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Convergence of Singular Difference Approximations for the Discrete Ordinate Equations in x-y Geometry

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Abstract. The solutions to two well-known finite difference approximations are shown to converge to the solution of the discrete ordinate equations which are an approximation to the linear Boltzmann equation. These difference schemes are the diamond approximation of Carlson, and the central difference approximation. These schemes are known to give singular systems of algebraic equations in certain cases. Despite this singularity, convergence is shown for all cases when solutions exist.

1. Introduction. In this paper, we analyze some of the characteristics of certain numerical approximations to the time-independent one-velocity linear Boltzmann equation which is commonly known as the neutron transport equation. The transport equation is an integro-differential equation whose characteristics and derivation may be found in [1].

In practical applications, it is rare to encounter a neutron transport problem that can be solved exactly. Therefore, many different numerical techniques have been developed to approximate the solution of the transport equation. Our attention in this paper will be focused on one method, the method of discrete ordinates [1]. The discrete ordinate approximation was first introduced by Wick [2] and Chandrasekhar [3]. Discretization error estimates for the discrete ordinate approximation are found in [4], [5], [6].

After the discrete ordinate approximation is made, there remains a coupled system of partial differential equations. Again, in most practical applications it is unusual to be able to solve these equations explicitly. Various finite difference methods have been used to approximate the solution of the discrete ordinate equations and, in this paper, we concern ourselves primarily with the diamond difference approximation of Carlson [7]. The diamond approximation is a second order scheme and is considered for vacuum, reflecting, and periodic boundary conditions.

If a finite difference formulation leads to a nonsingular system of algebraic equations, then the existence of a unique solution is guaranteed. However, if the difference formulation leads to a singular system, then a solution need not be unique and may not even exist. It is known [8] that for vacuum boundary conditions the diamond scheme gives a nonsingular system of equations. For periodic boundary conditions the diamond scheme gives a singular or nonsingular system depending on the particular mesh chosen, [8]. Finally, for reflecting conditions, the diamond scheme always leads to a singular system [9]. For these last two singular cases, it is known, however,

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that the singular system always has a solution which, in fact, is unique in a certain sense, [8], [9].

In this paper, we show that for any of the above boundary conditions (including the singular cases), the solution of the diamond difference equations converges to the solution of the discrete ordinate equations. The convergence is shown in two norms: a discrete L_2 norm, and a maximum norm. The convergence rate is $O(h^2)$ for the discrete L_2 norm, where h is the maximum mesh spacing. These results answer some of the questions raised by Gelbard et al. in [10]. We also show how these same results can be obtained for the central difference approximation considered in [9].

2. Diamond Difference Approximation. The one-velocity form of the discrete ordinate equations in x-y geometry may be written as

$$\Omega_x^m \frac{\partial \phi^m}{\partial x} + \Omega_y^m \frac{\partial \phi^m}{\partial y} + \Sigma^T \phi^m - \sum_{n=1}^{\tau} w^n \Sigma^{m,n} \phi^n = S^m, \qquad m = 1, 2, \cdots, \tau, \tag{1}$$

where

ϕ^m is the flux in direction $\mathbf{\Omega}^m$,
Σ^T is the total cross section,
S^m is the source term,
w^n represents the quadrature weights,
$\Sigma^{m,n}$ is the scattering cross section from direction $\mathbf{\Omega}^n$ to direction $\mathbf{\Omega}^m$,
Ω_x^m, Ω_y^m, Ω_z^m are the direction cosines of $\mathbf{\Omega}^m$,
τ is the number of discrete directions used.

Equations (1) are the two-dimensional discrete ordinate equations and will be considered in the domain D defined by $0 \leqq x \leqq L_x$, $0 \leqq y \leqq L_y$. The Eqs. (1) will be subject to certain conditions prescribed on ∂D, the boundary of D. The vacuum conditions are:

$$\text{If } (x, y) \in \partial D \text{ and } \mathbf{\Omega}^m \cdot \mathbf{n} < 0, \text{ where } \mathbf{n} \text{ is an outward drawn normal at } (x, y), \text{ then } \phi^m(x, y) = 0. \tag{2}$$

The periodic conditions are:

$$\begin{aligned} \phi^m(0, y) &= \phi^m(L_x, y), \qquad 0 \leqq y \leqq L_y,\ m = 1, 2, \cdots, \tau, \\ \phi^m(x, 0) &= \phi^m(x, L_y), \qquad 0 \leqq x \leqq L_x,\ m = 1, 2, \cdots, \tau. \end{aligned} \tag{3}$$

Kellogg [11] has shown that reflecting boundary conditions are really a subclass of the periodic conditions, so vacuum and periodic boundary conditions are all that need be considered (the results of this paper can be directly verified for the reflecting conditions using exactly the same techniques).

To approximate the solution of Eqs. (1), we first impose a rectangular mesh on D with the lines

$$\begin{aligned} x &= x_0, \quad x = x_1, \cdots, x = x_I, \qquad 0 = x_0 < x_1 < \cdots < x_I = L_x, \\ y &= y_0, \quad y = y_1, \cdots, y = y_J, \qquad 0 = y_0 < y_1 < \cdots < y_J = L_y. \end{aligned}$$

The mesh spacings $\Delta x_i = x_i - x_{i-1}$ and $\Delta y_j = y_j - y_{j-1}$ are not assumed uniform. We introduce the mesh variables

$$N^m_{i,j}, \quad 1 \leqq i \leqq I,\ 1 \leqq j \leqq J,\ 1 \leqq m \leqq \tau,$$
$$V^m_{i,j}, \quad 0 \leqq i \leqq I,\ 1 \leqq j \leqq J,\ 1 \leqq m \leqq \tau,$$
$$H^m_{i,j}, \quad 1 \leqq i \leqq I,\ 0 \leqq j \leqq J,\ 1 \leqq m \leqq \tau.$$

These variables are associated with the imposed mesh as shown in Fig. 1. The discrete ordinate equations for the (i, j) mesh box are now approximated by the equations

$$\Omega^m_x\left(\frac{V^m_{i,j} - V^m_{i-1,j}}{\Delta x_i}\right) + \Omega^m_y\left(\frac{H^m_{i,j} - H^m_{i,j-1}}{\Delta y_j}\right) + \Sigma^T_{i,j} N^m_{i,j} - \sum_{n=1}^{\tau} w^n \Sigma^{m;n}_{i,j} N^n_{i,j} = S^m_{i,j}, \tag{4}$$

$$N^m_{i,j} = \tfrac{1}{2}(V^m_{i,j} + V^m_{i-1,j}) = \tfrac{1}{2}(H^m_{i,j} + H^m_{i,j-1}), \tag{5}$$

where $\Sigma^T_{i,j}$, $\Sigma^{m;n}_{i,j}$, and $S^m_{i,j}$ are the respective values of Σ^T, $\Sigma^{m,n}$, and S^m at the center of the (i, j) mesh box.

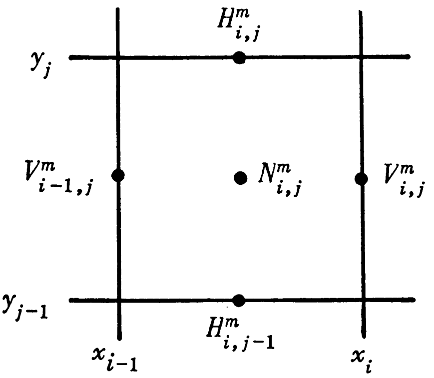

FIGURE 1. *Unknowns for the Diamond Approximation*

The vacuum boundary conditions are approximated by

$$\begin{aligned} V^m_{0,j} &= 0, \quad 1 \leqq j \leqq J, \text{ for all } m \text{ such that } \Omega^m_x > 0,\\ V^m_{I,j} &= 0, \quad 1 \leqq j \leqq J, \text{ for all } m \text{ such that } \Omega^m_x < 0,\\ H^m_{i,0} &= 0, \quad 1 \leqq i \leqq I, \text{ for all } m \text{ such that } \Omega^m_y > 0,\\ H^m_{i,J} &= 0, \quad 1 \leqq i \leqq I, \text{ for all } m \text{ such that } \Omega^m_y < 0, \end{aligned} \tag{6}$$

and the periodic boundary conditions are approximated by

$$\begin{aligned} V^m_{0,j} &= V^m_{I,j}, \quad 1 \leqq j \leqq J,\ 1 \leqq m \leqq \tau,\\ H^m_{i,0} &= H^m_{i,J}, \quad 1 \leqq i \leqq I,\ 1 \leqq m \leqq \tau. \end{aligned} \tag{7}$$

Equations (4) and (5), together with boundary conditions (6) or (7), define the diamond difference approximation to the discrete ordinate equations with vacuum or periodic boundary conditions, respectively.

It is convenient to define

$$\Sigma_{i,j}^{a;m} = \Sigma_{i,j}^{T} - \sum_{n=1}^{\tau} w^n \Sigma_{i,j}^{m;n}. \tag{8}$$

For the remainder of the paper, we make the following assumptions:

$$\sum_{m=1}^{\tau} w^m = 4\pi \quad \text{and} \quad w^m > 0 \quad \text{for all } m, \tag{9a}$$

$$\Sigma_{i,j}^{a;m} \geqq \Sigma_0 > 0 \quad \text{for all } i, j, m, \tag{9b}$$

$$\Sigma_{i,j}^{m;n} = \Sigma_{i,j}^{n;m} \quad \text{for all } i, j, m, n, \tag{9c}$$

$$\Sigma_{i,j}^{m;n} \geqq 0 \quad \text{for all } i, j, m, n. \tag{9d}$$

If $\phi = (\phi^1, \phi^2, \cdots, \phi^\tau)$ is a vector whose components are functions of the variables x and y which have partial derivatives with respect to x and y up to order p, then we define

$$||\phi||_k = \max_m \max_{|\alpha| \leq k} \sup_{(x,y) \in D} \left| \frac{\partial^{|\alpha|} \phi^m}{\partial x^{\alpha_1} \partial y^{\alpha_2}} \right|, \qquad 1 \leqq k \leqq p,$$

where $\alpha = (\alpha_1, \alpha_2)$, $|\alpha| = \alpha_1 + \alpha_2$.

For any mesh function $\mathbf{N} = (N_{i,j}^m)$, we define the maximum norm of $\mathbf{N}$ as

$$||\mathbf{N}||_\infty = \max_{i,j,m} |N_{i,j}^m|,$$

and the discrete L_2 norm as

$$||\mathbf{N}|| = \left[\sum_{i,j,m} \Delta x_i \, \Delta y_j w^m (N_{i,j}^m)^2 \right]^{1/2}.$$

With the preceding definitions and assumptions we can prove the following theorem.

THEOREM 1 (BASIC INEQUALITY). *If* $\mathbf{N} = (N_{i,j}^m)$, $\mathbf{V} = (V_{i,j}^m)$, $\mathbf{H} = (H_{i,j}^m)$, *and* $\mathbf{S} = (S_{i,j}^m)$ *are vectors whose components satisfy* (4), (5), *and* (6) *or* (7), *then*

$$||\mathbf{N}|| \leqq \frac{1}{\Sigma_0} ||\mathbf{S}||.$$

Proof. Multiplying both sides of Eq. (4) by $w^m N_{i,j}^m \, \Delta x_i \, \Delta y_j$ and summing over all appropriate i, j, and m, we find that

$$\begin{aligned} &\sum_{i,j,m} \Omega_x^m \, \Delta y_j w^m N_{i,j}^m (V_{i,j}^m - V_{i-1,j}^m) + \sum_{i,j,m} \Omega_y^m \, \Delta x_i w^m N_{i,j}^m (H_{i,j}^m - H_{i,j-1}^m) \\ &\qquad + \sum_{i,j} \Delta x_i \, \Delta y_j \left[\sum_m \Sigma_{i,j}^T w^m (N_{i,j}^m)^2 - \sum_{m,n} w^n w^m \Sigma_{i,j}^{m;n} N_{i,j}^m N_{i,j}^n \right] \\ &= \sum_{i,j,m} \Delta x_i \, \Delta y_j \; w^m N_{i,j}^m S_{i,j}^m. \end{aligned} \tag{10}$$

Using (5) and (6) or (7), one can show that the first two summations appearing in (10) are nonnegative. Using (8), we may rewrite the third summation in (10) as

$$\sum_{i,j,m} \Delta x_i \, \Delta y_j w^m \Sigma_{i,j}^{a;m} (N_{i,j}^m)^2 + \sum_{i,j,m,n} \Delta x_i \, \Delta y_j w^m w^n \Sigma_{i,j}^{m;n} (N_{i,j}^m - N_{i,j}^n) N_{i,j}^m. \tag{11}$$

Using (9c), we rewrite the second sum in (11) as

$$\frac{1}{2} \sum_{i,j,m,n} \Delta x_i \, \Delta y_j w^m w^n \Sigma_{i,j}^{m;n} (N_{i,j}^m - N_{i,j}^n) N_{i,j}^m$$
$$+ \frac{1}{2} \sum_{i,j,m,n} \Delta x_i \, \Delta y_j w^n w^m \Sigma_{i,j}^{n;m} (N_{i,j}^n - N_{i,j}^m) N_{i,j}^n$$
$$= \frac{1}{2} \sum_{i,j,m,n} \Delta x_i \, \Delta y_j w^m w^n \Sigma_{i,j}^{m;n} (N_{i,j}^m - N_{i,j}^n)^2$$

which is, by (9d), nonnegative. Now, combining these results, from (10), we see that

$$\sum_{i,j,m} \Delta x_i \, \Delta y_j w^m \Sigma_{i,j}^{a;m} (N_{i,j}^m)^2 \leqq \sum_{i,j,m} \Delta x_i \, \Delta y_j w^m N_{i,j}^m S_{i,j}^m .$$

Using Schwarz's inequality and (9b), we have

$$\Sigma_0 \, ||\mathbf{N}||^2 \leqq ||\mathbf{N}|| \, ||\mathbf{S}|| \quad \text{or} \quad ||\mathbf{N}|| \leqq \frac{1}{\Sigma_0} ||\mathbf{S}||.$$

We remark that if $(\mathbf{N}, \mathbf{V}, \mathbf{H})$ is a solution of the diamond approximation, then the Basic Inequality establishes the uniqueness of $\mathbf{N}$.

3. Convergence of the Method. If $\boldsymbol{\phi} = (\phi^1, \phi^2, \cdots, \phi^r)$ is the solution to the discrete ordinate equations, and if $\mathbf{N} = (N_{i,j}^m)$, $\mathbf{V} = (V_{i,j}^m)$, and $\mathbf{H} = (H_{i,j}^m)$ are the solutions to the diamond scheme, then we define the error vector $\mathbf{e} = (e_{i,j}^m)$ by

$$e_{i,j}^m = \phi^m(x_i - \tfrac{1}{2} \Delta x_i, y_j - \tfrac{1}{2} \Delta y_j) - N_{i,j}^m .$$

Using the Basic Inequality, Taylor's theorem, and a simple averaging technique, the convergence of the diamond scheme is now easily demonstrated.

THEOREM 2. *Let $\boldsymbol{\phi} = (\phi^1, \phi^2, \cdots, \phi^r)$ be in $C^2[D]$ and have bounded third partial derivatives. If assumptions* (9) *are satisfied, then there exists a positive constant C independent of h and $\boldsymbol{\phi}$ such that $||\mathbf{e}|| \leqq C||\boldsymbol{\phi}||_3 \cdot h^2$, where $h = \max_{i,j} (\Delta x_i, \Delta y_j)$.*

Proof. Using $\boldsymbol{\phi} = (\phi^1, \phi^2, \cdots, \phi^r)$, we define the averaged vectors $\mathfrak{N} = (\mathfrak{N}_{i,j}^m)$, $\mathfrak{V} = (\mathfrak{V}_{i,j}^m)$ and $\mathfrak{H} = (\mathfrak{H}_{i,j}^m)$ by

$$\mathfrak{N}_{i,j}^m = \tfrac{1}{4}[\phi^m(x_i, y_j) + \phi^m(x_i, y_{j-1}) + \phi^m(x_{i-1}, y_j) + \phi^m(x_{i-1}, y_{j-1})],$$
$$\mathfrak{V}_{i,j}^m = \tfrac{1}{2}[\phi^m(x_i, y_j) + \phi^m(x_i, y_{j-1})],$$
$$\mathfrak{H}_{i,j}^m = \tfrac{1}{2}[\phi^m(x_i, y_j) + \phi^m(x_{i-1}, y_j)].$$

We remark that these vectors satisfy Eq. (5) exactly. Defining a vector $\mathbf{e}_1 = \mathfrak{N} - \mathbf{N}$, we see that the vector $\mathbf{e} - \mathbf{e}_1$ has components $\phi^m(x_i - \frac{1}{2} \Delta x_i, y_j - \frac{1}{2} \Delta y_j) - \mathfrak{N}_{i,j}^m$ and hence, by Taylor's theorem,

$$||\mathbf{e} - \mathbf{e}_1|| \leqq C' \, ||\boldsymbol{\phi}||_2 \cdot h^2 .$$

Therefore, it will suffice to estimate $||\mathbf{e}_1||$. Substituting $\mathfrak{N}$, $\mathfrak{V}$, $\mathfrak{H}$, and $\mathbf{N}$, $\mathbf{V}$, $\mathbf{H}$ into (4) and (5), subtracting the two respective resulting sets of equations, and applying the Basic Inequality shows that

$$||\mathbf{e}_1|| \leqq \frac{1}{\Sigma_0} ||\boldsymbol{\delta}||,$$

where $\boldsymbol{\delta}$ satisfies $||\boldsymbol{\delta}|| \leqq C''||\boldsymbol{\phi}||_3 \cdot h^2$. The last inequality is obtained by several applications of Taylor's theorem. Therefore, there exists a constant C such that

$$||\mathbf{e}|| \leqq C\,||\Phi||_3 \cdot h^2.$$

COROLLARY. *Let* $h' = \min_{i,j}(\Delta x_i, \Delta y_j)$, $h = \max_{i,j}(\Delta x_i, \Delta y_j)$, *and suppose there exists a positive constant* C_1 *such that, for all meshes chosen,* $h \leqq C_1 h'$. *Then, under the assumptions of Theorem* 2, *we have the following estimate for the maximum norm of* $\mathbf{e}$. *There exists a constant C independent of h and* Φ *such that*

$$||\mathbf{e}||_\infty \leqq C\,||\Phi||_3 \cdot h.$$

Proof. Let $|e^{m_0}_{i_0,j_0}| = ||\mathbf{e}||_\infty$. Then we have

$$\Delta x_{i_0}\, \Delta y_{j_0} w^{m_0} (e^{m_0}_{i_0,j_0})^2 \leqq \sum_{i,j,m} \Delta x_i\, \Delta y_j w^m (e^m_{i,j})^2 = ||\mathbf{e}||^2.$$

Solving for $|e^{m_0}_{i_0,j_0}|$, we have from Theorem 2 and the hypotheses that

$$||\mathbf{e}||_\infty = |e^{m_0}_{i_0,j_0}| \leqq \frac{(w^{m_0})^{-1/2}}{(\Delta x_{i_0}\, \Delta y_{j_0})^{1/2}}\, ||\mathbf{e}|| \leqq \frac{C_2\, ||\Phi||_3 \cdot h^2}{h'}$$

$$\leqq \frac{C_1 C_2\, ||\Phi||_3 \cdot h^2}{h} \leqq C\,||\Phi||_3 \cdot h.$$

Using the transformation given in [9] which relates the diamond difference approximation to the central difference approximation considered in [8] and [9], it is easy to show that the results of this paper apply to the central difference approximation when solutions to it exist. The questions of existence of a solution to the central difference approximation for the various boundary conditions are considered in [8], [9].

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