} + (\sigma_g^a + \sigma_g^u)\bar{N}_g V] = \sum_{g,R} (\sigma^u \bar{N}_g^p + Q_g)V + \sum_R F^p V \tag{3-107}$$

Above, the fission spectrum normalization was used to perform the g sum of the fission source. From Eq. (3-107) an upscatter scale factor is determined as for inner iteration,

$$f_{up} = \sum_R V(F^p + \sum_g Q_g)/\sum_R V\{F^p + \sum_g [Q_g + \sigma_g^u(\bar{N}_g^p - \bar{N}_g)]\} \tag{3-108}$$

As with self-scatter scaling, more complicated recipes might be applied to effect balance over sub-portions of the whole system.

Convergence tests for upscattering are analogous to those of Eqs. (3-100) and (3-101):

$$\left| \sum_{g,R} V\sigma_g^u (\bar{N}_g^p - \bar{N}_g) \right| < \epsilon \sum_R V\left(F^p + \sum_g Q_g\right) = \epsilon S_{TOT} \tag{3-109}$$

and

$$\sum_{g,R} V\sigma_g^u \left| \bar{N}_g^p - \bar{N}_g \right| < \epsilon \sqrt{GHS_{TOT}} \tag{3-110}$$

If there is no external source, the total fission source is normalized to a specified level, and all flux data are made consistent with this normalization. After an outer iteration the fission source is recomputed, and the ratio

$$\lambda = \left(\sum_R VF\right) / \left(\sum_R VF^p\right) \tag{3-111}$$

is calculated before the fission source and flux are renormalized. λ is the multiplication ratio. Before each succeeding outer iteration the fission spectrum is multiplied by $1/\lambda$ so that λ tends towards unity as iteration proceeds. In these terms the system multiplication constant is the product of the successive λ. Convergence of λ is deemed sufficient when

$$\left| \lambda - \lambda^p \right| < \epsilon \tag{3-112}$$

and when

$$\sum_{R} V \left| F - \lambda^{p} F^{p} \right| < \epsilon \sqrt{HS_{avg}} \qquad (3\text{-}113)$$

where S_{avg} is the average total source in the group (as in Eq. (3-100)) and can, in a subcritical system, contain an external source as well as fission.

After both upscatter and fission convergence tests are passed the outer iteration cycle is terminated. However, the calculation itself may not be finished. Although the procedures so far described are sufficient for source and criticality problems, more sophisticated problems may be posed.

3.7.3 Parametric Eigenvalue Searches

Once an outer iteration cycle is converged, an alteration of the system may be made, by adjusting suitable parameters, in an attempt to achieve a given multiplication level, usually criticality. Parameters customarily altered are system dimensions (whole-system or zone), time absorption, or material composition. In each case an iterative search, involving a sequence of converged outer iteration cycles, is necessary to find that value of the varied parameter which gives the desired multiplication. At this point in the iterative process, every effort must be made to accelerate convergence since each converged outer cycle may be very time consuming. Alternately, the time required for outer solutions may be reduced by relaxing outer solution convergence criteria. That is, in a critical thickness calculation obtaining an outer solution to

six significant digits is wasted effort if the system dimensions are yet to be modified by large amounts. A related method which has been successful in reducing total iteration time uses artificial restriction of the number of inner iterations until the eigenvalue sought has converged to within, say, ten times the specified accuracy. This restriction is based on the philosophy that early values of inner solutions need not be extremely precise to give reasonable values of integral parameters such as the multiplication, and that precision is most efficiently obtained when the entire calculation is nearly complete. In practice this strategy has materially shortened computation times. Usually it is found that by the time the parametric eigenvalue has converged to within ten times specified accuracy, inner iteration values have already been obtained very accurately.

The search for parametric eigenvalues is usually made by parabolic or linear extrapolation/interpolation. However, when convergence is nearly complete, the numerical derivatives involved may become unreliable. This difficulty is overcome by fixing the slope when λ is within a specified distance of unity. Iteration is terminated at that value of the parametric eigenvalue for which λ is within ϵ of unity.

3.7.4 Implicit Boundary Conditions

While the boundary condition of no incoming flux is easily satisfied by using zero values of the flux for incoming directions at the boundary, more complicated boundary conditions require iterative solution.

For instance, a reflective boundary condition on the right of a plane slab requires that the incoming flux in each direction be equal to the outgoing flux in the reflected direction, i.e., the direction with the same magnitude of direction cosine. Because the calculation proceeds by following the flux flow from the right to the left for incoming directions and then from left to right for outgoing directions, the outgoing flux on the right depends upon the modification, by an entire sequence of calculations, of the right boundary incoming flux. Thus, with a reflective boundary condition, inner iteration must continue until incoming and outgoing fluxes match in detail as well as until the false within group scatter source converges. Unfortunately, the angular flux is, of all the fluxes, the least smoothed by integrating processes and is the most susceptible to oscillations. Thus, unless convergence is accelerated or unless a less stringent boundary convergence test is made, a reflective outer boundary is likely to require lengthy iteration. One method of improving the rate of convergence utilizes the linearity of the Boltzmann equation. First, one inward-outward pass is made in which the inward directed flux on the right is taken to be, in detail, the last available right boundary outgoing flux. Then, before normal inner iteration control tests are made, the outgoing flux from this computation is used as an incoming flux source for another inward-outward pass. The second pass is made with all other sources set equal to zero. Next, a multiple of the second solution is added to the first solution in such a way that the total right current is zero. Normal

inner iteration procedures are executed on the combined results of each set of two passes. Rather than insist on detailed agreement between ingoing and outgoing fluxes, this iterative process may be terminated when the right current is zero (within ϵ) after the first of the two inward-outward passes.

Other implicit boundary conditions can be handled in a similar fashion. The "white" boundary condition is an isotropic return condition; i.e., the incoming partial current is made up of equal angular components. In this case a zero net current on the outer boundary is a precise convergence requirement. Another implicit condition, the periodic boundary condition, requires that angular fluxes on the left boundary equal their counterparts on the right. This condition can be satisfied in detail or by requiring that the net flow through the system vanish (within ϵ).

In multidimensional systems, if integral convergence criteria are used, all outer boundaries with the same type of condition can be lumped together and treated as a single surface.

3.8 A Numerical Example

To clarify some of the techniques and procedures that have been described, consider a simple problem. Suppose the flux and multiplication constant are to be determined in a homogeneous sphere of radius 2 cm. Assume, for the sake of simplicity, that two energy groups, four equal spatial intervals, and a $n = 4$ angular representation will provide a

sufficiently accurate solution. Again for simplicity, assume that scattering is isotropic, that there is no upscattering, and that most of the fission neutrons which are created by reactions in the second group are released in the first group. Geometric and angular coefficients, cross sections, and a fission spectrum reflecting these assumptions are given in Table III-2.

Table III-2

Apart from the relative coarseness of the geometric mesh and the arbitrarily selected cross sections the input data of Table III-2 defines a typical problem.

For a one-dimensional sphere the applicable form of the recursion relation, Eq. (3-74), is

$$N_{i+\frac{1}{2},m} = \frac{|\mu_m|AN_{i+1,m} + \alpha N_{i+\frac{1}{2},m-\frac{1}{2}}/w_m + V_{i+\frac{1}{2}}S_{i+\frac{1}{2}}}{|\mu_m|A + \alpha/w_m + V_{i+\frac{1}{2}}\sigma} \qquad (3\text{-}114)$$

where, for m = 1 the α terms are absent and for m = 4 and 5 $N_{i,m}$ is used instead of $N_{i+1,m}$. Values of $|\mu_m|A$ and α/w_m, which remain constant for the entire calculation, are listed in Table III-3. $\alpha_{1/2}$, for the

Table III-3

starting direction, is zero.

To begin calculation it is assumed that all fluxes are zero and that the only source is due to one fission neutron uniformly distributed over the system. For the first group, then, the source $V_{i+\frac{1}{2}}S_{i+\frac{1}{2}}$ is $0.9V_{i+\frac{1}{2}}/(\sum_{i=1}^{4} V_{i+\frac{1}{2}})$. That is, the fission source of Eq. (3-21) is the

same in each cell and is normalized to unity when integrated over the whole system. Nine-tenths or χ_1 of this source is released in the first group. The calculation begins with the straight inward direction, m = 1, at the outside of the sphere. A vacuum boundary condition is assumed; i.e., the neutron flux in the incoming directions on the boundary is zero. The space-direction mesh and calculation flow are shown in Fig. III-6. With $N_{4,1} = 0$, Eq. (3-114) (with $\alpha = 0$) gives $N_{7/2,1} = 0.0063134$.

Fig. III-6

Because there is no angular redistribution in this direction $N_{7/2,\frac{1}{2}} = N_{7/2,3/2}$; and by the diamond difference scheme, Eq. (3-71), these are both equal to $N_{7/2,1}$. Again from the diamond relations $N_{3,1} + N_{4,1} = 2N_{7/2,1}$ so that $N_{3,1} = 0.0126268$. In this fashion calculation continues inward for m = 1. $N_{3,1}$ provides input for computation of $N_{5/2,1}$ so that $N_{2,1}$ and $N_{5/2,3/2}$ can be extrapolated and so on. The values of $N_{i+\frac{1}{2},3/2}$ generated by the inward traverse serve as input for the next direction. After the first three directions have been traversed, calculation begins at the center and proceeds to the outer boundary. Since the geometry is spherical, center boundary values for directions four and five are obtained from the central values of the flux in the reflected directions, i.e., $N_{0,9/2} = N_{0,7/2}$ and $N_{0,11/2} = N_{0,5/2}$. Cell average flux values, $N_{i+\frac{1}{2},m}$, obtained from a complete traverse of the mesh, i.e., from one inner iteration, are displayed in Fig. III-7. The Figure also displays values of the average flux, $\bar{N}_{i+\frac{1}{2}} = \sum_1^5 w_m N_{i+\frac{1}{2},m}$.

Fig. III-7

Before the second iteration is begun, convergence tests are made. The left side of Eq. (3-100) is

$$\left| \sum_{i=1}^{4} \sigma^{s}_{ogg} \left(\overline{N}_{i+\frac{1}{2}} - \overline{N}^{p}_{i+\frac{1}{2}}\right) V_{i+\frac{1}{2}} \right| = 0.0675174 \qquad (3\text{-}115)$$

which is larger than ϵS^{p}_{avg} with $\epsilon = 0.0001$ and $S^{p}_{avg} = 0.5$. The test of Eq. (3-101) also fails. The scale factor f of Eq. (3-99) is easily found, since the volume sum of the group source is 0.9, to be f = 0.9/(0.9-0.0675174) = 1.081104. This scale factor is used to adjust the flux level of $\overline{N}_{i+\frac{1}{2}}$ with results as shown in Fig. III-7. With first iterate values of $\overline{N}_{i+\frac{1}{2}}$ available, the group source is corrected by adding $\sigma^{s}_{ogg}\overline{N}_{i+\frac{1}{2}}V_{i+\frac{1}{2}}$ to the unaltered fission source. As inner iteration proceeds, this portion of the source is continuously revised while the fission source remains fixed. A second inner iteration produces fluxes as shown in Fig. III-8. Note that the scale factor, in addition to pro-

Fig. III-8

viding system-wide neutron conservation, accelerates convergence since the second iterate fluxes are indeed larger than the first iterate fluxes. Also note that the new scale factor is much closer to but still larger than unity. The second iterate flux values do not yet pass the convergence tests; and a third iteration, with results as shown in parentheses in Fig. III-8, is needed to finish inner iteration in the first group.

Calculation next proceeds to the second group. The fission source in this group, 0.1 of the total fission source, is supplemented by a down-scatter source calculated with converged first group fluxes:

$$V_{i+\frac{1}{2}}S_{i+\frac{1}{2},g=2} = \sigma_{21}V_{i+\frac{1}{2}}\bar{N}_{i+\frac{1}{2},g=1} + 0.1V_{i+\frac{1}{2}}/\left(\sum_{i=1}^{4} V_{i+\frac{1}{2}}\right) \qquad (3\text{-}116)$$

The above source is the fixed source for the second group and is corrected by addition of a self-scatter source. This self-scatter source is calculated as soon as second group fluxes are available and corrected after each inner iteration. The results of three iterations necessary for second group inner iteration convergence are summarized in Table III-4. With inner iteration converged in both groups, outer convergence

Table III-4

tests are made. When the fission source is recomputed, Eq. (3-111) gives

$$\lambda = \left(\sum_{i=1}^{4} V_{i+\frac{1}{2}}F_{i+\frac{1}{2}}\right)/\left(\sum_{i=1}^{4} V_{i+\frac{1}{2}}F^{p}_{i+\frac{1}{2}}\right) = 0.0901929 \qquad (3\text{-}117)$$

After six more outer iterations and a total of twenty-seven inner iterations a converged outer iteration terminates the calculation. The behavior of fluxes, multiplication constant, and λ are summarized in Table III-5.

Table III-5

For the problem defined, the sphere is so small that most (94.12%) of the neutrons escape, and consequently the system is very subcritical.

Most of the numerical values computed above were hand-calculated and then checked by comparing with a special edit of a current version of a Los Alamos one-dimensional transport code.

Indeed, almost all of the methods described in this chapter are presently (1965) applied in one- and two-dimensional, multigroup transport codes for orthogonal geometries. In addition to the capabilities here described these existing codes also solve the adjoint transport equation by making simple transformations of sources and cross sections entered for a regular computation.

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TABLE III-1 AREA AND VOLUME ELEMENTS

Geometry	Variables	V	A	B	C
Rectangular	x	Δx_i	1		
	x, y	$\Delta x_i \Delta y_j$	Δy_j	Δx_i	
	x, y, z	$\Delta x_i \Delta y_j \Delta z_k$	$\Delta y_j \Delta z_k$	$\Delta x_i \Delta z_k$	$\Delta x_i \Delta y_j$
Cylindrical[a]	r	R_i	$2\pi r_i$		
	r, θ	$R_i \Delta\theta_j$	$2\pi r_i \Delta\theta_j$	Δr_i	
	r, z	$R_i \Delta z_k$	$2\pi r_i \Delta z_k$		R_i
	r, θ, z	$R_i \Delta\theta_j \Delta z_k$	$2\pi r_i \Delta z_k \Delta\theta_j$	$\Delta r_i \Delta z_k$	$2\pi r_i \Delta r_i \Delta\theta_j$
Spherical[a]	r	S_i	$4\pi r_i^2$		
	r, φ	$S_i S_k$	$4\pi r_i^2 S_k$		$R_i \cos 2\pi\varphi_k$
	r, θ, φ	$S_i S_k \Delta\theta$	$4\pi r_i^2 S_k \Delta\theta$	$R_i \Delta\varphi$	$R_i \cos 2\pi\varphi_k \Delta\theta$

[a] θ and φ measured in revolutions

$R_i = \pi(r_{i+1}^2 - r_i^2)$, $S_i = 4\pi(r_{i+1}^3 - r_i^3)/3$, $S_k = (\sin 2\pi\varphi_{k+1} - \sin 2\pi\varphi_k)/2$,

$\Delta x_i = x_{i+1} - x_i$ and similarly for other variables.

TABLE III-2 INPUT DATA FOR EXAMPLE PROBLEM

Geometric Functions

i	Radii - r_i cm	Area Elements - A_i cm^2	Volume Elements - $V_{i+\frac{1}{2}}$ cm^3
0	0.0	0.0	0.523598
1	0.5	3.14159	3.665188
2	1.0	12.56636	9.948368
3	1.5	28.27431	19.373140
4	2.0	50.26544	--

Quadrature Coefficients

m	Direction Cosine μ_m	Direction Weight w_m	Product $w_m\mu_m$
1	-1.0	0.0	0.0
2	-0.8819171	0.1666667	-0.1469862
3	-0.3333333	0.3333333	-0.1111111
4	+0.3333333	0.3333333	+0.1111111
5	+0.8819171	0.1666667	+0.1469862

Macroscopic Cross Sections (cm^{-1}) and Fission Spectrum

Group, g	σ^a	$\nu\sigma^f$	σ	$\sigma_{g,g+1}$	σ_{gg}	$\sigma_{g,g-1}$	χ_g
1	0.02	0.0	0.2	0.0	0.06	--	0.9
2	0.08	0.24	0.22	--	0.14	0.12	0.1

TABLE III-3 EXAMPLE PROBLEM GEOMETRIC AND CURVATURE FUNCTIONS

i	0			1			2			3		
m	$\alpha_{m+\frac{1}{2}}$	$\lvert\mu_m\rvert A$	α/w	$\alpha_{m+\frac{1}{2}}$	$\lvert\mu_m\rvert A$	α/w	$\alpha_{m+\frac{1}{2}}$	$\lvert\mu_m\rvert A$	α/w	$\alpha_{m+\frac{1}{2}}$	$\lvert\mu_m\rvert A$	α/w
1	0.0	3.1416		0.0	15.7079		0.0	40.8407		0.0	78.5397	
2	0.4618	2.7706	2.7706	1.3853	13.8531	8.3119	2.3088	36.0181	13.8531	3.2324	69.2655	19.3944
3	0.8108	1.0472	3.8178	2.4325	5.2360	11.4534	4.0542	13.6136	19.0891	5.6758	26.1799	26.7247
4	0.4618	1.0472	3.8178	1.3853	5.2360	11.4534	2.3088	13.6136	19.0891	3.2324	26.1799	26.7247
5	0.0	2.7706	2.7706	0.0	13.8531	8.3119	0.0	36.0181	13.8531	0.0	69.2655	19.3944

TABLE III-4 EXAMPLE PROBLEM - SECOND GROUP

INNER ITERATION

INNER ITERATION NUMBER	Average Flux $\bar{N}_{i+\frac{1}{2}}$				SCALE FACTOR
	i = 0	i = 1	i = 2	i = 3	
1	0.0123561	0.0120812	0.0107605	0.0077786	1.21253
2	0.0152062	0.0148435	0.0131309	0.0094156	1.000767
3	0.0152358	0.0148695	0.0134622	0.0094215	1.000050

TABLE III-5 EXAMPLE PROBLEM - OUTER ITERATION

OUTER ITERATION NUMBER	AVERAGE FLUX $\bar{N}_{i+\frac{1}{2}}$								MULTIPLICATION CONSTANT
	GROUP 1				GROUP 2				
	i = 0	i = 1	i = 2	i = 3	i = 0	i = 1	i = 2	i = 3	
1	0.046255	0.045544	0.041882	0.031603	0.015236	0.014870	0.013147	0.009422	0.090193
2	0.054482	0.052780	0.045139	0.031148	0.017253	0.016646	0.014091	0.009606	0.095117
3	0.056497	0.054400	0.045713	0.031023	0.017719	0.017031	0.014269	0.009634	0.096074
4	0.056963	0.054761	0.045830	0.030994	0.017826	0.017118	0.014307	0.009640	0.096279
5	0.057071	0.054843	0.034856	0.030988	0.017850	0.017137	0.014315	0.009641	0.096324
6	0.057094	0.054860	0.045861	0.030986	0.017856	0.017142	0.014317	0.0096415	0.096334
7	0.057100	0.054865	0.045863	0.030986	0.017858	0.017143	0.014317	0.0096416	0.096338

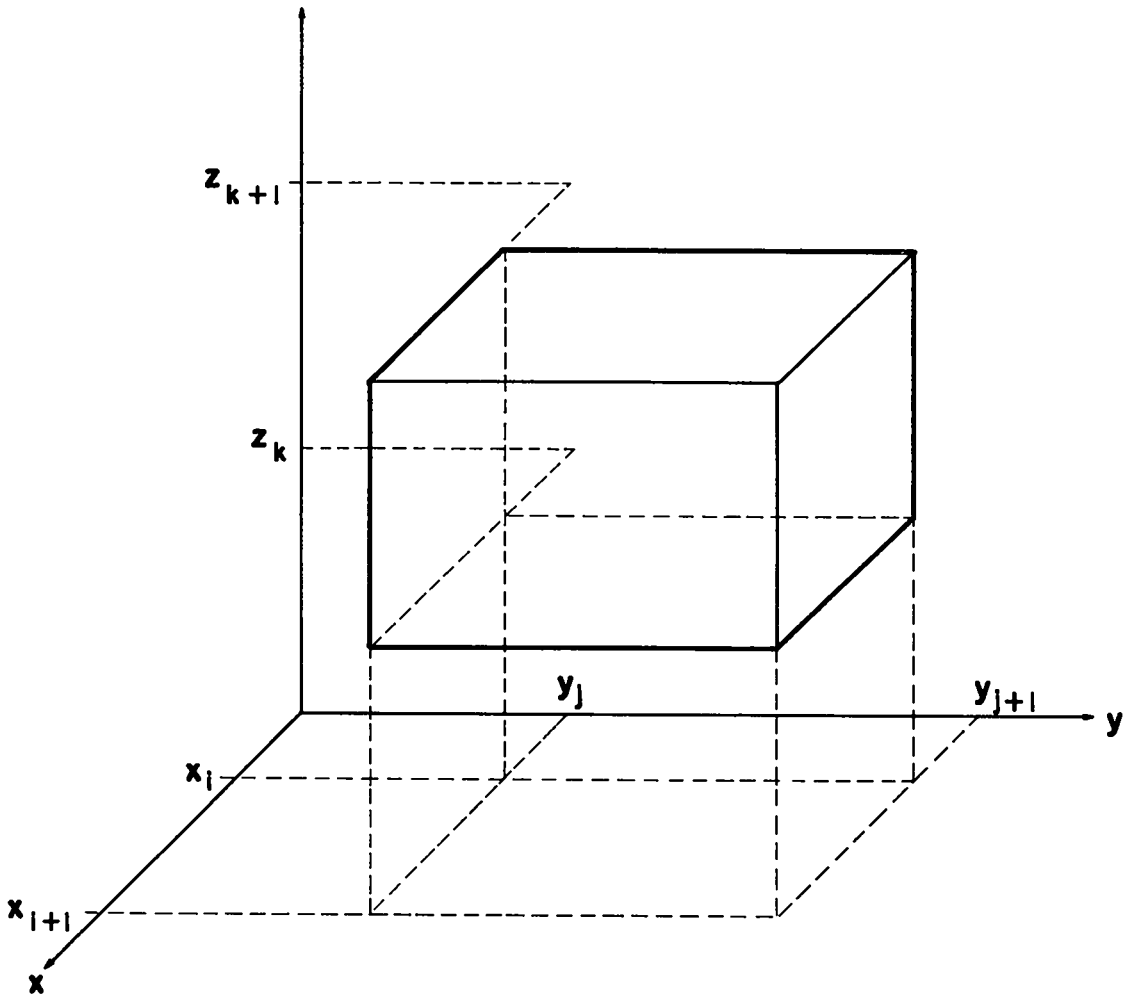


Fig. III-1 Mesh Cell in Rectangular Geometry

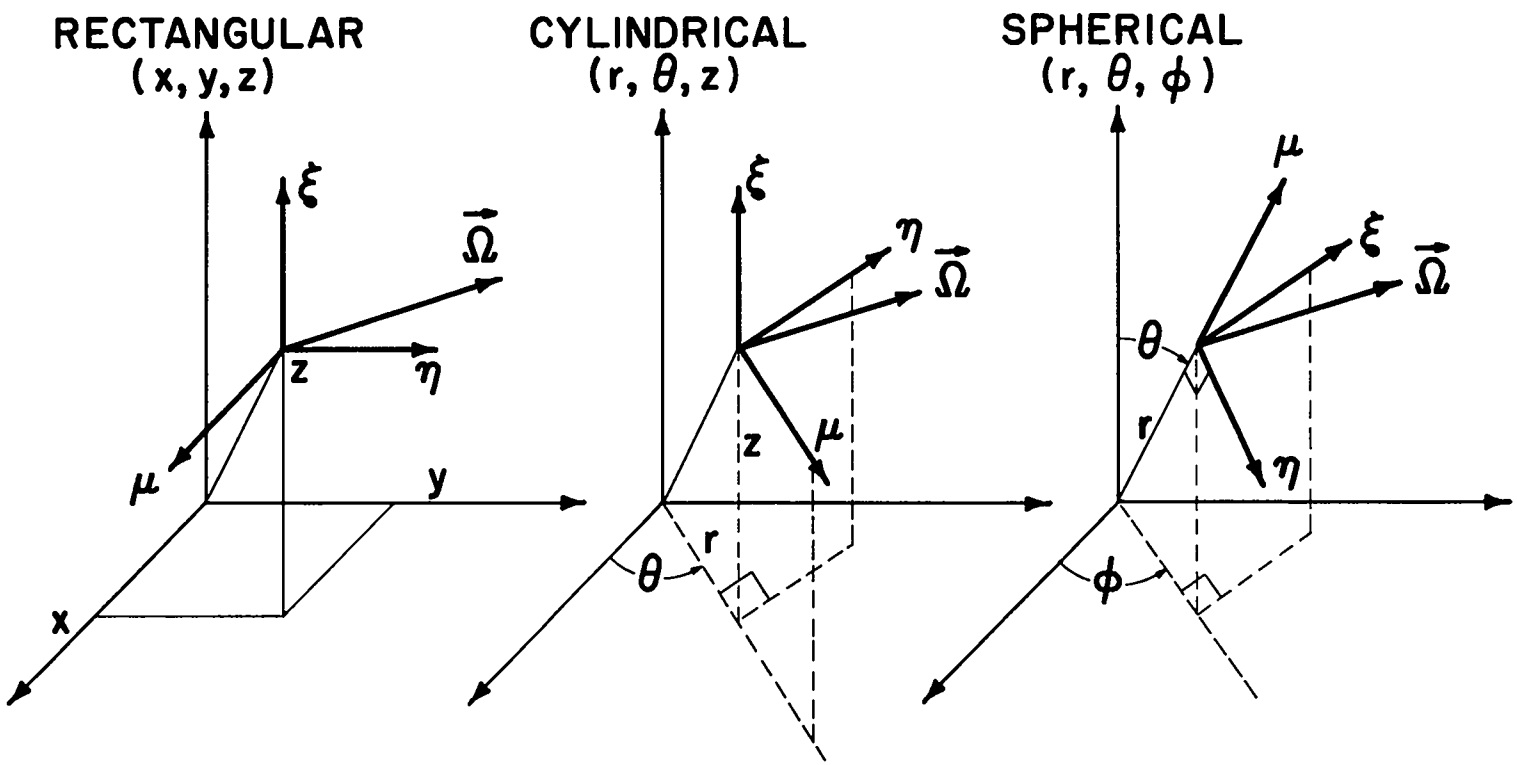


Fig. III-2 Orientation of Angular Coordinate System

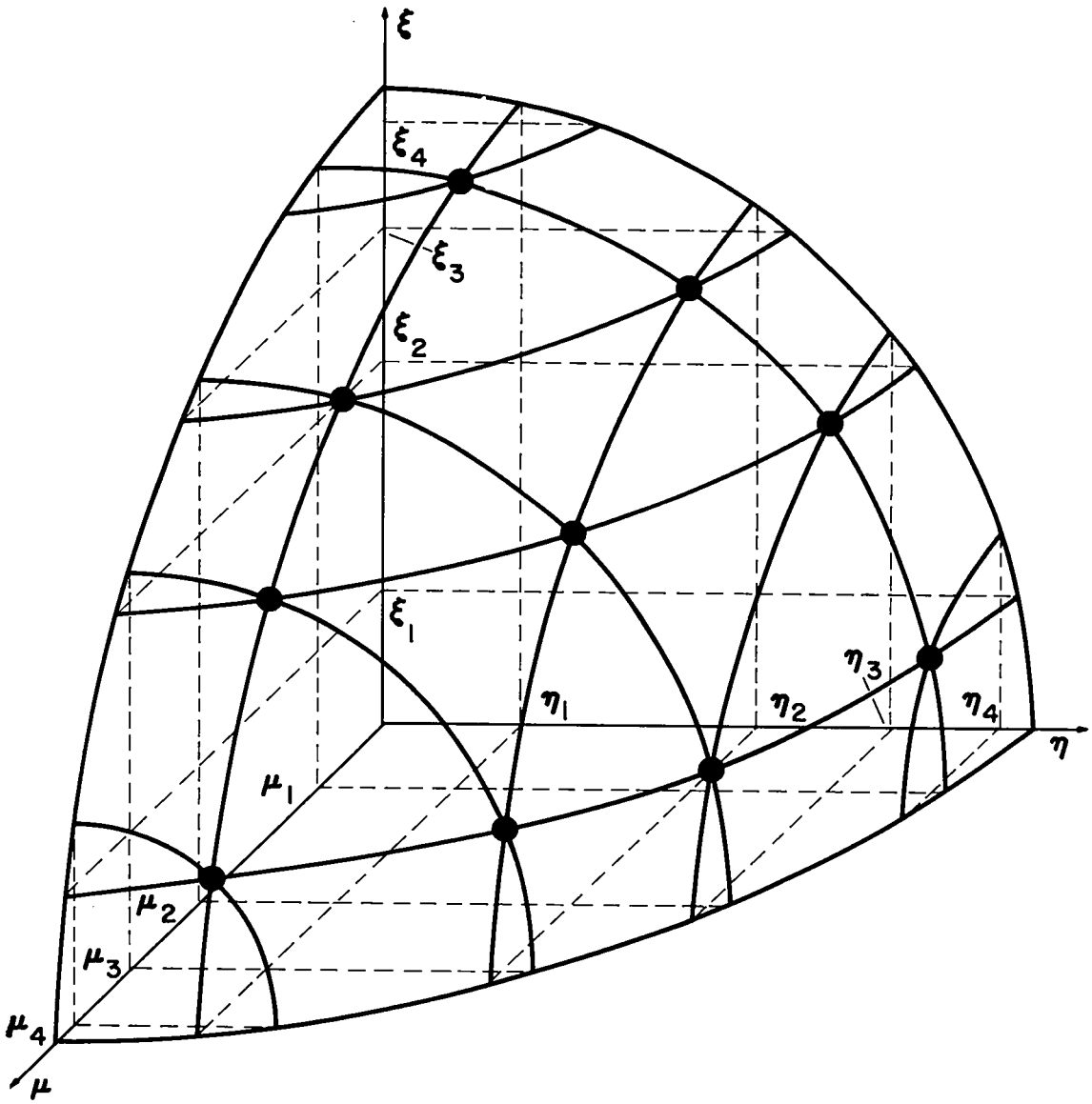


Fig. III-3 Completely Symmetric Point Arrangement, n = 8

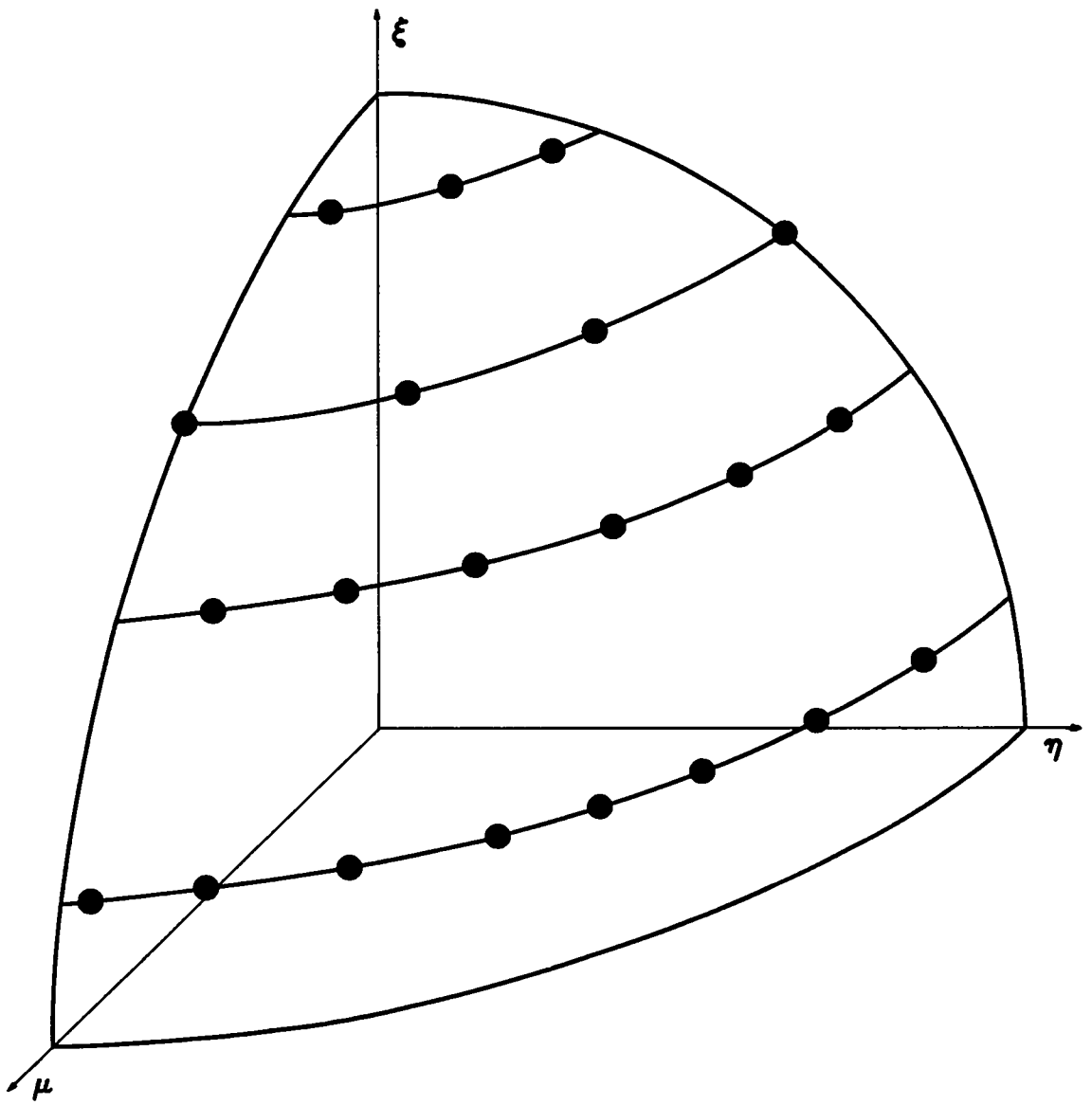


Fig. III-4 Latitudinal Point Arrangement - Relaxation of Symmetry

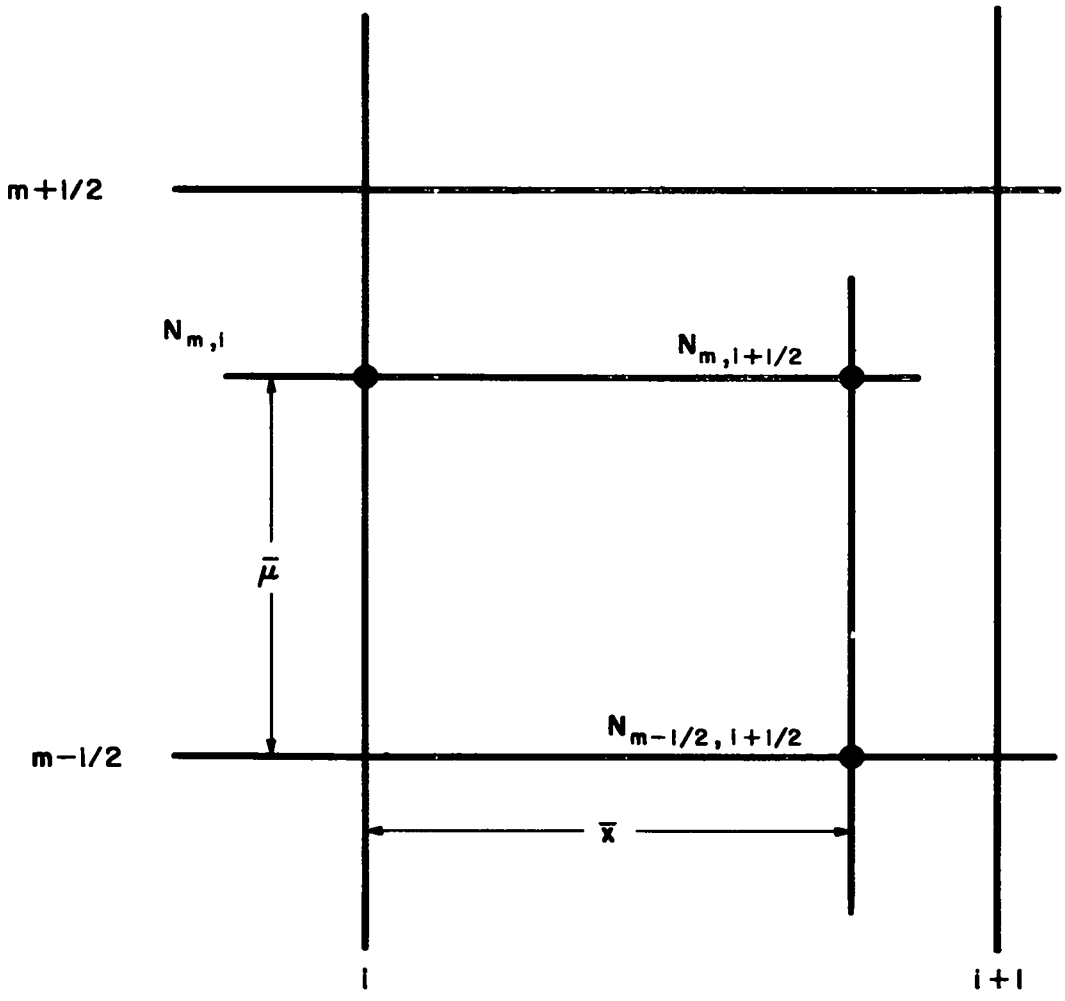
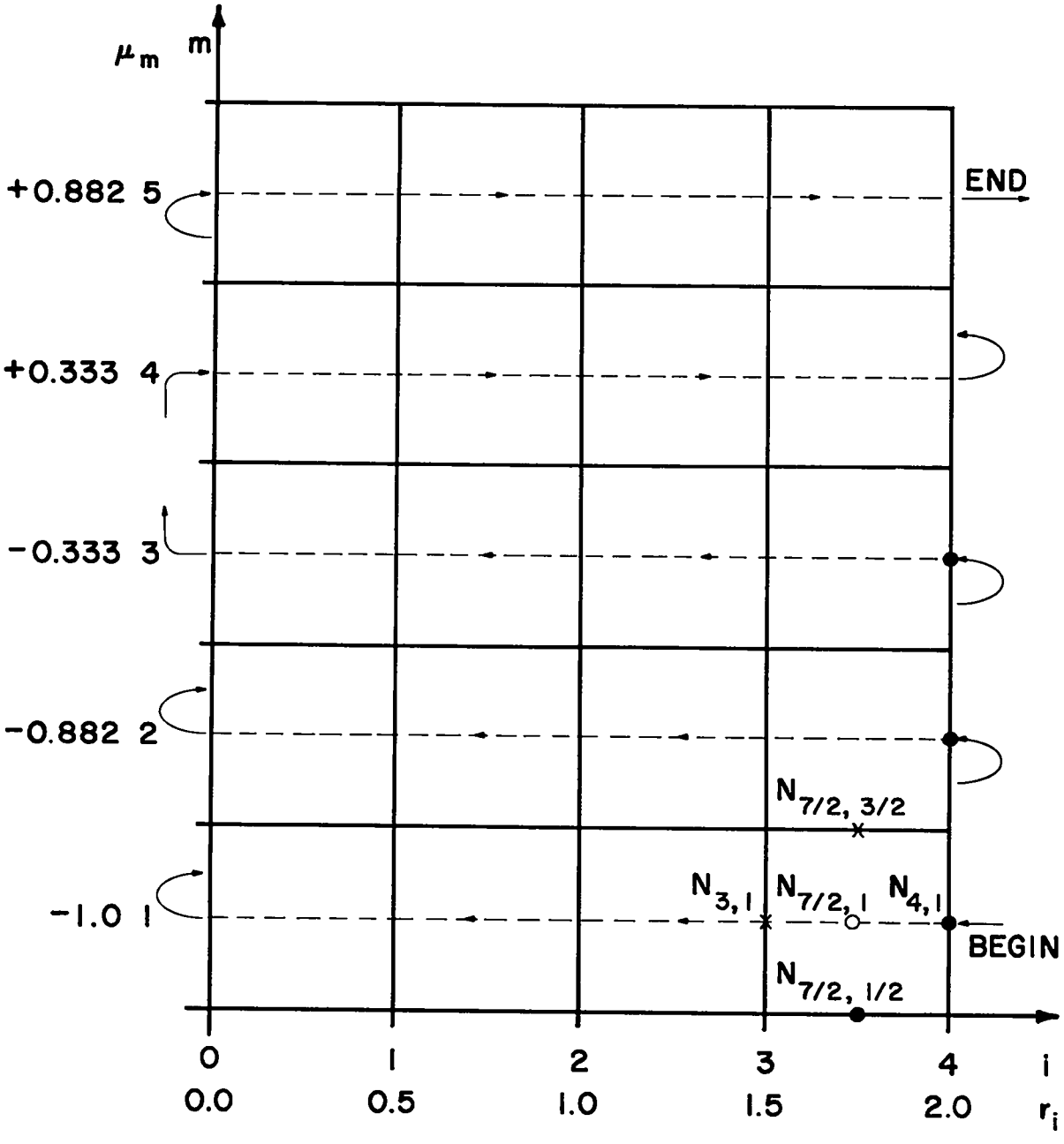
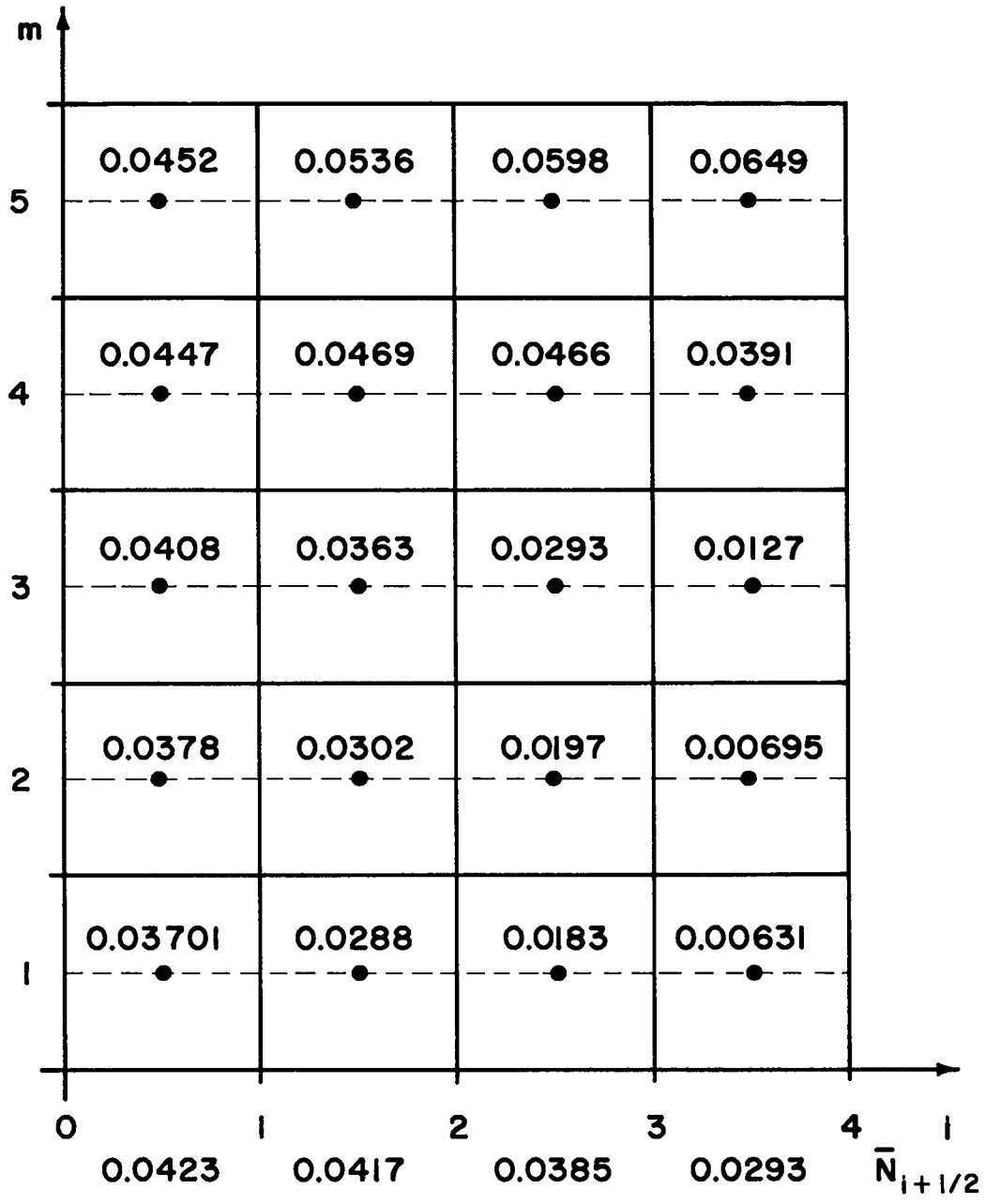


Fig. III-5 Space - Direction Mesh



● BOUNDARY VALUES
○ CALCULATED VALUES
× EXTRAPOLATED VALUES

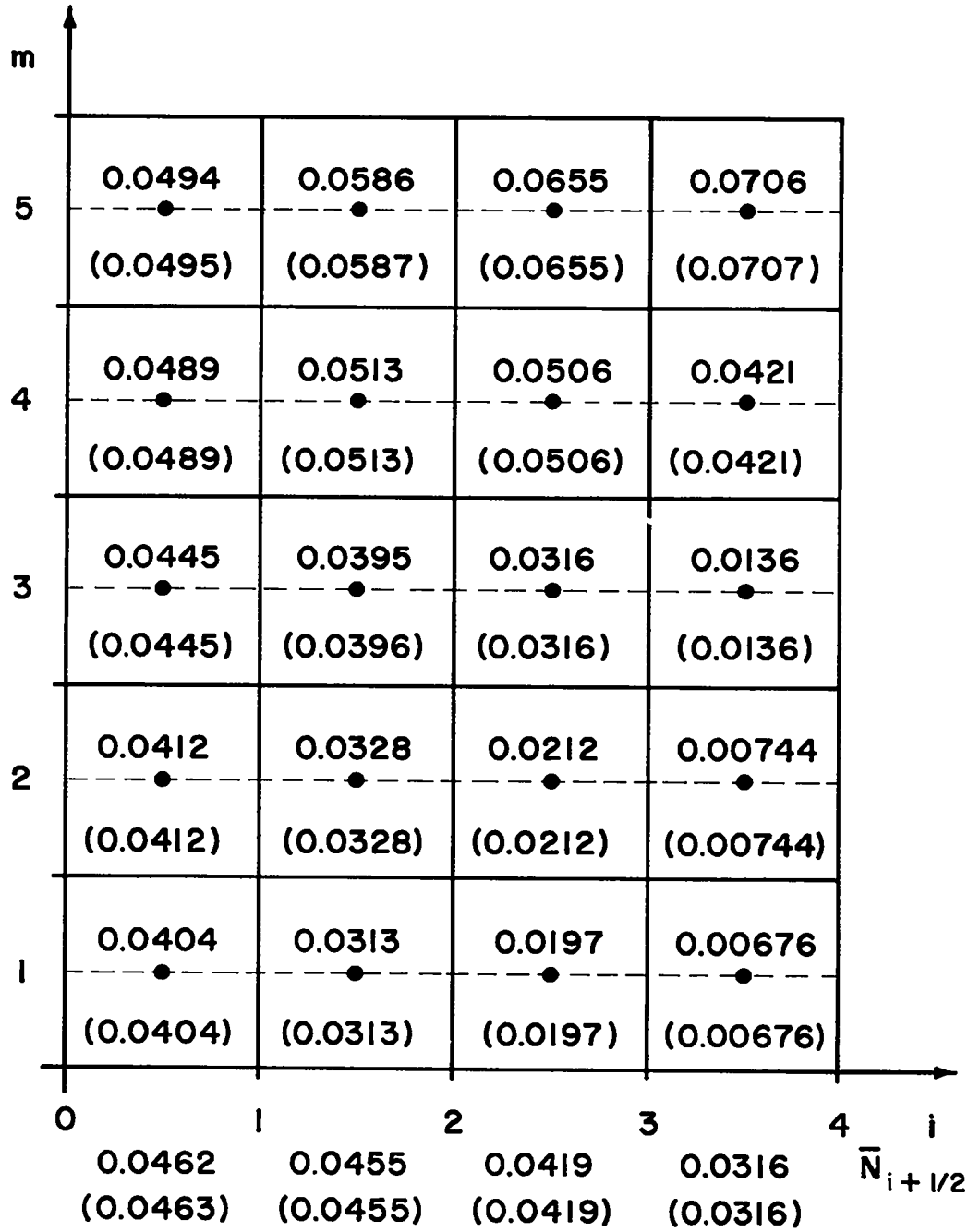
Fig. III-6 Example Problem Space - Direction Mesh



$$\sum_i V_{i+1/2}\sigma_{gg}\,(\bar{N}_{i+1/2}-\bar{N}^{p}_{i+1/2}) = 0.0675$$

SCALE FACTOR, f = 1.0811

Fig. III-7 Example problem - First group fluxes after first inner iteration



$$\sum_i V_{i+1/2}\sigma_{gg}\,(\bar{N}_{i+1/2}-\bar{N}^{p}_{i+1/2}) = 0.00019\ (0.0000054)$$

SCALE FACTOR, f = 1.00021 (1.000006)

Fig. III-8 Example problem - First group fluxes, second and third (in parentheses) inner iterations