NUCLEAR SCIENCE AND ENGINEERING: 100, 142-148 (1988)

Boundary Treatment of the Diffusion Synthetic Acceleration Method for Fixed-Source Discrete-Ordinates Problems in x-y Geometry

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Received July 24, 1987
Accepted January 18, 1988

Abstract — *A study on the development of acceleration equations for boundary cells and the associated boundary conditions for the diffusion synthetic acceleration method of neutron transport problems in x-y geometry is described. Alcouffe's algebraic manipulation of the P_1 equations resulting in a single diffusion equation is modified to obtain explicit acceleration equations for the boundary cells. To accomplish this, the discretization in space is performed according to the ordinary box-centered method. The resulting synthetic computation scheme is linear in its differenced form. The boundary cell difference equations are derived in a manner that exactly parallels the discretization of the diffusion equation for interior mesh cells and that of the transport equation. The importance of these equations in improving overall efficiency without sacrificing stability is discussed, as is the optimum choice of the boundary conditions associated with these equations.*

I. INTRODUCTION

The diffusion synthetic acceleration (DSA) method[1-6] has been extensively used to accelerate the slow convergence of the standard source iteration (SI) method for discrete ordinates problems in optically thick regions with scattering ratios c near unity. Stability difficulties of early versions of the DSA method have been resolved by Alcouffe[4] by altering the differencing of the diffusion equation.

One important issue not discussed in the fundamental work of Alcouffe[4] is the problem of establishing difference equations to accelerate the scalar flux at the physical boundaries of the problem under consideration. It is well known that to have an unconditionally stable iteration-acceleration scheme, the differencing of the diffusion equation must precisely parallel the differencing of the transport equation. For this reason, differenced acceleration equations at the boundary cells that possess this compatibility are very important in preserving the efficiency of the DSA method without sacrificing stability. In the present work, we derive acceleration equations for cells on the problem boundary, called boundary acceleration equations, possessing a spatial discretization that is consistent with the discretization of the diffusion equation. We also find the optimum choice of boundary conditions associated with these equations to improve the efficiency of the acceleration scheme. Some progress on this problem has been made by Larsen,[5] but the success there is limited to problems in slab geometry.

The derivation of compatible differenced boundary acceleration equations in x-y geometry turns out to be a nontrivial problem. As we demonstrate in the present work, the standard difference form of the two-dimensional DSA method[4] must be altered. The spatial discretization is performed according to the box-centered difference scheme,[7] which is a natural extension of the diamond-difference (DD) approximation. We point out that the resulting acceleration scheme is linear in its difference form. The reliability, in general, of a linear acceleration technique compared

to a nonlinear one has been pointed out by Gelbard et al.,[8,9] both for fixed-source[8] and eigenvalue[9] computations.

The organization of this paper is as follows. In Sec. II, the development of the box-centered difference transport and diffusion equations for interior mesh points is given. The extension of this algebraic procedure for boundary mesh points along with the derivation of certain boundary conditions is described in Sec. III. In Sec. IV, numerical results are presented and, finally, Sec. V contains a brief summary and conclusions. It should be emphasized that our analysis is based on the DD transport equation.

II. FORMULATION OF THE BOX-CENTERED DIFFERENCE EQUATIONS

In this section, the differenced form of the transport equation and the diffusion acceleration equation for interior points is derived in x-y geometry. The implemented spatial discretization scheme has been introduced by Keller[7] in the context of numerical solutions of partial differential equations. It is well known as the box method and is a simple extension of the DD scheme.

Let us divide the rectangle x-y domain into cells as seen in Fig. 1, with $i = 1, \ldots, I$ and $j = 1, \ldots, J$. The cross sections σ and σ_s are taken to be piecewise constant and can change values only at the (half-integer) cell boundaries. The standard DD discrete ordinates equations with isotropic scattering and fixed sources are

$$\mu_m k_j \left(\psi^{l+1/2}_{mi+1/2,j} - \psi^{l+1/2}_{mi,j}\right) + \eta_m h_i \left(\psi^{l+1/2}_{mij+1/2} - \psi^{l+1/2}_{mij-1/2}\right) + \sigma_{ij} V_{ij} \psi^{l+1/2}_{mij} = \sigma_{s_{ij}} V_{ij} \varphi^{l}_{00_{ij}} + V_{ij} S_{ij} \quad , \tag{1}$$

where

l = iteration index

μ_m, η_m = direction cosines with respect to x and y axes

h_i, k_j = mesh spacings

$V_{ij} = h_i k_j$

and the diamond equations

$$\psi_{mij} = \frac{1}{2}\left(\psi_{mi+1/2,j} + \psi_{mi-1/2,j}\right) = \frac{1}{2}\left(\psi_{mij+1/2} + \psi_{mij-1/2}\right) \quad . \tag{2}$$

The flux moments are calculated by the approximation

$$\varphi^{l+1/2}_{rs_{ij}} = \sum_m w_m Y_{rs}(\mu_m, \eta_m) \psi^{l+1/2}_{mij} \quad , \tag{3}$$

where

w_m = integration weight factors

$Y_{rs}(\mu_m, \eta_m)$ = spherical harmonics.

Formulating the desired acceleration scheme, we derive a set of synthetic equations by taking the zeroth and the two first discrete moments (with respect to μ and η) of Eq. (1). To carry this out, Eq. (1) is multiplied successively by w_m, $w_m \mu_m$ and $w_m \eta_m$. Following the procedure developed by Larsen,[5,6] we define the acceleration equations as

$$k_j \left(f^{l+1}_{10_{i+1/2,j}} - f^{l+1}_{10_{i,j}}\right) + h_i \left(f^{l+1}_{01_{i,j+1/2}} - f^{l+1}_{01_{ij}}\right) + \sigma_{r_{ij}} V_{ij} f^{l+1}_{00_{ij}} = \sigma_{s_{ij}} V_{ij} \left(\varphi^{l+1/2}_{00_{ij}} - \varphi^{l}_{00_{ij}}\right) \quad , \tag{4a}$$

$$D_{ij} \left(f^{l+1}_{00_{i+1/2,j}} - f^{l+1}_{00_{i-1/2,j}}\right) + h_i f^{l+1}_{10_{ij}} = 0 \quad , \tag{4b}$$

and

$$D_{ij} \left(f^{l+1}_{00_{ij+1/2}} - f^{l+1}_{00_{ij-1/2}}\right) + k_j f^{l+1}_{01_{ij}} = 0 \quad , \tag{4c}$$

where

$$D_{ij} = 1/(3\sigma_{ij}) \quad ,$$

$$\sigma_{r_{ij}} = \sigma_{ij} - \sigma_{s_{ij}} \quad ,$$

and

$$f^{l+1}_{rs} = \varphi^{l+1}_{rs} - \varphi^{l}_{rs} \quad . \tag{5}$$

Equations (4) are a discretized form of the P_1 equations.

We now seek the form of a single difference diffusion type equation. Alcouffe[4] presented an algebraic procedure that allows the system of P_1 acceleration equations to collapse down to a single diffusion equation. Adding to Eq. (4a) the corresponding equations for the adjacent cells $(i+1,j)$, $(i,j+1)$, and $(i+1,j+1)$ and introducing to the resulting equation the DD approximations for the first moments f_{10} and f_{01}, we obtain

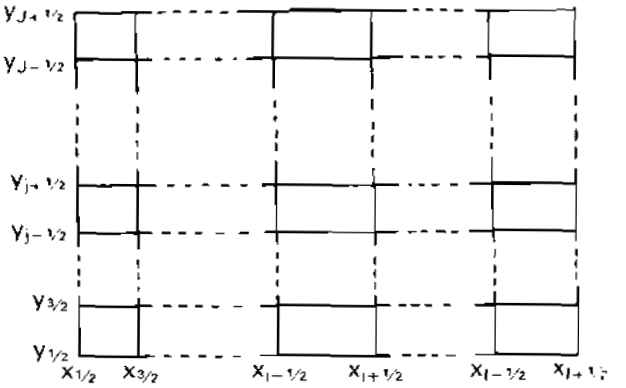

Fig. 1. Cell-centered mesh in x-y geometry.

$$-2k_j f_{10_{ij}}^{l+1} + 2k_j f_{10_{i+1j}}^{l+1} - 2k_{j+1} f_{10_{ij+1}}^{l+1} + 2k_{j+1} f_{10_{i+1j+1}}^{l+1} - 2h_i f_{01_{ij}}^{l+1} - 2h_{i+1} f_{01_{i+1j}}^{l+1} + 2h_i f_{01_{ij+1}}^{l+1} + 2h_{i+1} f_{01_{i+1j+1}}^{l+1}$$
$$+ \sigma_{r_{ij}} V_{ij} f_{00_{ij}}^{l+1} + \sigma_{r_{i+1j}} V_{i+1j} f_{00_{i+1j}}^{l+1} + \sigma_{r_{ij+1}} V_{ij+1} f_{00_{ij+1}}^{l+1} + \sigma_{r_{i+1j+1}} V_{i+1j+1} f_{00_{i+1j+1}}^{l+1} = g_{i+\frac{1}{2}j+\frac{1}{2}} \ , \tag{6}$$

where

$$g_{i+\frac{1}{2}j+\frac{1}{2}} = \sum_{p=i}^{i+1} \sum_{q=j}^{j+1} \sigma_{s_{pq}} V_{pq} (\varphi_{00_{pq}}^{l+\frac{1}{2}} - \varphi_{00_{pq}}^{l}) \ .$$

Then we substitute Eqs. (4b) and (4c) into Eq. (6) to find

$$2\left[D_{ij} \frac{k_j}{h_i} \left(f_{00_{i+\frac{1}{2}j}} - f_{00_{i-\frac{1}{2}j}} \right)^{l+1} - D_{i+1j} \frac{k_j}{h_{i+1}} \left(f_{00_{i+\frac{3}{2}j}} - f_{00_{i+\frac{1}{2}j}} \right)^{l+1} + D_{ij+1} \frac{k_{j+1}}{h_i} \left(f_{00_{i+\frac{1}{2}j+1}} - f_{00_{i-\frac{1}{2}j+1}} \right)^{l+1} \right.$$
$$- D_{i+1j+1} \frac{k_{j+1}}{h_{i+1}} \left(f_{00_{i+\frac{3}{2}j+1}} - f_{00_{i+\frac{1}{2}j+1}} \right)^{l+1} + D_{ij} \frac{h_i}{k_j} \left(f_{00_{ij+\frac{1}{2}}} - f_{00_{ij-\frac{1}{2}}} \right)^{l+1}$$
$$+ D_{i+1j} \frac{h_{i+1}}{k_j} \left(f_{00_{i+1j+\frac{1}{2}}} - f_{00_{i+1j-\frac{1}{2}}} \right)^{l+1} - D_{ij+1} \frac{h_i}{k_{j+1}} \left(f_{00_{ij+\frac{3}{2}}} - f_{00_{ij+\frac{1}{2}}} \right)^{l+1}$$
$$\left. - D_{i+1j+1} \frac{h_{i+1}}{k_{j+1}} \left(f_{00_{i+1j+\frac{3}{2}}} - f_{00_{i+1j+\frac{1}{2}}} \right)^{l+1} \right]$$
$$+ \sigma_{r_{ij}} V_{ij} f_{00_{ij}}^{l+1} + \sigma_{r_{i+1j}} V_{i+1j} f_{00_{i+1j}}^{l+1} + \sigma_{r_{ij+1}} V_{ij+1} f_{00_{ij+1}}^{l+1} + \sigma_{r_{i+1j+1}} V_{i+1j+1} f_{00_{i+1j+1}}^{l+1} = g_{i+\frac{1}{2}j+\frac{1}{2}} \ . \tag{7}$$

Since this equation contains a lot of variables, Alcouffe approximated two adjacent cell-edge fluxes with an arithmetic average of the flux value at the intermediate cell vertex, e.g.,

$$D_{ij} k_j f_{00_{i+\frac{1}{2}j}} + D_{ij+1} + k_{j+1} f_{00_{i+\frac{1}{2}j+1}} = (D_{ij} k_j + D_{ij+1} k_{j+1}) f_{00_{i+\frac{1}{2}j+\frac{1}{2}}} \ .$$

In addition, he introduced a nonlinear approximation on the removal term. However, although the implementation of these approximations leads to a tractable five-point diffusion equation, it does not allow the construction of compatible differenced boundary acceleration equations.

To avoid this drawback, the scalar fluxes at intermediate mesh points and at mesh centers are eliminated, according to the ordinary box-centered difference method, by the use of

$$f_{00_{i+\frac{1}{2}j}} = \frac{1}{2} \left(f_{00_{i+\frac{1}{2}j+\frac{1}{2}}} + f_{00_{i+\frac{1}{2}j-\frac{1}{2}}} \right) \ , \tag{8a}$$

$$f_{00_{ij+\frac{1}{2}}} = \frac{1}{2} \left(f_{00_{i+\frac{1}{2}j+\frac{1}{2}}} + f_{00_{i-\frac{1}{2}j+\frac{1}{2}}} \right) \ , \tag{8b}$$

and

$$f_{00_{ij}} = \frac{1}{4} \left(f_{00_{i-\frac{1}{2}j-\frac{1}{2}}} + f_{00_{i-\frac{1}{2}j+\frac{1}{2}}} + f_{00_{i+\frac{1}{2}j-\frac{1}{2}}} + f_{00_{i+\frac{1}{2}j+\frac{1}{2}}} \right) \ , \tag{8c}$$

respectively. As a result, we obtain the following equation:

$$-R_{ij} f_{00_{i-\frac{1}{2}j-\frac{1}{2}}}^{l+1} + (S_{ij} + S_{i+1j}) f_{00_{i+\frac{1}{2}j-\frac{1}{2}}}^{l+1} - R_{i+1j} f_{00_{i+\frac{3}{2}j-\frac{1}{2}}}^{l+1} + (T_{ij} + T_{ij+1}) f_{00_{i-\frac{1}{2}j+\frac{1}{2}}}^{l+1}$$
$$+ (Q_{ij} + Q_{i+1j} + Q_{ij+1} + Q_{i+1j+1}) f_{00_{i+\frac{1}{2}j+\frac{1}{2}}}^{l+1} + (T_{i+1j} + T_{i+1j+1}) f_{00_{i+\frac{3}{2}j+\frac{1}{2}}}^{l+1} - R_{ij+1} f_{00_{i-\frac{1}{2}j+\frac{3}{2}}}^{l+1}$$
$$+ (S_{ij+1} + S_{i+1j+1}) f_{00_{i+\frac{1}{2}j+\frac{3}{2}}}^{l+1} - R_{i+1j+1} f_{00_{i+\frac{3}{2}j+\frac{3}{2}}}^{l+1} = g_{i+\frac{1}{2}j+\frac{1}{2}} \ . \tag{9}$$

where

$$Q_{ij} = D_{ij} \left(\frac{k_j}{h_i} + \frac{h_i}{k_j} \right) + \frac{1}{4} V_{ij} \sigma_{ij} \ , \tag{10a}$$

$$R_{ij} = D_{ij} \left(\frac{k_j}{h_i} + \frac{h_i}{k_j} \right) - \frac{1}{4} V_{ij} \sigma_{ij} \ , \tag{10b}$$

$$S_{ij} = D_{ij} \left(\frac{k_j}{h_i} - \frac{h_i}{k_j} \right) + \frac{1}{4} V_{ij} \sigma_{ij} \ , \tag{10c}$$

and

$$T_{ij} = D_{ij} \left(-\frac{k_j}{h_i} + \frac{h_i}{k_j} \right) + \frac{1}{4} V_{ij} \sigma_{ij} \ . \tag{10d}$$

From the nine-point diffusion equation, Eq. (9), we can calculate the correction term $f_{00_{i+\frac{1}{2}j+\frac{1}{2}}}^{l+1}$. We now complete the acceleration scheme by shifting the unknowns in Eq. (1) from cell-average and cell-edge angular fluxes to cell-vertex angular fluxes. Substituting the box scheme approximations into Eq. (1) yields

$$(2\mu_m k_j + 2\eta_m h_i + \sigma_{ij}V_{ij})\psi^{l+1/2}_{mi+1/2j+1/2} + (2\mu_m k_j - 2\eta_m h_i + \sigma_{ij}V_{ij})\psi^{l+1/2}_{mi+1/2j-1/2}$$
$$+ (-2\mu_m k_j + 2\eta_m h_i + \sigma_{ij}V_{ij})\psi^{l+1/2}_{mi-1/2j+1/2} + (-2\mu_m k_j - 2\eta_m h_i + \sigma_{ij}V_{ij})\psi^{l+1/2}_{mi-1/2j-1/2}$$
$$= \sigma_{s_{ij}}V_{ij}\left(\varphi^l_{00_{i+1/2j+1/2}} + \varphi^l_{00_{i-1/2j+1/2}} + \varphi^l_{00_{i+1/2j-1/2}} + \varphi^l_{00_{i-1/2j-1/2}}\right) + 4V_{ij}S_{ij} , \quad (11)$$

which determines the corner angular fluxes only.

The acceleration scheme now consists of the vertex-differenced transport and diffusion equations, Eqs. (11) and (9), respectively. The present approach is characterized by the absence of any approximations that destroy the consistency and the full compatibility of the equations in their difference form. The synthetic iteration process is linear and the nine-point diffusion equation has been derived in a way that exactly parallels the differencing of the transport equation. In Sec. III, we use a similar procedure to give consistent boundary equations for the discretized diffusion equation, Eq. (9), defined for interior mesh points only.

III. FORMULATION OF THE DIFFERENCE SCHEME AT THE BOUNDARIES

We now turn to the question of providing boundary cell equations to the discretized diffusion equation, Eq. (9), defined for interior net points. It is obvious that these equations associated with certain boundary conditions will improve the convergence rate of the acceleration scheme, and we accomplish this without sacrificing stability. In this section, we first develop consistent boundary conditions and then derive explicit acceleration equations on f^{l+1}_{00} at the boundary mesh points.

III.A. Boundary Conditions

The objective is to generate the diffusion boundary conditions from the transport boundary conditions,[5] and the guiding principle is the assumption that the exact transport solution is a linear function of μ and η. We first treat the left boundary, at $x = x_{1/2}$ and $y = y_{j+1/2}$, $j = 0,1,\ldots,J$. If there is a prescribed incident flux, then we consider

$$\psi_{1/2j+1/2}(\mu,\eta) = \varphi_{00_{1/2j+1/2}} + 3\mu\varphi_{10_{1/2j+1/2}} + 3\eta\varphi_{01_{1/2j+1/2}} \quad (12a)$$

for $0 \le \mu \le 1$, $-(1-\mu^2)^{1/2} \le \eta \le (1-\mu^2)^{1/2}$, and the integral that defines the flux moments has been transformed to the corresponding integral over a disk. If we require the diffusion angular flux on this boundary defined by

$$\psi^{l+1}_{1/2j+1/2}(\mu,\eta) = \varphi^{l+1}_{00_{1/2j+1/2}} + 3\mu\varphi^{l+1}_{10_{1/2j+1/2}} + 3\eta\varphi^{l+1}_{01_{1/2j+1/2}} \quad (12b)$$

to satisfy the same boundary conditions as the transport flux, then we obtain the following condition on the correction term:

$$f^{l+1}_{00_{1/2j+1/2}} + 3\mu f^{l+1}_{10_{1/2j+1/2}} + 3\eta f^{l+1}_{01_{1/2j+1/2}} = 0 ,$$
$$0 \le \mu \le 1 , \quad -(1-\mu^2)^{1/2} \le \eta \le (1-\mu^2)^{1/2} , \quad (13)$$

which becomes exact on convergence. Multiplying Eq. (13) by $(1/2\pi)(1-\mu^2-\eta^2)^{-1/2}w(\mu)$ and integrating over $0 \le \mu \le 1$ and $-(1-\mu^2)^{1/2} \le \eta \le (1-\mu^2)^{1/2}$ yields

$$f^{l+1}_{10_{1/2j+1/2}} = -\lambda f^{l+1}_{00_{1/2j+1/2}} , \quad j = 0,1,\ldots,J , \quad (14)$$

where

$$\lambda = \frac{1}{3}\frac{\displaystyle\int_0^1 \int_{-(1-\mu^2)^{1/2}}^{(1-\mu^2)^{1/2}} w(\mu)(1-\mu^2-\eta^2)^{-1/2}\,d\eta\,d\mu}{\displaystyle\int_0^1 \int_{-(1-\mu^2)^{1/2}}^{(1-\mu^2)^{1/2}} \mu w(\mu)(1-\mu^2-\eta^2)^{-1/2}\,d\eta\,d\mu} . \quad (15)$$

By setting $w(\mu) = \mu^n$, $n = 1,2,\ldots$, we find $\lambda = (n+1)/3n$. For a prescribed incident flux, including the case of vacuum boundary conditions, any choice of the function $w(\mu)$ leading to a parameter λ greater than zero is physically justified, while for reflecting boundary conditions $\lambda = 0$. Finally, in the limit as $\lambda \to \infty$, the correction term f^{l+1}_{00} becomes zero, which corresponds to a DSA method without acceleration at the boundaries. In Sec. IV, we present a detailed experimental study on the effect of the parameter λ.

Next, we treat the bottom boundary at $x = x_{i+1/2}$, $i = 0,1,\ldots,I$, and $y = y_{1/2}$. For a prescribed incident flux on this boundary, we find

$$f^{l+1}_{00_{i+1/2\,1/2}} + 3\mu f^{l+1}_{10_{i+1/2\,1/2}} + 3\eta f^{l+1}_{01_{i+1/2\,1/2}} = 0 ,$$
$$-1 \le \mu \le 1 , \quad 0 \le \eta \le (1-\mu^2)^{1/2} . \quad (16)$$

Multiplying Eq. (16) by $(1/2\pi)(1-\mu^2-\eta^2)^{-1/2}w(\eta)$ and integrating over $-1 \le \mu \le 1$ and $0 \le \eta \le (1-\mu^2)^{1/2}$, we obtain the condition

$$f^{l+1}_{01_{i+1/2\,1/2}} = \lambda f^{l+1}_{00_{i+1/2\,1/2}} , \quad i = 0,1,\ldots,I . \quad (17)$$

Following the same procedure, we find

$$f^{l+1}_{10_{i+1/2j+1/2}} = -\lambda f^{l+1}_{00_{i+1/2j+1/2}} , \quad j = 0,1,\ldots,J \quad (18)$$

and

$$f^{l+1}_{01_{i+1/2J+1/2}} = \lambda f^{l+1}_{00_{i+1/2J+1/2}} , \quad i = 0,1,\ldots,I \quad (19)$$

at the two remaining boundaries of the two-dimensional grid.

III.B. Boundary Acceleration Equations

We now seek difference boundary equations, which associated with Eqs. (14), (17), (18), and (19) may yield explicit acceleration equations on f_{00}^{l+1} at the boundary net points. A detailed derivation of these equations is presented only at one of the four boundaries and also at one of the four corners. Similar analysis may be carried out to deduce the remaining equations.

We choose the left boundary at $x = x_{1/2}$ and $y = y_{j+1/2}$, $j = 1, \ldots, J-1$. Summing Eq. (4a) over two boundary adjacent cells $(1,j)$ and $(1,j+1)$ yields

$$k_j\left(f_{10_{1/2j}}^{l+1} - f_{10_{3/2j}}^{l+1}\right) + k_{j+1}\left(f_{10_{1/2j+1}}^{l+1} - f_{10_{3/2j+1}}^{l+1}\right) + h_1\left(f_{01_{1j+1}}^{l+1} - f_{01_{1j}}^{l+1}\right) + \sigma_{r_{1j}} V_{1j} f_{00_{1j}}^{l+1} + \sigma_{r_{1j+1}} V_{1j+1} f_{00_{1j+1}}^{l+1} = g_{1/2j+1/2} \ , \tag{20}$$

where

$$g_{1/2j+1/2} = \sum_{q=j}^{j+1} \sigma_{s_{1q}} V_{1q} \left(\varphi_{00_{1q}}^{l+1/2} - \varphi_{00_{1q}}^{l}\right) \ .$$

We introduce the DD approximation into Eq. (20) to obtain

$$2\left[k_j\left(f_{10_{1j}}^{l+1} - f_{10_{3/2j}}^{l+1}\right) + k_{j+1}\left(f_{10_{1j+1}}^{l+1} - f_{10_{3/2j+1}}^{l+1}\right) + h_1\left(f_{01_{1j+1}}^{l+1} - f_{01_{1j}}^{l+1}\right)\right] + \sigma_{r_{1j}} V_{1j} f_{00_{1j}}^{l+1} + \sigma_{r_{1j+1}} V_{1j+1} f_{00_{1j+1}}^{l+1} - g_{1/2j+1/2} \ . \tag{21}$$

Evaluating Eqs. (4b) and (4c) at $i = 1$ and $j = j, j+1$ and substituting the resulting equations for $f_{10_{1j}}$, $f_{10_{1j+1}}$, $f_{01_{1j}}$, and $f_{01_{1j+1}}$ into Eq. (21) gives

$$2\Bigg[D_{1j}\frac{h_1}{k_j}\left(f_{00_{1j+1/2}} - f_{00_{1j-1/2}}\right)^{l+1} - D_{1j+1}\frac{h_1}{k_{j+1}} \times \left(f_{00_{1j+3/2}} - f_{00_{1j+1/2}}\right)^{l+1} - k_j f_{10_{3/2j}}^{l+1} - D_{1j}\frac{k_j}{h_1}\left(f_{00_{3/2j}} - f_{00_{1/2j}}\right)^{l+1} - D_{1j+1}\frac{k_{j+1}}{h_1} \times \left(f_{00_{3/2j+1}} - f_{00_{1/2j-1}}\right)^{l+1} - k_{j+1} f_{10_{3/2j+1}}^{l+1}\Bigg] + \sigma_{r_{1j}} V_{1j} f_{00_{1j}}^{l+1} + \sigma_{r_{1j+1}} V_{1j+1} f_{00_{1j+1}}^{l+1} = g_{1/2j+1/2} \ . \tag{22}$$

Finally, we use the box method approximations, Eqs. (8), and the boundary condition, Eq. (14), to obtain the following six-point acceleration equation on $f_{00_{1/2j+1/2}}^{l+1}$, $j = 1, \ldots, J-1$:

$$(S_{1j} + \lambda k_j) f_{00_{1/2j-1/2}}^{l+1} - R_{1j} f_{00_{1/2j+1/2}}^{l+1} + [Q_{1j} + Q_{1j+1} + \lambda(k_j + k_{j+1})] f_{00_{1/2j-1/2}}^{l+1} + (T_{1j} + T_{1j+1}) f_{00_{3/2j+1/2}}^{l+1} + (S_{1j+1} + \lambda k_{j+1}) f_{00_{3/2j-1/2}}^{l+1} - R_{1j+1} f_{00_{3/2j+1/2}}^{l+1} = g_{1/2j+1/2} \ , \tag{23}$$

where the quantities Q, R, S, and T are as defined earlier.

In deriving the acceleration equation for the corner scalar flux at $(\frac{1}{2},\frac{1}{2})$, we use the system of P_1 equations, Eqs. (4), with $i = j = 1$. After we introduce the DD approximation into the resulting balance equation and replace the first moments of f at the cell center using the remaining two equations, we obtain

$$2\Bigg[-D_{11}\frac{k_1}{h_1}\left(f_{00_{3/2}} - f_{00_{1/2}}\right)^{l+1} - D_{11}\frac{h_1}{k_1} \times \left(f_{00_{1/2}} - f_{00_{1/2}}\right)^{l+1} - k_1 f_{10_{3/2}}^{l+1} - h_1 f_{01_{1/2}}^{l+1}\Bigg] + \sigma_{r_{11}} V_{11} f_{00_{11}}^{l+1} = \sigma_{s_{11}} V_{11}\left(\varphi_{00_{11}}^{l+1/2} - \varphi_{00_{11}}^{l}\right) \ . \tag{24}$$

Imposing the box-centered method approximations, Eqs. (8), and the boundary conditions, Eqs. (14) and (16), we find

$$[Q_{11} + \lambda(k_1 - h_1)] f_{00_{1/2,1/2}}^{l+1} + (T_{11} - h_1\lambda) f_{3/2,1/2}^{l+1} + (S_{11} + k_1\lambda) f_{00_{1/2,3/2}}^{l+1} - R_{11} f_{00_{3/2,3/2}}^{l+1} = \sigma_{s_{11}} V_{11}\left(\varphi_{00_{11}}^{l+1/2} - \varphi_{00_{11}}^{l}\right) \ . \tag{25}$$

The remaining boundary acceleration equations may be obtained easily operating in a similar fashion. This set of equations along with the diffusion equation, Eq. (9), result in a linear system where the number of equations is equal to the number of unknowns and overall to a complete DSA scheme.

IV. NUMERICAL RESULTS

Here we shall consider a model problem to demonstrate the convergence of the discretized linear synthetic scheme and to illustrate the effectiveness of the acceleration equations at the boundaries associated with the optimum boundary conditions. The physical system consists of a homogeneous square $L \times L$, with L equal to 30 mfp, purely reflective boundary conditions on the left and bottom boundaries, vacuum boundary conditions on the right and top boundaries, and a flat source.

Test computations have been carried out for various quadrature approximations and scattering ratios c, without negative angular flux fixup. The mesh intervals h_i and k_j are altered from 1 to 15 mfp. For the reflecting boundaries, the choice of $\lambda = 0$ in the boundary conditions is clear. For the vacuum boundaries, there are many ways that the parameter λ can be assigned and the choice, it turns out, can affect the rates of convergence significantly. A pointwise convergence criterion of 10^{-4} for the scalar flux is used. The DSA acceleration equations that arise from the box-centered difference method are solved efficiently using standard iterative methods (e.g., symmetric successive

overrelaxation). The CPU time of the implemented acceleration scheme compared to the CPU time of the standard SI method for the model problem ($c = 1.0$) is reduced by a factor of ~100. For all cases tested, no convergence difficulties were encountered.

Primary characteristics and typical results for our computations are given in Table I. The numerical results are for $c = 1.0$ (worst case), S_8 quadrature set, and $h_i = k_j$, and they present the number of iterations required for convergence with increasing mesh size and different values of λ including $\lambda = (n + 1)/3n$, $n = 1,2,\ldots$. The stability of the proposed linear DSA method against mesh size for this problem is demonstrated. We find experimentally $\frac{1}{3} \leq \lambda \leq \frac{2}{3}$ to be the optimum range of the parameter λ. This result is in agreement with the linear extrapolated distances,[10] which are used to obtain boundary conditions in diffusion theory. For $\lambda \geq 10$, the number of iterations required for convergence is constant, while as λ approaches zero, the numerical scheme, as expected, becomes unstable. The presented results, including the choice of $\lambda = \frac{4}{9}$ as the optimum diffusion boundary parameter, remain consistent for all test computations performed.

Finally, we address the issue of the importance of an acceleration method supplemented with explicit boundary acceleration equations. In Table II, we compare the complete acceleration technique consisting of acceleration equations for interior and boundary net points, with a similar incomplete acceleration scheme that does not accelerate the scalar flux f_{00} at the boundaries ($f_{00} = 0$). Although both algorithms are convergent, the improvement to the convergence rate obtained with the complete acceleration method is significant. It is seen that the inefficiency of the incomplete acceleration scheme exists on coarse and dense grid systems.

Note that the convergence performance of the incomplete DSA scheme is identical with the convergence performance of the complete DSA scheme as $\lambda \to \infty$, which is a limit situation in the framework of the complete acceleration method.

TABLE I

Number of Iterations Required for Convergence with Linear DSA Scheme for Varying Mesh Size and Boundary Condition Parameter λ

h (mfp)	λ									
	$\frac{1}{5}$	$\frac{1}{4}$	$\frac{1}{3}$	$\frac{2}{5}$	$\frac{4}{9}$	$\frac{1}{2}$	$\frac{2}{3}$	1	10	100
1	11	10	6	5	4	5	6	6	9	10
5	19	13	7	5	4	5	6	8	11	11
10	24	14	7	5	4	5	7	8	13	14
15	27	14	8	5	4	5	7	9	14	14

TABLE II

Convergence Performance of Linear DSA With and Without Acceleration of the Scalar Flux at the Boundaries

Cell Width (mfp)	Complete DSA ($\lambda = \frac{4}{9}$)	Incomplete DSA
1	4	12
5	4	13
10	4	14
15	4	14

V. CONCLUSIONS

A study has been carried out for accelerating the zeroth moment of the angular flux at boundary mesh points in x-y geometry resulting in a complete DSA method. The main advantage of the present work is that the derived nine-point vertex-differenced diffusion equation and the six-point vertex-differenced boundary acceleration equations are consistent with the difference transport equation. The iteration-acceleration algorithm is independent of the mesh width and has proven to be stable for the model problem. The importance of providing acceleration equations at the boundaries, associated with the best choice of the boundary condition parameter λ, has been demonstrated. The functions $w(\mu)$ and $w(\eta)$ that are involved in the computation of λ can be chosen in an arbitrary way. Our conclusion that the DSA method becomes optimum for $\frac{1}{3} \leq \lambda \leq \frac{2}{3}$ is valid only for the DD discrete ordinates transport equation. However, our results indicate that any acceleration scheme that provides consistently differenced boundary mesh point equations for the discretized diffusion equation can be expected to be significantly more efficient without sacrificing stability.

Another interesting feature of the proposed scheme, which is peripheral to the main purpose of this paper, is that it is linear in its difference form. An issue that we intend to investigate in future work on this subject is the comparison of the proposed linear technique with the standard nonlinear technique.

ACKNOWLEDGMENTS

The author would like to acknowledge many enlightening discussions about synthetic acceleration methods with E. W. Larsen.

This work was supported in part by U.S. Department of Energy Grant DE-AS05-80ER10711 and National Science Foundation Grant DMS-8312451.

REFERENCES

1. H. J. KOPP, *Nucl. Sci. Eng.*, **17**, 65 (1963).

2. E. M. GELBARD and I. A. HAGEMAN, *Nucl. Sci. Eng.*, **37**, 288 (1969).

3. W. H. REED, *Nucl. Sci. Eng.*, **45**, 237 (1971).

4. R. E. ALCOUFFE, *Nucl. Sci. Eng.*, **64**, 344 (1977).

5. E. W. LARSEN, *Nucl. Sci. Eng.*, **82**, 47 (1982).

6. E. W. LARSEN, *TTSP*, **13**, 107 (1984).

7. H. B. KELLER, *Numerical Solution of Partial Differential Equations—II*, B. HUBBARD, Ed., Academic Press, New York (1970).

8. E. M. GELBARD, D. R. McCOY, and E. W. LARSEN, *Trans. Am. Nucl. Soc.*, **39**, 462 (1981).

9. E. M. GELBARD, C. H. ADAMS, D. R. McCOY, and E. W. LARSEN, *Trans. Am. Nucl. Soc.*, **41**, 309 (1981).

10. K. M. CASE and P. F. ZWEIFEL, *Linear Transport Theory*, Addison-Wesley Publishing Company Inc., Reading, Massachusetts (1967).