JOURNAL OF COMPUTATIONAL PHYSICS 2, 173-197 (1967)

Numerical Solution of the Boltzmann Transport Equation*

K. LATHROP AND B. CARLSON

Los Alamos Scientific Laboratory,
University of California,
Los Alamos, New Mexico

ABSTRACT

A numerical model for solution of the linear Boltzmann Transport Equation is formulated. By applying the same techniques used in the derivation of the analytic equation, a discrete analog of the Boltzmann equation is derived for a finite cell in phase space. Initially undetermined coefficients in the analog are determined by requiring the numerical formulation to include properties (e.g., particle conservation) of the analytic equation. Terms occurring in the finite-cell analog are defined, and two treatments of the angular dependence are illustrated. A discrete ordinates representation is derived based on a connected straight-line–angular representation. This formulation maintains optical reciprocity and may be generalized.

The second portion of the paper describes the systematic derivation of difference relations necessary to complete solution of the numerical formulation. Both representation schemes, based on assumed forms of particle fluxes in the cell, and characteristic schemes are examined. Difficulties encountered in extrapolations made by the use of representation schemes are clarified, and insight is gained for methods that can be used to prevent flux oscillations in numerical calculations.

INTRODUCTION

The linear Boltzmann transport equation [1], which describes the transport of neutrons or photons through matter, does not readily yield to analytical solution. Although the method of singular integral equations introduced by Case [2] has been extended to curved one-dimensional geometries [3], at present there are

* This work was performed under the auspices of the U.S. Atomic Energy Commission.

no analytic solutions for finite two- or three-dimensional geometries. Such analytic solutions as exist are useful primarily to provide standards for direct numerical solution, because the analytic solutions require comparable numerical effort to evaluate and are not nearly as flexible as direct-solution procedures for solving complex problems. But, other than in one-dimensional geometries, there are no such standards available and direct numerical solution proceeds in relatively uncharted territory. This lack of mathematical guidance is regrettable, for when solution methods are proposed, errors cannot be analyzed and one is reduced to comparing results from what may be equally imprecise algorithms. In this paper we describe procedures for numerically solving the Boltzmann equation. In formulating these procedures we attempt to compensate for the lack of analytic solutions by making maximum use of the physics that is contained in the Boltzman equation. We insist, as a fundamental principle, that the numerical approximation, or finite-cell analog, to the analytic equation be based on the same physical properties as the analytic equation. For instance, the Boltzmann equation is a statement of particle conservation; therefore numerical approximations should also conserve particles, a principle that is sometimes [4] overlooked in an attempt to find more accurate algorithms. As another example, if the equation adjoint to the Boltzmann equation is to be solved numerically, then it is desirable that the numerical formulation of the adjoint equation be adjoint to the numerical formulation of the direct equation [5].

In this paper we concentrate on the treatment of the divergence operator of the Boltzmann equation and on the difference relations necessary to solve the resulting formulation. Elsewhere [6, 7] we have described symmetry restrictions on angular quadrature set which are necessary to ensure particle path ("optical") reciprocity. To simplify the discussion that follow, we restrict our attention to the monoenergetic time-independent Boltzmann equation. In general problems, energy dependence has been treated successfully by the multigroup approximation [5], and time dependence can be handled by simple extension of the difference schemes described below. Although we are interested in general geometries, we frequently examine the equation in one space dimension for the sake of simplicity.

We first formulate an analog of the analytic Boltzmann equation for a finite cell in phase space, reasoning from the same principles which lead to the analytic equation. We then examine various assumptions relating to the angular variable. As one example of such assumptions we derive the equations for a connected straight-line representation of the angular variable that was used in the original S_n method [8]. This original method was set aside in favor of an approach closer to that of Wick and Chandrasekar [9] because it did not preserve optical recipro-

city, but we show this difficulty can be overcome, thus making feasible very general formulations of the Boltzmann equation. As another example, we give the conditions necessary for our numerical approximations to the Boltzmann equation to yield the solutions of the diffusion approximation to the transport equation.

In the second portion of the paper we examine the problem of determining the additional approximations, called difference relations, which make possible solution of the numerical Boltzmann equation. We first examine the problems encountered by using relations based on locally smooth behavior of the flux and then turn to formulations derived from the integral form of the analytic Boltzmann equation. These formulations not only make possible the systematic derivation of more general and, hopefully, more accurate approximations, but they provide guidance for meaningful recipes with which, for example, negative fluxes can be prevented. Both midvalue (diamond difference) and corner-point (central difference) schemes are examined.

The methods described here lead to discrete ordinates equations for finite cells in phase space. The main effect is that a single, complex equation is reduced to a system of simpler equation, the ray equations, in which the size of the system is related to the order, n, of approximation. It is also possible to formulate discrete ordinates equations equivalent to moments equations which approximate the Boltzmann equation. This approach, beginning from a general moments equation approximation [10, 11], seems promising and may be explored in a future paper.

Formluation of a Discrete Approximation to the Boltzmann Equation

The monoenergetic time-independent linear Boltzmann transport equation can be written

$$\nabla \cdot \mathbf{\Omega} N(\mathbf{r}, \mathbf{\Omega}) + \sigma(\mathbf{r}) N(\mathbf{r}, \mathbf{\Omega}) = S(\mathbf{r}, \mathbf{\Omega}) \tag{1}$$

where $\mathbf{r}$ is the particle position vector and $\mathbf{\Omega}$ is a unit vector in the direction of the particle motion. The particle flux (particle speed times particle density) is denoted by N, S represents particle sources, and σ is the macroscopic cross section for particle collisions. Equation (1) is a detailed statement of particle conservation in an infinitesimal volume of phase space, with losses due to neutron streaming (leakage), $\nabla \cdot \mathbf{\Omega} N$, and collisions, σN, being balanced by sources, S. In general problems, S may be composed of components proportional to N (scattering or neutron fission) as well as sources independent of N. Here we do not specify S further, but refer the reader to Reference [5] for a detailed discussion of the nu-

merical treatment of scattering, fission, and independent sources. It should be noted that although we have assumed a monoenergetic problem, Eq. (1) is also the equation solved in each group of a multigroup calculation where, even if S depends on fluxes in other groups, it is assumed known for calculations within the groups.

The fact that Eq. (1) is a conservation relation has several ramifications that are useful in formulating numerical approximations. First, when the equation is integrated over all solid angles, the neutron balance equation is obtained:

$$\nabla \cdot \mathbf{J}(\mathbf{r}) + \sigma(\mathbf{r})\bar{N}(\mathbf{r}) = \bar{S}(\mathbf{r}) \tag{2}$$

where $\mathbf{J}$ is the current

$$\mathbf{J}(\mathbf{r}) = \int \mathbf{\Omega} N(\mathbf{r}, \mathbf{\Omega}) d\mathbf{\Omega}\,, \tag{3}$$

$\bar{N}$ is the scalar flux

$$\bar{N} = \int N(\mathbf{r}, \mathbf{\Omega}) d\mathbf{\Omega}\,, \tag{4}$$

and $\bar{S}$ is a similar average of $S(\mathbf{r}, \mathbf{\Omega})$. When (2) is integrated over a finite volume V, with surface area A, the balance of particles is clearly evident:

$$\int_A \mathbf{J} \cdot d\mathbf{A} + \int_V \sigma \bar{N} dV = \int_V \bar{S} dV \tag{5}$$

with losses due to flow through the surface plus collisions in the volume-balancing sources in the volume. When we write a numerical approximation to (1) we insist that it satisfy relations analogous to (2) and (5); that is, we write the numerical approximation in conservation form.[1] In this fashion we develop a numerical equation analogous to the conservation form of the Boltzmann equation. For instance, in one-dimensional spherical geometry, N and S are assumed to depend only on the radial coordinate r and the cosine $\mu = \mathbf{\Omega} \cdot \mathbf{e}_r$ where $\mathbf{e}_r = \mathbf{r}/r$. Then the analytic form of (1) can be written

$$\mu \frac{\partial N}{\partial r} + \frac{(1 - \mu^2)}{r} \frac{\partial N}{\partial \mu} + \sigma N(r, \mu) = S(r, \mu)\,. \tag{6}$$

While this equation can be integrated to give a balance equation, the same is not

[1] The importance of including conservation relations in numerical approximations was first noted by Lax [12] in the hydrodynamics equations. Strictly speaking, (7) and (8) should be multiplied by r^2 so that the coefficient of each derivative is independent of the variable being differentiated.

usually true of numerical approximations to this form of the equation. The desired conservation form is

$$\frac{\mu\partial(r^2N)}{r^2\partial r} + \frac{\partial[(1-\mu^2)N]}{r\,\partial\mu} + \sigma N = S \tag{7}$$

which, when integrated over the unit sphere of directions with $(-1 \leq \mu \leq 1)$, gives

$$\frac{1}{r^2}\frac{\partial(r^2I)}{\partial r} + \sigma\bar{N} = \bar{S} \tag{8}$$

as a specific form of (2) with $I \equiv \mathbf{J}\cdot\mathbf{e}_r$. Notice that the angular derivative vanishes in this integration. Because the orientation of the angular coordinate system is a function of position in curved geometry, a particle changes angular coordinates as it moves through the system. The angular derivative in (7) provides a mechanism for this directional transfer, and the vanishing of the term in passing from (7) to (8) shows that this process has no net effect on particle balance. This, then, is another useful condition to impose on any numerical approximation to (1).

Integrating Eq. (8) over a finite volume $0 \leq r \leq a$ with $dV = 4\pi r^2 dr$ gives as in (5)

$$r^2I\Big|_{r=0}^{r=a} + \int_0^a r^2\bar{N}dr = \int_0^a r^2\bar{S}dr\,, \tag{9}$$

where r^2I contributes only as the flow through the system boundaries.

Finally, if N is constant, (1) shows that $\sigma N = S$ so that in this situation the derivative terms of (7) must and do cancel identically. Thus, when (1) is approximated numerically, this property should be maintained.

To recapitulate, when Eq. (1) is formulated for numerical solution, we insist that the approximation express neutron conservation for a cell in phase space in a manner such that

(a) angular integration results in a cell balance and a zero net flow due to angular redistribution,

(b) spatial integration results in a balance statement involving boundary currents only,

(c) when N is constant, the approximations to the derivatives of the divergence operator are such that they cancel identically.

We now formulate an approximation which incorporates these properties of the Boltzmann equation. Rather than attempt trial and error, we insert unspe-

cified constants in the formulation and determine these constants so that the above conditions are satisfied. We restrict our attention to one-dimensional spherical geometry, but adopt a notation which permits generalization to other geometries and more dimensions. We distinguish between noncentered subscripts (i and $i + 1$, $m - \frac{1}{2}$ and $m + \frac{1}{2}$) and centered subscripts ($i + \frac{1}{2}$ or m). The noncentered subscripts refer to specific values of the independent variable (r_i or $\mu_{m+1/2}$), but the centered subscripts refer to averages over the range of the independent variables and not to specific values of the variables.

Consider the phase-space cell of Fig. 1 which is applicable to the (r, μ) geometry

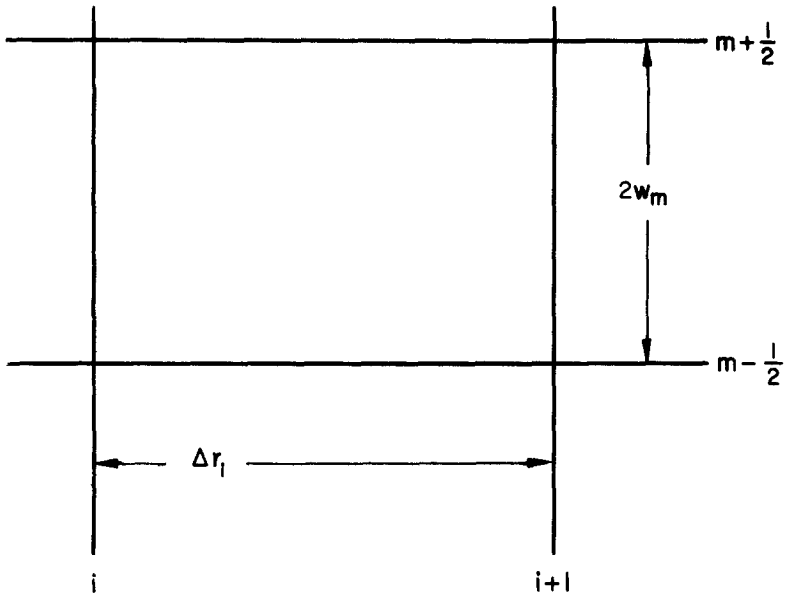

FIG. 1.

of Eq. (7). In spherical geometry, the area of the cell face at $r = r_i$ is $4\pi r_i^2 \equiv A_i$. Similarly, the area of the face at $r = r_{i+1}$ is $A_{i+1} = 4\pi r_{i+1}^2$ and the volume of the cell is $V_{i+1/2} = 4\pi(r_{i+1}^3 - r_i^3)/3$. We define the average flux on the cell face at $r = r_i$ that is in the direction range $2w_m = \mu_{m+1/2} - \mu_{m-1/2}$ about an average cosine μ_m to be $N_{i,m}$. The similar flux at $r = r_{i+1}$ is defined to be $N_{i+1,m}$. In these terms, if μ_m is positive, the net loss from the vertical faces of the cell is the number that flow out of the cell through the right face minus the number that flow into the cell through the left face:

$$2w_m(A_{i+1}\mu_m N_{i+1,m} - A_i\mu_m N_{i,m}). \tag{10}$$

In an analogous fashion we define the average flux at $\mu = \mu_{m+1/2}$ in the range of r between r_{i+1} and r_i to be $N_{i+1/2,m+1/2}$ and represent the net number of particles leaving the cell by passing through the horizontal faces by

$$2\alpha_{m+1/2,i+1/2}N_{m+1/2,i+1/2} - 2\alpha_{m-1/2,i+1/2}N_{m-1/2,i+1/2}\,, \tag{11}$$

where the coefficients α are as yet unspecified. Next, assuming the collision cross section is constant within the cell, we define the average number of particles removed from the cell by collisions to be

$$2w_m\sigma_{i+1/2}V_{i+1/2}N_{i+1/2,m}\,. \tag{12}$$

Similarly, the average number of particles produced in the cell by sources is

$$2w_mV_{i+1/2}S_{i+1/2,m}\,. \tag{13}$$

Combining (10) through (13) we have a statement of neutron conservation for the finite cell:

$$w(A_{i+1}\mu_mN_{i+1} - A_i\mu_mN_i) + \alpha_{m+1/2}N_{m+1/2} - \alpha_{m-1/2}\,N_{m-1/2} + w\sigma VN = wVS. \tag{14}$$

In writing Eq. (14) we have dropped centered subscripts which refer to averages over faces or volumes. Except in situations which require emphasis we henceforth adopt this convention. Equation (14) corresponds to Eq. (7) multiplied by $4\pi r^2drd\mu \sim dVd\Omega/2\pi$.

We now determine the α-coefficients in accordance with the criteria established above. First, in the angular integration of Eq. (14), the α-terms should vanish. That is, the m sum of Eq. (14), which is a discrete angular quadrature, should give

$$A_{i+1}I_{i+1} - A_iI_i + \sigma\bar{N}V = \bar{S}V\,, \tag{15}$$

where[2]

$$\begin{aligned} I_i &= \sum_{m=1}^{M} w_m\mu_mN_{i,m}\,, \\ \bar{N}_{i+1/2} &= \sum_{m=1}^{M} w_mN_{i+1/2,m}\,, \\ \bar{S}_{i+1/2} &= \sum_{m=1}^{M} w_mS_{i+1/2,m}\,, \end{aligned} \tag{16}$$

[2] The factor of two included in the definition of w in effect normalizes these integrals, e.g., $I = \int_{-1}^{1} \mu N d\mu/2$.

in analogy to Eq. (8). In these terms the discrete angular quadrature set consists of M direction cosines,[3] μ_m, with an equal number of associated weights w_m. In order that Eq. (15) be valid it is necessary that

$$\sum_{m=1}^{M} (\alpha_{m+1/2}N_{m+1/2} - \alpha_{m-1/2}N_{m-1/2}) = \alpha_{M+1/2}N_{M+1/2} - \alpha_{1/2}N_{1/2} = 0. \quad (17)$$

This can be accomplished independently of M by choosing $\alpha_{1/2} = \alpha_{M+1/2} = 0$.

Next, it is a simple exercise to verify that the volume integral, that is, the i sum, of (15) involves only boundary values of the currents.

Finally, when all fluxes in (14) are constant and $\sigma N = S$, the two terms approximating the divergence operator should cancel which gives

$$\alpha_{m+1/2} - \alpha_{m-1/2} = -w\mu_m(A_{i+1} - A_i). \quad (18)$$

Given the w's and μ's and the initial condition $\alpha_{1/2} = 0$, Eq. (18) determines the α recursively. Because $\alpha_{M+1/2}$ is also zero, the left-side m-sum of (18) vanishes which implies that the right side sum must also vanish. That is, we must have

$$\sum_{m=1}^{M} w_m\mu_m = 0, \quad (19)$$

which imposes a mild restraint on the quadrature coefficients. Equation (19) is satisfied identically by symmetric (in this case with respect to $\mu = 0$) sets needed to preserve optical reciprocity. With symmetric sets, the α-coefficients are positive and symmetric; and $\alpha_{M+1/2}$ is in fact zero, provided that directions are ordered so that $m = 1$ corresponds to the most negative direction cosine and increasing m index corresponds to a monotone increase of direction cosine.

Except for the restriction of (19), and the requirement that the angular quadrature weights sum to one-half the length of the integration interval, the formulation of (14) imposes no conditions on the quadrature set. It has been found useful to require, in the limit of linearly varying angular flux, $N(\mu) \sim \bar{N} + 3\mu I$, that the formulation of (14) yield the diffusion theory equations. That is, in this limit, when (1) is multiplied by $\boldsymbol{\Omega}$ and integrated over $d\Omega$, the result can be expressed [1] in terms of equations relating derivatives of the flux, the current, and the linearly anisotropic part of the source. Corresponding to Eqs. (7) and (14) these current equations are, respectively,

$$\frac{\partial \bar{N}}{\partial r} + 3\sigma I = 0 \quad (20)$$

[3] In one-dimensional plane or spherical geometry $M = n$ of the S_n discrete ordinates schemes.

and

$$\tfrac{1}{2}(A_{i+1} + A_i)(\bar{N}_{i+1} - \bar{N}_i) + 3\sigma VI = 3VS_I \tag{21}$$

where S_I is the linearly anisotropic component of S. It can be shown [5] that, provided

$$\sum_{m=1}^{M} w_m \mu_m{}^2 = \frac{1}{3}, \tag{22}$$

this property of the analytic equations is preserved by the discrete formulation of (14).

Definitions of the Fluxes in the Discrete Formulation

So far, we have not defined the fluxes that occur in Eq. (14). Basically, the discrete form of the transport equation is obtained by averaging the analytic equation over a finite cell in phase space, and therefore the fluxes in (14) can be defined in terms of ratios of definite integrals. We illustrate by averaging the analytic equation for a one-dimensional sphere. Multiplying (7) by $4\pi r^2 dr d\mu$ and integrating we have for the first term

$$\begin{aligned} 4\pi \int_{r_i}^{r_{i+1}} dr \int_{\mu_{m-1/2}}^{\mu_{m+1/2}} \frac{\mu \partial(r^2 N) d\mu}{\partial r} &= A_{i+1} \int_{\mu_{m-1/2}}^{\mu_{m+1/2}} \mu N_{i+1}(\mu) d\mu \\ &\quad - A_i \int_{\mu_{m-1/2}}^{\mu_{m+1/2}} \mu N_i(\mu) d\mu , \end{aligned} \tag{23}$$

where we have used our previous definition of A_i and written $N_{i+1}(\mu)$ for $N(r_{i+1}, \mu)$. We now see that, if we let

$$\int_{\mu_{m-1/2}}^{\mu_{m+1/2}} \mu N_i(\mu) d\mu \equiv 2 w_m \mu_m N_{i,m} \qquad \text{for } i \text{ or } i+1, \tag{24}$$

Eq. (23) is the same as (10). We therefore have

$$N_{i,m} = \int_{\mu_{m-1/2}}^{\mu_{m+1/2}} \mu N_i(\mu) d\mu \Big/ \left(\mu_m \int_{\mu_{m-1/2}}^{\mu_{m+1/2}} d\mu \right) \tag{25}$$

for the average flux at left face of the cell in Fig. 1. The average clearly depends upon the choice of the angular quadrature, but such a definition permits μ_m to be arbitrarily selected.

Integration of the second term of (7) over the finite cell gives

$$4\pi \int_{\mu_{m-1/2}}^{\mu_{m+1/2}} d\mu \int_{r_i}^{r_{i+1}} \frac{r\partial[(1-\mu^2)N]dr}{\partial\mu} \tag{26}$$
$$= 4\pi(1-\mu_{m+1/2}^2)\int_{r_i}^{r_{i+1}} rN_{m+1/2}(r)dr - 4\pi(1-\mu_{m-1/2}^2)\int_{r_i}^{r_{i+1}} rN_{m-1/2}(r)d\mu$$

where we have written $N_{m\pm1/2}(r)$ for $N(r, \mu_{m\pm1/2})$. Comparing (26) to (11), we identify

$$2\alpha_{m\pm1/2,i+1/2}N_{m\pm1/2,i+1/2} = 4\pi(1-\mu_{m\pm1/2}^2)\int_{r_i}^{r_{i+1}} rN_{m\pm1/2}(r)dr \tag{27}$$

thereby defining

$$N_{m\pm1/2,i+1/2} = \frac{4\pi(1-\mu_{m\pm1/2}^2)\int_{r_i}^{r_{i+1}} rN_{m\pm1/2}(r)dr}{2\alpha_{m\pm1/2,i+1/2}}. \tag{28}$$

From the definition (18) we see that all the α-coefficients are proportional to $A_{i+1} - A_i = 4\pi(r_{i+1}^2 - r_i^2)$. Writing $\alpha_{m\pm1/2,i+1/2} = (A_{i+1} - A_i)\beta_{m\pm1/2,i+1/2}$, we see that the definition of Eq. (28) can be written as

$$N_{m\pm1/2,i+1/2} = \frac{(1-\mu_{m\pm1/2}^2)\int_{r_i}^{r_{i+1}} rN_{m\pm1/2}(r)dr}{4\beta_{m\pm1/2,i+1/2}\int_{r_i}^{r_{i+1}} rdr}. \tag{29}$$

Finally, for the third term of (7), we identify with (12) to find

$$4\pi \int_{r_i}^{r_{i+1}} r^2dr \int_{\mu_{m-1/2}}^{\mu_{m+1/2}} N(r,\mu)d\mu = 2w_mV_{i+1/2}N_{i+1/2,m}, \tag{30}$$

which defines

$$N_{i+1/2,m} = \frac{\int_{r_i}^{r_{i+1}} r^2dr \int_{\mu_{m-1/2}}^{\mu_{m+1/2}} N(r,\mu)d\mu}{\int_{r_i}^{r_{i+1}} r^2dr \int_{\mu_{m-1/2}}^{\mu_{m+1/2}} d\mu}. \tag{31}$$

While the definitions of (25), (29), and (31) apply to one-dimensional spherical geometry, similar definitions can easily be found for other geometries.

CONSISTENCY OF THE DIFFERENCE EQUATION

With the definitions of A_i and $V_{i+1/2}$ that we have used, we have a discrete analog of Eq. (7). Hence we should be able to obtain (7) from (14) in the limit of small intervals as $2w \to d\mu$ and $r_{i+1} - r_i \to dr$. Examining Eq. (18) we see that

$$\lim_{2w \to d\mu} \frac{\alpha_{m+1/2} - \alpha_{m-1/2}}{2w} = \frac{\partial \alpha}{\partial \mu} = -\mu \left[\frac{1}{2} (A_{i+1} - A_i) \right]. \tag{32}$$

Integrating this equation gives

$$\alpha = (\text{constant} - \tfrac{1}{2}\mu^2)[\tfrac{1}{2}(A_{i+1} - A_i)]. \tag{33}$$

Since α must vanish at both ends of the direction range the constant is $\frac{1}{2}$. In the same vein,

$$\lim_{2w \to d\mu} \frac{2\alpha_{m+1/2}N_{m+1/2} - 2\alpha_{m-1/2}N_{m-1/2}}{2w} = \frac{2\partial(\alpha N)}{\partial \mu} = \frac{A_{i+1} - A_i}{2} \frac{\partial[(1-\mu^2)N]}{\partial \mu} \tag{34}$$

by using Eq. (33). Dividing Eq. (14) by wV thus gives, as $2w \to d\mu$ and $\mu_m \to \mu$,

$$\frac{3\mu(r_{i+1}^2 N_{i+1} - r_i^2 N_i)}{(r_{i+1}^2 + r_i r_{i+1} + r_i^2)(r_{i+1} - r_i)} + \frac{3(r_{i+1}^2 - r_i^2)}{2(r_{i+1}^3 - r_i^3)} \frac{\partial[(1-\mu^2)N]}{\partial \mu} + \sigma N = S, \tag{35}$$

which, as $r_{i+1} - r_i \to dr$ and $r_{i+1} \to r_i \to r$, becomes (7).

We thus have derived a neutron-conserving approximation that is simple and that reduces to the analytic equation in the limit of small interval sizes. Equation (14) is quite general and can be used as a transport equation for the common one-dimensional geometries simply by defining A_i and $V_{i+1/2}$ properly. For example, in plane geometry, $A_{i+1} = A_i = 1$, and the terms in α vanish. In cylindrical geometry it is necessary to treat both components of $\boldsymbol{\Omega}$, but Eq. (14) can still be used by careful ordering of the angular quadrature set [5]. Any two-dimensional geometry that is curved in at most one direction, e.g., (r, z) and (r, θ) cylindrical or (x, y) rectangular geometries, can be treated by inserting a term

$$w\eta(B_{j+1}N_{j+1} - B_j N_j) \tag{36}$$

in Eq. (14), where N_{j+1} is an abbreviation for $N_{i+1/2,j+1,m}$ and all fluxes depend on the j subscript. The B_j are area elements of the cell faces perpendicular to the j direction and η is a direction cosine similar to μ. For instance, in (x, y)

geometry, $\eta \equiv \mathbf{\Omega} \cdot \mathbf{e}_y$. The absence of curvature in the j direction implies that $B_{j+1} = B_j$. In the same fashion, (14) can be extended to three-dimensional geometries. If the geometry is curved in more than one direction, another curvature term is added and the curvature coefficients determined exactly as the α coefficients.

It is worth noting that the α-coefficients provide a minimal direction coupling of fluxes. In discrete ordinates equations that are equivalent to the spherical harmonics equations [13], all the directions are coupled by a directional transfer matrix, a situation which is difficult and laborious to treat numerically. In the above derivation of the α-coefficients we used a number of undetermined coefficients just sufficient to be determined by the conditions imposed, but the use of more general assumptions is not precluded.

An Alternate Formulation of a Discrete Approximation

We refer to the above formulation, in which the position of the direction cosine within the direction interval is unspecified, as the general discrete S_n(GDS_n) method. This approach is used in the DSN codes [14], but in these the treatment of the curvature terms is somewhat different. Curvature coefficients defined by (18) and the GDS_n method are used in more recent codes, e.g., DTF-IV [15].

An alternate approach is possible; μ may be specified to be $\bar{\mu} = \frac{1}{2}(\mu_{m+1/2} + \mu_{m-1/2})$ and an intermediate N determined on the basis of some assumed variation of N with respect to μ in Eq. (24). We illustrate the possibilities by developing a consistent linear S_n (CLS_n) method in which the angular dependence of $N(\mu)$ in (24) is represented by connected straight-line segments. This type of representation was originally used in the first [8] S_n formulation which we here refer to as the linear S_n(LS_n) formalism. This LS_n development, although found to be very accurate in homogeneous systems, was replaced because of several disadvantages compared to the GDS_n method. Perhaps most importantly, the method failed to preserve optical reciprocity. This difficulty was traced to the fact that the method consists of a nonsymmetric angular quadrature [7]. In addition, the method required recursions with more terms and proved difficult to generalize to multidimensional geometries. These shortcomings are overcome by the CLS_n formulation described here.

A linear (in μ) function that assumes the value $N_{m+1/2}(r)$ at $\mu = \mu_{m+1/2}$ and the value $N_{m-1/2}(r)$ at $\mu_{m-1/2}$ is given by

$$N(r, \mu) = [(\mu - \mu_{m-1/2})N_{m+1/2}(r) + (\mu_{m+1/2} - \mu)N_{m-1/2}(r)]/2w_m . \quad (37)$$

If this function is evaluated at $r = r_i$, it assumes the corner values $N_{i,m\pm1/2}$ on the left side of Fig. 1. For this function the integral average of Eq. (24) is

$$\int_{\mu_{m-1/2}}^{\mu_{m+1/2}} \mu N(r_i, \mu) d\mu = 2w_m(pN_{i,m+1/2} + qN_{i,m-1/2}) \tag{38}$$

where

$$p = \tfrac{1}{6}(2\mu_{m+1/2} + \mu_{m-1/2}), \tag{39}$$
$$q = \tfrac{1}{6}(\mu_{m+1/2} + 2\mu_{m-1/2}).$$

In (14), by letting

$$\mu_m N_{i,m} = pN_{i,m+1/2} + qN_{i,m-1/2} \tag{40}$$

for

$$i \text{ or } i+1$$

and

$$2N_{m+1/2,i+1/2} = N_{m+1/2,i} + N_{m+1/2,i+1}; \tag{41}$$

the LS_n equations for spherical geometry can be obtained [16]. Equation (41) is consistent with the assumption of a constant or linear flux along the top and bottom faces of the cell of Fig. 1.

Instead of following this procedure we use only (40), substituting in (14) to obtain

$$w\bar{\mu}(A_{i+1}N_{i+1,m} - A_iN_{i,m}) + \frac{w^2}{6}A_{i+1}(N_{i+1,m+1/2} - N_{i+1,m-1/2}) \tag{42}$$
$$- \frac{w^2}{6}A_i(N_{i,m+1/2} - N_{i,m-1/2}) + \alpha_{m+1/2}N_{m+1/2} - \alpha_{m-1/2}N_{m-1/2} + \sigma NVw = SVw,$$

where

$$\bar{\mu} = \tfrac{1}{2}(\mu_{m+1/2} + \mu_{m-1/2}) \tag{43}$$

and

$$N_{i,m} = \tfrac{1}{2}(N_{i,m+1/2} + N_{i,m-1/2}) \text{ for } i \text{ or } i+1. \tag{44}$$

To eliminate the unwanted corner unknowns from (42) we make the expansion consistent with the assumed linearity of the angular flux,

$$N_{i,m\pm1/2} = \bar{N}_i + 3\mu_{m\pm1/2}I_i \text{ for } i \text{ or } i+1; \tag{45}$$

that is, we assume that the angular flux is adequately represented by the first two terms of a Legendre polynomial expansion. If Eqs. (22) and (19) are satisfied,

(45) is consistent with the definitions of (16) where $\bar{N}$ is the scalar flux and I is the current. Applying (45) to (42) we obtain

$$w\bar{\mu}(A_{i+1}N_{i+1} - A_iN_i) + w^3(A_{i+1}I_{i+1} - A_iI_i) + \alpha_{m+1/2}N_{m+1/2} - \alpha_{m-1/2}N_{m-1/2} + \sigma NVw = SVw\,, \tag{46}$$

which we call the CLS_n equations. Note that the additional term in (46) is a spatial derivative of the current which measures whether a cell is producing or absorbing particles and that the term is proportional to w^3 which becomes quite small as the direction mesh is refined. In order that (46) satisfy the balance equation (15) we must define

$$I_i = \sum_{m=1}^{M} w_m\bar{\mu}_m N_{im} + I_i \sum_{m=1}^{M} {w_m}^3\,; \tag{47}$$

that is, in terms of $\bar{\mu}$, the current is given by

$$I_i = \sum_{m=1}^{M} w_m\bar{\mu}_m N_{i,m} \Big/ \left(1 - \sum_{m=1}^{M} {w_m}^3\right). \tag{48}$$

Provided a symmetric quadrature set is used, it is not necessary to change the definition of the α-coefficients, for in the limit of constant flux, I, as given by (48), vanishes. Thus, the α-coefficients are defined by (18) with $\bar{\mu}$ replacing μ.

It can be shown that (46) reduces to the diffusion equations in the limit of slowly varying angular flux. In particular it is necessary that, similar to (22),

$$\Sigma w_m\bar{\mu}_m{}^2 + \tfrac{1}{3}\Sigma {w_m}^3 = \tfrac{1}{3}\,. \tag{49}$$

With the above definitions, (46) is a neutron-conserving formulation of the Boltzmann equation that incorporates a connected straight-line angular representation, and yet may be used with an arbitrary, symmetric angular quadrature set that satisfies (49). It can be shown [16] that, for two directions, the boundary condition of zero net inflow applied to (46) corresponds to the current-over-flux condition $I/N = \frac{1}{2}$ which is the same as the Double P_0 ratio. In general, boundary conditions are applied to the μ-weighted flux (40), which in the CLS_n case is $\bar{\mu}N_m + w^2I$.

Equation (46) can be generalized, in the same manner as (14), to two- and three-dimensional geometries and hence this difficulty in the original LS_n formulation is overcome. Instead of the four corner fluxes of (42), (46) contains only the two currents. However, since the currents depend on all angular fluxes, an iterative solution is implied. That is, currents cannot be computed until all angular fluxes are calculated, and, hence, currents will depend on previous in-

formation. Normally, S also must be recomputed iteratively so that no extra iterative effort is required. In fact, as described below, solution of (14) or (46) is facilitated by approximations which introduce the current, I.

The above GDS_n equations illustrate the use of the integral of (24) to formulate an approximation to the transport equation. It should be clear that much more general assumptions are possible both in (24) and (28). Any such assumptions used in these averages (or the averages appropriate to the geometry considered) will satisfy the zero divergence condition provided the assumed forms reduce to a constant when the fluxes in the representation are a constant. For example, in (37) if the two fluxes on the right are a constant, then $N(r, \mu)$ is constant.

It is worth noting that Eq. (42) can be derived in another manner. The finite-cell formulation is, in the limit of small w_m, given by

$$\mu[A_{i+1}N_{i+1}(\mu) - A_iN_i(\mu)] + \frac{A_{i+1} - A_i}{2}\frac{\partial[(1-\mu^2)N(\mu)]}{\partial\mu} + \sigma VN(\mu) = VS\,.$$

Equation (42) can be formed by substituting (37) in this equation and integrating over the $(\mu_{m-1/2}, \mu_{m+1/2})$ interval.

Solution of the Discrete Formulation of the Boltzmann Transport Equation

The equations derived in the preceding section contain more unknowns than there are determining relations. For instance, assuming that μ is positive and that one is preceding in order of increasing m index, N_i and $N_{m-1/2}$ can be assumed known from boundary conditions or calculations in adjoining cells, but N, N_{i+1} and $N_{m+1/2}$ are unknowns. The equations necessary to determine these unknowns are called difference relations. In this section we review the standard difference relations that have been used and discuss alternate approaches to formulating difference relations that have been motivated by shortcomings of the standard relations. Again we emphasize use of properties of the analytic transport equation.

Some of the methods described below have been carefully considered [17] in one-dimensional geometries. We are primarily interested in methods applicable to two-dimensional geometries. Our interest is motivated by the poor performance, in certain two-dimensional problems, of difference relations which seem to be entirely adequate in one dimension. We sometimes illustrate points in one-dimensional plane geometry for which a systematic treatment is possible in terms of tabulated approximations to the exponential function. However, such a treatment is not possible in general geometries, and here our discussions are explora-

tory. Similarly, we do not attempt to give error estimates for the various difference schemes proposed below. It is our feeling, based on computational experience, that such estimates are of less relative importance within the context of finite-cell equations which correctly incorporate basic physical principles. Nevertheless, one may want to know the effect, for a given difference relation, of refining spatial or angular quadratures. Such effects are most conventiently determined by solving a few typical problems for a progression of interval sizes. In one-dimensional plane geometry it can be shown, by comparing analytic solutions of the difference equations to analytic solutions of the transport equation in some simple problems, that the error in using the diamond relations described below is proportional to $\sigma\Delta x$ unless the weights are equal when the error is proportional to $(\sigma\Delta x)^2$. In the same situation, the methods based on the integral equation also have errors proportional to $(\sigma\Delta x)^2$. Here Δx is the (uniform) mesh spacing $x_{i+1} - x_i$.

A midvalue or diamond difference scheme is a set of difference relations which involve function values along the *sides* of a mesh cell; a corner-point or central difference scheme is a set of difference relations which involve function values at the *corners* of a mesh cell. Both usually also involve function values over the interior of a cell. Depending on *how* the relations are derived we distinguish between representation schemes, based on an assumed behavior or form of N and S over the cell, and characteristic schemes based on assumed forms for N and S and the physics of flow within a cell. In either case, additional degrees of freedom can be obtained by introducing weights on the function values. If the solution of the Boltzmann equation happen to possess the properties assumed, then no approximation is made in using the difference relations; the greater the disparity between the actual solution and the assumed properties, the greater the error that is made. Although certain of the assumptions that are made in deriving difference relations are consistent with assumptions made in formulating the transport equation, all of the difference relations displayed below may be used with any of the above formulations.

A set of diamond difference equations based on an assumed smooth behavior of the underlying function is the following:

$$\begin{aligned} N &= aN_{i+1} + (1-a)N_i\,, && \mu > 0\,, \\ N &= (1-a)N_{i+1} + aN_i\,, && \mu < 0\,, \\ N &= bN_{m+1/2} + (1-b)N_{m-1/2}\,, \end{aligned} \tag{50}$$

where a and b are constants on the interval $[\frac{1}{2}, 1]$. The above relations are designed for extrapolating N_{i+1} when $\mu > 0$, N_i when $\mu < 0$, and $N_{m+1/2}$ for all μ. When $a = b = \frac{1}{2}$ the equations, which are the same for all μ, can be pictured as a plane

surface passing through the fluxes at the midpoints of the cell boundaries in Fig. 1. If $a = b = 1$, the so-called step-function difference equations are obtained. These expressions equate the cell-centered fluxes to appropriate boundary fluxes.

If we suppose that $\mu < 0$ and that we are proceeding in the direction of increasing m index, then (50) can be used to eliminate N_i and $N_{m+1/2}$ from (14). By solving the resulting equation for N we obtain

$$N = \frac{|\mu| N_{i+1}[(1-a)A_i + aA_{i+1}]/a + N_{m-1/2}[(1-b)\alpha_{m+1/2} + b\alpha_{m-1/2}]/bw + SV}{|\mu| A_i/a + \alpha_{m+1/2}/wb + \sigma V}. \tag{51}$$

When $\mu > 0$ the appropriate equation is obtained by interchanging A_{i+1} and A_i and N_i and N_{i+1} in (51). Assuming that the source is known, from a previous iteration if necessary, N can be calculated from (51) and (50) can be used to extrapolate N_{i+1} or N_i and $N_{m+1/2}$. Thus, Eq. (51) can be used for a recursive solution for all directions and space cells. Boundary values furnish starting values for N_i (or N_{i+1}), but some initial value must be found for $N_{m-1/2}$ for $m = 1$. In practice this is accomplished by including in the direction set unweighted "singular" directions [5] ($\mu = -1$ in spherical geometry) in which there is no angular redistribution. Then with $w = 0$, the cell in Fig. 1 has zero height so that $N_{m+1/2} = N_{m-1/2}$ and, from (50), both equal N. This result and the fact that $\alpha_{m+1/2}w = -\mu(A_{i+1} - A_i)$ for these directions provide enough information to solve (14). The resultant expression is simply (51) without the term in $N_{m-1/2}$ in the numerator and with $b = 1$ in the denominator. The disadvantage of such procedure is that, in cylinders and many other geometries, there may be many such directions and the time spent in calculations to provide starting values may be excessive.

One way to eliminate the need for starting values is to use the step-function approximation, $b = 1$, for the angular difference relation. Then, because $\alpha_{1/2} = 0$ by definition, the coefficient of $N_{m-1/2}$ in the numerator of (51) vanishes and no starting value is needed.

Another possibility is to assume that (45) holds for $\mu = \mu_m$. Then the cell boundary flux is approximated by

$$N_{m+1/2} \approx N_m + \frac{\partial N_m}{\partial \mu}(\mu_{m+1/2} - \mu_m) = N_m + 3I(\mu_{m+1/2} - \mu_m). \tag{52}$$

The use of this approximation for the angular fluxes $N_{m+1/2}$ and $N_{m-1/2}$ in Eq. (14) produces the recursion[4]

[4] When this equation is solved, values of I from a previous iteration are used. An iterative process is usually necessary, in any case, to allow for a dependence of S on N, e.g., due to a scattering source. See Reference [5] for details of iteration procedures.

$$N = \frac{|\mu| N_{i+1}[(1-a)A_i + aA_{i+1}]/a + \alpha_{m-1/2}N_{m-1}(w + \beta I + SV)^{-1}}{|\mu| A_i/a + \alpha_{m+1/2}(w + \sigma V)^{-1}} \tag{53}$$

where N_{m-1} is N for the preceeding value of m and

$$\beta = 3[(\mu_{m-1/2} - \mu_{m-1})\alpha_{m-1/2} - (\mu_{m+1/2} - \mu_m)\alpha_{m+1/2}]/w. \tag{54}$$

This approximation (with $a = \frac{1}{2}$) seems to be of accuracy comparable to the diamond difference [$a = \frac{1}{2}$, $b = \frac{1}{2}$ in (51)] equations when used in the calculation of homogeneous-sphere critical radii. Although (52) can be used with either the GDS_n or the CLS_n formulations, the approach is particularly consistent with the CLS_n method which, in addition, already requires the use of the current I.

We now turn to an examination of some of the shortcomings of the difference relations of Eq. (50). In plane geometry, Eq. (51) becomes, with $\Delta x = x_{i+1} - x_i$,

$$N = \frac{|\mu| N_{i+1} + S\Delta x a}{|\mu| + \sigma \Delta x a}, \tag{55}$$

which gives a positive result for N whenever S and N_{i+1} are positive. The extrapolation for N_i, using (50), gives

$$N_i = \frac{[|\mu| - \sigma\Delta x(1-a)]N_{i+1} + S\Delta x}{|\mu| + a\sigma\Delta x}. \tag{56}$$

Now notice that, in this extrapolation, it is possible for the coefficient of N_{i+1} to become negative. Whenever

$$\frac{\sigma\Delta x(1-a)}{|\mu|} > 1 \tag{57}$$

that is, whenever the particle path across the cell measured in mean free paths is too large, the coefficient of N_i is negative. If this negative contribution is less than $S\Delta x/(|\mu| + \sigma\Delta x a)$, N_i remains positive; however, in this case, damped (because for $a > \frac{1}{2}$ the coefficient of N_{i+1} is less than unity in magnitude) oscillations can be propagated through the spatial mesh. If, on the other hand, the contribution is so negative that N_i is negative, the effect may very well be catastrophic. That is, if a sufficient number of angular fluxes are negative, the scalar flux $\bar{N}$ can be negative. Because S usually depends strongly on $\bar{N}$, even S for the next iteration may be negative. In plane geometry the remedy is usually simple—decrease Δx. However, this is not always practical. An artifice that is presently used is the following: If N_i calculated by (56) is negative, N_i is set equal to zero. To conserve particles this information is used in Eq. (14) and N is calculated from

$$N = (|\mu| N_i + S\Delta x)/\sigma\Delta x . \tag{58}$$

While this procedure works, and can be generalized to all geometries, it has several disadvantages. First, it stops only the negative fluxes and does nothing to improve possible oscillations. Second, it has only a pragmatic basis and there is no way to assess the accuracy or validity of the method. Below we describe a more useful method which is based on the physical properties of the transport equation.

In two-dimensional (x, y) geometry with $\mu = \mathbf{\Omega} \cdot \mathbf{e}_x$ and $\eta = \mathbf{\Omega} \cdot \mathbf{e}_y$, the equation corresponding to (55) is

$$\begin{aligned} N &= [|\mu| \Delta y N_i/a + |\eta| \Delta x N_j/b + S\Delta x\Delta y]/D , \\ D &= [|\mu| \Delta y/a + |\eta| \Delta x/b + \sigma\Delta x\Delta y] . \end{aligned} \tag{59}$$

As written, the above equation is for μ and η greater than zero and the difference assumptions are $N = (1 - a)N_i + aN_{i+1}$ and $N = (1 - b)N_j + bN_j$. In this geometry the appropriate equations for the other three combinations of $\pm\mu$, $\pm\eta$ can be obtained by interchanging N_i for N_{i+1} and N_j for N_{j+1}. Here the extrapolation process leads to more-serious difficulties than in plane geometry. Calculating N_{i+1} and N_{j+1} from (59) gives

$$\begin{aligned} N_{i+1} = \langle N_i[|\mu| \Delta y - (1 - a)|\eta| \Delta x/b - (1 - a)\sigma\Delta x\Delta y] \\ + |\eta| \Delta x N_j/b + S\Delta x\Delta y\rangle/aD , \end{aligned} \tag{60a}$$

$$\begin{aligned} N_{j+1} = \langle N_j[|\eta| \Delta x - (1 - b)|\mu| \Delta y/b - (1 - b)\sigma\Delta x\Delta y] \\ + |\mu| \Delta y N_i/a + S\Delta x\Delta y\rangle/bD . \end{aligned} \tag{60b}$$

Now, for some value of the ratio $\varrho = |\eta\Delta x/\mu\Delta y|$, either the coefficient of N_i in (60a) or that of N_j in (60b) is negative (regardless of the size of $\sigma\Delta x\Delta y$) provided $a < 1$ and $b < 1$. When $a = b = \frac{1}{2}$, one of the coefficients is negative for all values of ϱ, that is, with the diamond difference relations, damped oscillations (at least) are propagated at all times. To understand the cause of this difficulty, it is necessary to remember that the particle flux at a point is due to the contributions from sources which lie along a straight line in the direction of particle motion. In Fig. 2 we have drawn two such characteristic lines, assuming that μ and η are greater than zero. It is clear that for this direction, N_{j+1} depends more strongly on N_i than it does on N_j and N as assumed by the diamond equations. The difficulty in the extrapolations in (60) can thus be related to the "crossing" of char-

acteristic lines. This suggests a modified approach based on the method of characteristics.

Consider the cell shown in Fig. 3, where, instead of centered edge fluxes we use corner fluxes. In this case we assume μ and η to be greater than zero and that

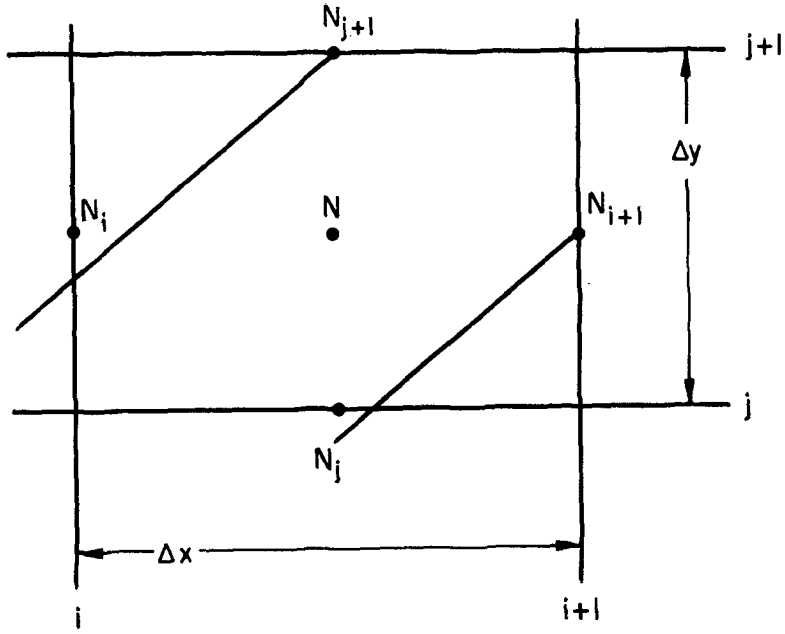

FIG. 2.

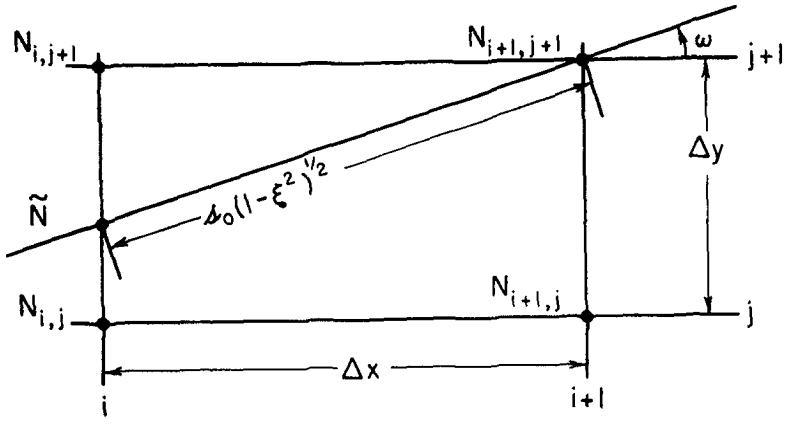

FIG. 3.

all the corner fluxes except $N_{i+1,j+1}$ are known. We now determine $N_{i+1,j+1}$ by using the integral form of the transport equation which can be written

$$N(\mathbf{r}, \mathbf{\Omega}) = N_0(\mathbf{r} - s_0\mathbf{\Omega}, \mathbf{\Omega})\exp(-\sigma s_0) + \int_0^{s_0} \exp(-\sigma s)S(\mathbf{r} - s\mathbf{\Omega}, \mathbf{\Omega})ds. \quad (61)$$

In (61), N_0 is a boundary value of the flux, and s_0 is the distance back along the direction of particle motion from $\mathbf{r}$ to the system boundary. For the cell of Fig. 3 the boundary flux is $\tilde{N}$ and particles travel a distances s_0 within the cell to reach $x = x_{i+1}$, $y = y_{j+1}$. The projection of s_0 onto the plane of the figure is s_0 times the sine of the angle between $\mathbf{\Omega}$ and the z axis, i.e., $s_0(1 - \xi^2)^{1/2}$ where $\xi = \mathbf{\Omega} \cdot \mathbf{e}_z$. Since $s_0(1 - \xi^2)^{1/2} \cos \omega = \Delta x$ and $(1 - \xi^2)^{1/2} \cos \omega = \mu$, $s_0 = \Delta x/\mu$. Applying this information to (61) we have

$$N_{i+1,j+1} = \tilde{N} \exp(-\sigma \Delta x/\mu) + \int_0^{x/\mu} \exp(-\sigma s)S \, ds. \quad (62)$$

We now assume that S is constant over the cell so that

$$N_{i+1,j+1} = \tilde{N} \exp(-\sigma \Delta x/|\mu|) + S[1 - \exp(-\sigma \Delta x/|\mu|)]/\sigma. \quad (63)$$

A further assumption is necessary to determine $\tilde{N}$. Since $N_{i,j+1}$ and N_{ij} are assumed known, $\tilde{N}$ can be determined by linear interpolation which gives

$$\tilde{N} = \varrho N_{ij} + (1 - \varrho)N_{i,j+1}, \quad (64)$$

where $\varrho = |\eta \Delta x/\mu \Delta y|$ as before. In the event the characteristic intercepts the horizontal cell boundary in Fig. 3., $s_0 = \Delta y/\eta$ and $\tilde{N}$ is interpolated from the bottom corner fluxes. These equations determine $N_{i+1,j+1}$, but the cell-centered flux, N, is as yet unknown. To maintain particle conservation, N is determined from the appropriate form of Eq. (14) assuming that

$$\begin{aligned} 2N_i &= N_{i,j+1} + N_{i,j}, \\ 2N_{i+1} &= N_{i+1,j+1} + N_{i+1,j}, \\ 2N_j &= N_{i,j} + N_{i+1,j}. \end{aligned} \quad (65)$$

It is helpful to examine this approach in plane geometry. Then (62) becomes

$$N_{i+1} = N_i \exp(-\sigma \Delta x/|\mu|) + S(1 - \exp(-\sigma \Delta x/|\mu|))/\sigma. \quad (66)$$

Substituting this expression in the appropriate form of (14) we find

$$N = [S(t - u)/\sigma + uN_i]/t, \tag{67}$$

where

$$t = \sigma\Delta x/|\mu|, u = 1 - \exp(-t). \tag{68}$$

When S/σ is eliminated from (66) by using (67) the result is a difference scheme

$$N = aN_{i+1} + (1 - a)N_i \qquad a = 1/u - 1/t, \tag{69}$$

with a assuming values in the range $\frac{1}{2} \leq a \leq 1$ as a function of t. When $\mu < 0$, the appropriate equations are obtained by interchanging N_i and N_{i+1} in (66), (67), and (69).

In this instance, recourse to the analytic transport equation is productive; values of the weighting coefficient a are obtained from the physics of the Boltzmann equation rather than by arbitrary selection. It is illuminating to examine (67) as the exponential is approximated. We find that for

$$\exp(-t) \approx (1 - \tfrac{1}{2}t)/(1 + \tfrac{1}{2}t), \tag{70}$$

Eq. (69) becomes the diamond difference relation with $a = \frac{1}{2}$. Further, for $\exp(-t) \approx 1/(1 + t)$, the step-function equations are obtained. Thus, a systematic means of producing difference relations is provided. In addition we see that the difficulty encountered in (54) is due to the approximation $\exp(-t) \approx [1 - (1 - a)t](1 + at)^{-1}$, which can assume negative values. Therefore, a possibility which eliminates negative coefficients is to approximate the exponential by, say, (70); but if $t > 2$, replace the exponential by zero. Table I shows the

TABLE I

SLAB CRITICAL HALF-THICKNESSES

Number of spatial intervals	Half-thickness in mean free paths
2	9.7403
5	5.9959
10	5.7153
20	5.6739
40	5.6668
80	5.6660
exact [8]	5.6655

results of using this approximation to calculate slab critical half-thicknesses. For these calculations, the neutron secondaries ratio, $c = (\nu\sigma_f + \sigma_s)/\sigma$, is 1.02. Many other nonnegative approximations for the exponential are possible.

In the computations of Table I double Gauss–Legendre quadrature [6] of order DP_7 was used. It is interesting to note that, for 5 spatial intervals, the exponential is replaced by zero in 12 of 16 directions, but yet the result is in error by less than 6%. Similar results are obtained for larger values of c.

As has been pointed out, it is not possible to eliminate all negative coefficients in the extrapolations of Eq. (60) when weighted difference equations similar to those of (50) are used. However, it is possible to ameliorate the difficulty by utilizing information about the orientation of the characteristic. We illustrate such a method by using a variant of (66). Suppose that, in plane geometry, we only go half-way across the cell with (66), letting

$$N = \nu N_i + (1 - \nu)S/\sigma \quad \nu = \exp(-t/2). \tag{71}$$

Then, using this value of N, we proceed the rest of the way by letting

$$N_{i+1} = \nu N + (1 - \nu)S/\sigma\,. \tag{72}$$

Subtracting these two equations we find a weighted difference scheme

$$(1 + \nu)N = N_{i+1} + \nu N_i. \tag{73}$$

In two-dimensional (x, y) geometry, (73) is an appropriate difference scheme for x-extrapolation when the characteristic is horizontal, that is, when $\varrho = \eta\Delta x/\mu\Delta y = 0$ because $\eta = 0$. In this situation, with S constant in the cell we have

$$N_{j+1} = N\,. \tag{74}$$

On the other hand, when $\varrho = 1$, the characteristics in Fig. 2 pass through N_i and N_j and we can write

$$\begin{aligned} N_{i+1} &= \nu N_j + (1 - \nu)S/\sigma\,, \\ N_{j+1} &= \nu N_i + (1 - \nu)S/\sigma\,, \end{aligned} \tag{75}$$

which is equivalent to

$$N_{i+1} + \nu N_i = N_{j+1} + \nu N_j\,. \tag{76}$$

When $\varrho = 1$ we must, as in this equation, have symmetry, i.e., similar difference

relations for N_{i+1} and N_{j+1} extrapolations. This symmetry is not affected if, instead of (76), we write

$$\begin{aligned} N_{i+1} + \nu N_i &= (1 + \nu)N, \\ N_{j+1} + \nu N_j &= (1 + \nu)N. \end{aligned} \tag{77}$$

For general ϱ in the range [0, 1], then, we can interpolate linearly between the equations for $\varrho = 0$ and those for $\varrho = 1$. This process gives (73) for all N_{i+1} extrapolations and

$$(1 + \varrho\nu)N = N_{j+1} + \varrho\nu N_j. \tag{78}$$

With this scheme the coefficient of N_i is always positive in the extrapolation for N_{i+1}, and while the coefficient of N_j can sometimes be negative in the extrapolation for N_{j+1}, the negative coefficient is relatively small compared to the coefficient of N_i in the same extrapolation.

Clearly, many such variants are possible. One variation, more elementary than the one described above, has been tested. In the test problem, fluxes produced using (50) (with $a = b = \frac{1}{2}$) displayed anomalous oscillations, but fluxes calculated using the variant were much smoothed.

In the aforegoing we have by no means exhausted the possibilities for deriving difference relations. We have demonstrated the principles which are applicable, and have noted that characteristic schemes can be constructed without disturbing neutron conservation. We have also gained insight into difficulties occurring in presently used schemes, and obtained more meaningful recipes for lessening or preventing flux oscillations as a result of extrapolation.

References

1. B. Davison, "Neutron Transport Theory." Oxford University Press, London (1957).
2. K. M. Case, *Ann. Phys. (N. Y.)* **9**, 1 (1960).
3. G. J. Mitsis, "Transport Solutions to the Monoenergetic Critical Problems," Argonne National Laboratory Report ANL-6787 (1963).
4. J. H. Bennett, *Nucl. Sci. Eng.* **19**, 209 (1964).
5. B. Carlson and K. Lathrop, "Transport Theory, The Method of Discrete Ordinates," Los Alamos Scientific Laboratory Report LA-3251-MS (Revised) (1965).
6. B. Carlson and C. Lee, "Mechanical Quadrature and the Transport Equation," Los Alamos Scientific Laboratory Report LAMS-2573 (1961).

7. K. LATHROP and B. CARLSON, "Discrete Ordinates Angular Quadrature of the Neutron Transport Equation," Los Alamos Scientific Laboratory Report LA-3186.

8. B. CARLSON and G. BELL, P/2386 *in* "Proceedings of the Second United Nations International Conference on the Peaceful Uses of Atomic Energy." United Nations, Geneva (1958).

9. S. CHANDRESKHAR, "Radiative Transfer." Oxford University Press, London (1950).

10. B. CARLSON, "A Method of Moments for Solving the Neutron Transport Equation," Los Alamos Scientific Laboratory Report LA-3060 (1965).

11. B. CARLSON and K. LATHROP, *Trans. Am. Nucl. Soc.* **8**, 487 (1965).

12. P. D. LAX, *Commun. Pure Appl. Math.* **7**, 159 (1954).

13. G. GOERTZEL, *Nucl. Sci. Eng.* **4**, 581 (1958).

14. B. CARLSON, C. LEE, and J. WORLTON, "The DSN and TDC Neutron Transport Codes," Los Alamos Scientific Laboratory Report LAMS-2346 (1960).

15. K. LATHROP, "DTF-IV, a FORTRAN-IV Program for Solving the Multigroup Transport Equation with Anisotropic Scattering," Los Alamos Scientific Laboratory Report LA-3373 (1965).

16. B. CARLSON and K. LATHROP, "Relation Between Present and Original S_n Method," Los Alamos Internal Memo, T-1-450 (1965).

17. E. H. Bareiss, "A Survey and Classification of Transport Theory Calculation Techniques," P/639 *in* Reference 8.