Journal Title: Transport Theory and Statistical Physics

Volume: 13
Issue:
Month/Year: 1987
Pages: pp.107-??

Article Author: Larsen, E. W.

Article Title: Diffusion Synthetics Acceleration Methods for Discrete Ordinates Problems

TRANSPORT THEORY AND STATISTICAL PHYSICS, 13(1&2), 107-126 (1984)

DIFFUSION-SYNTHETIC ACCELERATION METHODS FOR DISCRETE-ORDINATES PROBLEMS*

Edward W. Larsen

University of California
Los Alamos National Laboratory
Los Alamos, New Mexico 87545

ABSTRACT

The diffusion-synthetic acceleration (DSA) method is an iterative procedure for obtaining numerical solutions of discrete-ordinates problems. The DSA method is operationally more complicated than the standard source-iteration (SI) method, but if encoded properly it converges much more rapidly, especially for problems with diffusion-like regions. In this article we describe the basic ideas behind the DSA method and give a (roughly chronological) review of its long development. We conclude with a discussion which covers additional topics, including some remaining open problems and the status of current efforts aimed at solving these problems.

I. INTRODUCTION

The diffusion-synthetic acceleration (DSA) method[1-30] has, in recent years, emerged as a powerful and reliable tool for obtaining very rapidly convergent solutions of discrete-ordinates problems[18,20,29,30]. However, the method has had a lengthy and uneven development[1-28]. Many of its basic ideas were first proposed by Kopp[1] (1963) in a general transport setting, and then were specialized to discrete-ordinates problems by Gelbard and Hageman[2] (1969). However, Reed[3] (1971) showed that, in its then current form, the numerical method was unstable for problems having spatial cells with optical widths larger than only about one mean free path. This instability was severe

*This work was performed under the auspices of the U.S. Department of Energy. Also, this article is a revision of a paper presented at (and published in the proceedings of) the ANS topical meeting "Advances in Reactor Computations," held in Salt Lake City, March 28-30, 1983.

0041-1405/84/1301-0107$3.50/0

enough that it prevented the method from being of general use for practical problems. Alcouffe[14] (1977) later explained the source of this instability, showed how to overcome it for the diamond-differenced discrete-ordinates equations, and demonstrated for the first time that DSA could be used to affect a dramatic decrease in the total computing effort on practical problems. More recently, Larsen[25] has generalized Alcouffe's ideas and developed a procedure which has produced stable DSA equations for every standard spatially differenced form of the discrete-ordinates equations on which testing has been performed.

In spite of the long twenty-year effort that has preceded this article, there are still open problems concerning the DSA method. Briefly, the present status of the method is as follows:

(a) A simple Fourier stability analysis now exists to explain both the basic ideas behind the DSA method and how to spatially discretize the diffusion part of the algorithm to make the method numerically stable.

(b) The development of stable DSA equations for general differencing schemes in general geometries, although straightforward, can become quite complicated and detailed.

(c) Important open questions remain, particularly concerning the existence of efficient ways to solve the DSA equations referred to in (b).

In this article we give a complete presentation of the theory described in (a), a flavor of the detail referred to in (b), and a more explicit description of the open questions described in (c). Our goal is simplicity and unity of presentation. Thus, we describe the theory in the context of linear DSA methods (which are amenable to the Fourier stability analysis) and one-dimensional slab geometry. Nonlinear methods and certain other topics will only be mentioned briefly.

We begin, in Sec. II, with a description of the standard source-iteration (SI) method for both the analytic transport and diamond-differenced discrete-ordinates equations. We do this to establish notation, to introduce the Fourier analysis, and to motivate the reasons for attempting to develop the DSA method. Then in Sec. III we develop the DSA method for fixed source problems, again for both the analytic transport and the diamond-differenced discrete-ordinates equations. We conclude, in Sec. IV, with a discussion of further aspects of the DSA method, open questions, and the focus of current research efforts.

This article is an updated version of a previous article[28] which appeared in the proceedings of a recent ANS topical meeting.

II. SOURCE ITERATION METHOD

The SI method can be described by the equations

$$\mu \frac{\partial \psi^{(\ell+1/2)}}{\partial x}(x,\mu) + \psi^{(\ell+1/2)}(x,\mu) = c\, \phi_0^{(\ell)}(x) + Q(x) \quad , \tag{1}$$

$$\phi_0^{(\ell+1/2)}(x) = \frac{1}{2} \int_{-1}^{1} \psi^{(\ell+1/2)}(x,\mu')\, d\mu' \quad , \tag{2}$$

where $c \leq 1$ and we treat boundary conditions, for now, as unspecified. This method has the following physical interpretation: with a starting guess $\phi_0^{(0)}(x) = 0$, $\phi_0^{(\ell)}(x)$ is the scalar flux due to all particles which have undergone fewer than ℓ collisions after emission by the source Q. For a nearly conservative ($c \simeq 1$) and optically thick system, most of the particles undergo a very large number of collisions; thus, on the basis of its physical interpretation, one can expect the SI method to converge slowly for this type of problem.

To examine this in more detail, let us define

$$\Psi^{(\ell+1/2)}(x,\mu) = \psi^{(\ell+1/2)}(x,\mu) - \psi^{(\ell-1/2)}(x,\mu) \quad , \tag{3a}$$

$$\Phi_0^{(\ell+1)}(x) = \phi_0^{(\ell+1)}(x,\mu) - \phi_0^{(\ell)}(x) \quad , \tag{3b}$$

as the difference between successive iterates in Eqs. (1)-(2). Then Eqs. (1) and (2) describe a stable, convergent method if and only if $\Psi^{(\ell+1/2)}$ and $\Phi_0^{(\ell)}$ tend to zero as ℓ tends to ∞. Equations for $\Psi^{(\ell+1/2)}$ and $\Phi_0^{(\ell)}$ can be obtained by subtracting Eqs. (1) and (2) for successive values of ℓ, yielding

$$\mu \frac{\partial \Psi^{(\ell+1/2)}}{\partial x}(x,\mu) + \Psi^{(\ell+1/2)}(x,\mu) = c\, \Phi_0^{(\ell)}(x) \quad , \tag{4a}$$

$$\Phi_0^{(\ell+1)}(x) = \frac{1}{2} \int_{-1}^{1} \Psi^{(\ell+1/2)}(x,\mu')\, d\mu' \quad . \tag{4b}$$

We seek a separation-of-variables Fourier mode solution of these equations of the form

$$\left.\begin{aligned} \phi_0^{(\ell)}(x) &= \omega^\ell e^{i\lambda x} \quad , \\ \psi^{(\ell+1/2)}(x,\mu) &= \omega^\ell a(\lambda,\mu)\, e^{i\lambda x} \quad . \end{aligned}\right\} \qquad i = \sqrt{-1}, \ -\infty < \lambda < \infty \tag{5}$$

Here ω is the eigenvalue, which is a function of the parameter λ. The quantity

$$\rho = \sup_{\lambda} |\omega| \tag{6}$$

is termed the spectral radius; ρ measures the slowest possible reduction in the error from one iteration to the next. By the above remarks, the iterative method (1), (2) is stable and convergent if $\rho < 1$. Also, if two convergent methods have different values of ρ, then the method with the smaller ρ will generally converge faster.

Introducing the ansatz (5) into the two Eqs. (4) and solving for the two unknowns, a and ω, we easily obtain

$$a(\lambda,\mu) = \frac{c}{1 + i\lambda\mu} \quad , \tag{7}$$

$$\omega = c \int_0^1 \frac{d\mu}{1 + \lambda^2\mu^2} \quad . \tag{8}$$

Thus, the maximum value of $|\omega|$, which occurs for $\lambda = 0$, is $\rho = c$, and so the method (1), (2) is stable and convergent for $c < 1$. [With more work it can be proved that for a finite system, the $\lambda = 0$ mode, $a(0,\mu) = c$, cannot be present, and thus the method (1), (2) is stable for $c \leq 1$.]

The SI method thus has poor convergence properties for $\lambda \simeq 0$ and $c \simeq 1$ (an optically thick, nearly conservative system). This agrees with the physically motivated statements in the beginning of this section. We also note that for <u>any</u> value of c, the most slowly converging modes correspond to $\lambda \simeq 0$ and are nearly linear functions of μ:

$$a(\lambda,\mu) \simeq c\,(1 - i\lambda\mu) \quad \text{for } \lambda \simeq 0 \quad . \tag{9}$$

Next, let us consider the SI method for the diamond-differenced discrete-ordinates equations:

$$\frac{\mu_m}{h}\left(\psi^{(\ell+1/2)}_{m,k+1/2} - \psi^{(\ell+1/2)}_{m,k-1/2}\right) + \psi^{(\ell+1/2)}_{mk} = c\,\phi^{(\ell)}_{0k} + Q_k \quad , \tag{10a}$$

$$\psi^{(\ell+1/2)}_{mk} = \frac{1}{2}\left(\psi^{(\ell+1/2)}_{m,k+1/2} + \psi^{(\ell+1/2)}_{m,k-1/2}\right) \quad , \tag{10b}$$

$$\phi^{(\ell+1)}_{0k} = \sum_{m=1}^{N} \psi^{(\ell+1/2)}_{mk}\, w_m \quad . \tag{10c}$$

The notation is standard; the subscript m ($1 \le m \le N$) refers to the m-th discrete-ordinate direction, the subscript k refers to a cell-average quantity for the k-th spatial cell ($x_{k-1/2} < x < x_{k+1/2}$), the subscripts $k \pm 1/2$ refer to edge quantities for the k-th cell, $h = x_{k+1/2} - x_{k-1/2}$, and the angular weights w_m are normalized to satisfy

$$1 = \sum_{m=1}^{N} w_m \quad . \tag{11}$$

To determine the convergence properties of the iteration method (10), we define, as before,

$$\psi^{(\ell+1/2)}_{mk} = \psi^{(\ell+1/2)}_{mk} - \psi^{(\ell-1/2)}_{mk} \quad , \tag{12}$$

etc., and we obtain the equations

$$\frac{\mu_m}{h}\left(\psi^{(\ell+1/2)}_{m,k+1/2} - \psi^{(\ell+1/2)}_{m,k-1/2}\right) + \psi^{(\ell+1/2)}_{mk} = c\,\Phi^{(\ell)}_{0k} \quad , \tag{13a}$$

$$\psi^{(\ell+1/2)}_{mk} = \frac{1}{2}\left(\psi^{(\ell+1/2)}_{m,k+1/2} + \psi^{(\ell+1/2)}_{m,k-1/2}\right) \quad , \tag{13b}$$

$$\Phi^{(\ell+1)}_{0k} = \sum_{m=1}^{N} \psi^{(\ell+1/2)}_{mk}\, w_m \quad . \tag{13c}$$

Into these three equations we introduce, analogous to Eqs. (5), the separation-of-variables Fourier mode ansatz

$$\left.\begin{aligned} \phi_{0k}^{(\ell)} &= \omega^{\ell} e^{i\lambda x_k} \quad , \\ \psi_{mk}^{(\ell+1/2)} &= \omega^{\ell} a_m e^{i\lambda x_k} \quad , \end{aligned}\right\} \qquad x_k = \tfrac{1}{2}\,(x_{k+1/2} + x_{k-1/2}) \tag{14a,b}$$

$$\psi_{m,k+1/2}^{(\ell+1/2)} = \omega^{\ell} b_m e^{i\lambda x_{k+1/2}} \quad , \tag{14c}$$

and solve for the three unknowns a_m, ω, and b_m. We obtain for a_m and ω,

$$a_m = \frac{c}{1 + i\mu_m\left(\frac{2}{h}\tan\frac{\lambda h}{2}\right)} \quad , \tag{15}$$

$$\omega = c\sum_{m=1}^{N} \frac{w_m}{1 + \frac{1}{4}c^2\left(\frac{2}{h}\tan\frac{\lambda h}{2}\right)^2} \quad . \tag{16}$$

[Equation (16) was first derived by Reed[3].] Since ω is a periodic function of λ with period π/h, we need only consider λ on the interval $0 \le \lambda \le \pi/h$.

As before, we find that the maximum value of $|\omega|$, which occurs for $\lambda = 0$, is $\rho = c$, and so the discretized SI method (10) is stable for $c < 1$. (For finite systems, it is stable for $c \le 1$.) Also, as before, the most slowly converging modes, which correspond to $\lambda \simeq 0$, are nearly linear functions of μ_m:

$$a_m \simeq c(1 - i\mu_m\lambda) \qquad \text{for} \qquad \lambda \simeq 0 \quad . \tag{17}$$

To summarize, the SI method for the diamond-differenced discrete-ordinates equations has the desirable property that it is stable for all mesh sizes (this fact seems to have largely been taken for granted, but it is by no means obvious), and the undesirable property that its convergence rate is severely problem-dependent: as c tends to one and as the system increases in optical thickness, the error reduction from one iteration to the next becomes arbitrarily small. This creates two problems: the number of iterations required to achieve a given bound on the error tends to infinity, and at the same time it becomes increasingly difficult for a computer code to determine when to stop iterating so that this error is actually achieved. (This can lead to the phenomenon of "false convergence".) However, the most slowly converging

components of any solution are conveniently characterized as slowly varying in x and nearly linearly varying in μ. This type of solution, which can roughly be described as "diffusion-like", provides both the motivation and the starting point for the DSA method.

III. DIFFUSION SYNTHETIC ACCELERATION

The guiding principle behind the DSA method can be stated as follows:[14] retain Eq. (1), but replace Eq. (2) by new equations which produce the exact scalar flux ϕ_o in one iteration if the exact angular flux ψ is a linear function of μ. To do this, let us define

$$\phi_n^{(\ell+1/2)}(x) = \frac{1}{2}\int_{-1}^{1} P_n(\mu)\,\psi^{(\ell+1/2)}(x,\mu)\,d\mu \quad , \qquad n = 0,1,2 \quad , \tag{18}$$

where $P_0(\mu) = 1$, $P_1(\mu) = \mu$, $P_2(\mu) = (3\mu^2 - 1)/2$ are the first three Legendre polynominals.

We begin with Eq. (1),

$$\mu \frac{\partial \psi^{(\ell+1/2)}}{\partial x}(x,\mu) + \psi^{(\ell+1/2)}(x,\mu) = c\,\phi_0^{(\ell)}(x) + Q(x) \quad , \tag{19}$$

and compute its zeroth and first Legendre moments, obtaining

$$\frac{d\phi_1^{(\ell+1/2)}}{dx}(x) + \phi_0^{(\ell+1/2)}(x) = c\,\phi_0^{(\ell)}(x) + Q(x) \quad , \tag{20a}$$

$$\frac{2}{3}\frac{d\phi_2^{(\ell+1/2)}}{dx}(x) + \frac{1}{3}\frac{d\phi_0^{(\ell+1/2)}}{dx}(x) + \phi_1^{(\ell+1/2)}(x) = 0 \quad . \tag{20b}$$

Now we <u>define</u> acceleration equations as:

$$\frac{d\phi_1^{(\ell+1)}}{dx}(x) + (1-c)\,\phi_0^{(\ell+1)}(x) = Q(x) \quad , \tag{21a}$$

$$\frac{2}{3}\frac{d\phi_2^{(\ell+1/2)}}{dx}(x) + \frac{1}{3}\frac{d\phi_0^{(\ell+1)}}{dx}(x) + \phi_1^{(\ell+1)}(x) = 0 \quad . \tag{21b}$$

Equations (21) have the following properties: (a) they are two equations for the functions $\phi_0^{(\ell+1)}$ and $\phi_1^{(\ell+1)}$; (b) upon convergence, they agree with Eqs. (20), and; (c) if the angular flux is a linear function of angle, then $\phi_2^{(\ell+1/2)} = 0$ and Eqs. (21) determine $\phi_0^{(\ell+1)}$ and $\phi_1^{(\ell+1)}$ exactly. To proceed, we subtract Eqs. (20) from Eqs. (21) and obtain

$$\frac{df_1^{(\ell+1)}}{dx}(x) + (1 - c)\, f_0^{(\ell+1)}(x) = c\left(\phi_0^{(\ell+1/2)}(x) - \phi_0^{(\ell)}(x)\right) , \tag{22a}$$

$$\frac{1}{3}\frac{df_0^{(\ell+1)}}{dx}(x) + f_1^{(\ell+1)}(x) = 0 , \tag{22b}$$

where

$$f_n^{(\ell+1)}(x) = \phi_n^{(\ell+1)}(x) - \phi_n^{(\ell+1/2)}(x) . \tag{23}$$

We note that Eqs. (22) are similar in form to the standard P_1 equations[31]. Finally, we rearrange Eqs. (22) and obtain the diffusion equation

$$-\frac{1}{3}\frac{d^2 f_0^{(\ell+1)}}{dx^2}(x) + (1 - c)\, f_0^{(\ell+1)}(x) = c\,\phi_0^{(\ell+1/2)}(x) - \phi_0^{(\ell)}(x) , \tag{24a}$$

$$f_1^{(\ell+1)}(x) = -\frac{1}{3}\frac{df_0^{(\ell+1)}}{dx}(x) . \tag{24b}$$

The DSA method for the analytic transport equation is now described by Eqs. (19), (18) with n = 0, (24a), and (23) with n = 0, i.e.,

$$\mu\frac{\partial\psi^{(\ell+1/2)}}{\partial x}(x,\mu) + \psi^{(\ell+1/2)}(x,\mu) = c\,\phi_0^{(\ell+1/2)}(x) + Q(x) , \tag{25a}$$

$$\phi_0^{(\ell+1/2)}(x) = \frac{1}{2}\int_{-1}^{1}\psi^{(\ell+1/2)}(x,\mu')\, d\mu' , \tag{25b}$$

$$-\frac{1}{3}\frac{d^2 f_0^{(\ell+1)}}{dx^2}(x) + (1 - c)\left(f_0^{(\ell+1)}(x) = c\,\phi_0^{(\ell+1/2)}(x) - \phi_0^{(\ell)}(x)\right) , \tag{25c}$$

$$\phi_0^{(\ell+1)}(x) = \phi_0^{(\ell+1/2)}(x) + f_0^{(\ell+1)}(x) . \tag{25d}$$

Performing the same Fourier stability analysis on this method as was applied to the SI method in Sec. II, we obtain

$$\omega = c\left[\frac{\lambda^2}{\lambda^2 + 3(1 - c)}\right] \int_{-1}^{1} \frac{P_2(\mu)}{1 + \lambda^2\mu^2}\, d\mu \quad . \tag{26}$$

Therefore,

$$|\omega| \leq c \left| \int_{-1}^{1} \frac{P_2(\mu)}{1 + \lambda^2\mu^2}\, d\mu \right| \leq (0.2247)\, c \quad . \tag{27}$$

(The bound on the integral was obtained numerically). Thus, the DSA method for the analytic transport equation is stable and convergent for all $0 \leq c \leq 1$. Plots of ω versus λ for the SI method [Eq. (8)] and the DSA method [Eq. (26)] are given in Figure 1 for $c = 1$. Here it can be seen that the DSA eigenvalue is zero for $\lambda = 0$, as it was designed to be. However, Figure 1 additionally shows that the DSA eigenvalue is less than the SI eigenvalue for <u>all</u> values of λ.

Equations (25)-(27) were first derived by Gelbard and Hageman[2], who used a procedure, proposed originally by Kopp[1], which is substantially different from the procedure used above. (Other analyses, based on Kopp's procedure, have been performed by Wing[5] and Allen and Wing[6,16].) One of the unsatisfactory features of Kopp's procedure is that it provides no clues as to how to numerically difference Eqs. (25). Thus, for example, if one selects the diamond-difference scheme for Eq. (25a), then one is apparently at liberty to difference the remaining Eqs. (25b,c,d) in an arbitrary way. However, while in principle this is true, it turns out that any obvious choice of a differencing scheme produces an iterative method which is unstable for large enough spatial meshes. Reed[3] first demonstrated this analytically and numerically for the diamond-differenced Eq. (25a) and a simple centrally-differenced form of Eqs. (25b,c,d):

$$\phi_{0k}^{(\ell+1/2)} = \sum_{m=1}^{N} \psi_{mk}^{(\ell+1/2)} w_m \quad , \tag{28a}$$

$$-\frac{1}{3h^2}\left(f_{0,k+1}^{(\ell+1)} - 2f_{0k}^{(\ell+1)} + f_{0,k-1}^{(\ell+1)}\right) + (1 - c)\, f_{0k}^{(\ell+1)}$$

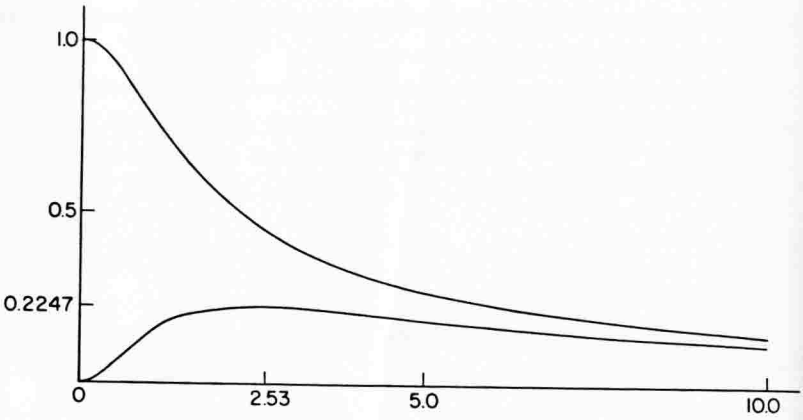

Figure 1. ω Versus λ for the SI Method (Upper Curve) and DSA Method (Lower Curve) for $c = 1.0$.

$$= c\left(\phi_{0k}^{(\ell+1/2)} - \phi_{0k}^{(\ell)}\right) , \tag{28b}$$

$$\phi_{0k}^{(\ell+1)} = \phi_{0k}^{(\ell+1/2)} + f_{0k}^{(\ell+1)} . \tag{28c}$$

For this method [i.e., Eqs. (10a,b) and (28)], we obtain, as in Sec. II,

$$\omega = c\left[\frac{\left(\frac{2}{h}\sin\frac{\lambda h}{2}\right)^2}{\left(\frac{2}{h}\sin\frac{\lambda h}{2}\right)^2 + 3(1-c)}\right]\sum_{m=1}^{N}\frac{\left(\cos\frac{\lambda h}{2}\right)^2 - 3\mu_m^2}{\left(\cos\frac{\lambda h}{2}\right)^2 + \mu_m^2\left(\frac{2}{h}\sin\frac{\lambda h}{2}\right)^2} w_m . \tag{29}$$

For any h, the most rapidly converging modes are the "flat" ($\lambda = 0$) ones:

$$\omega(0) = 0 , \tag{30a}$$

while the most poorly converging modes are the "oscillatory" ($\lambda = \pi/h$) ones:

$$\left|\omega\left(\frac{\pi}{h}\right)\right| = \frac{c}{\frac{4}{3h^2} + 1 - c} . \tag{30b}$$

Thus for $h^2(2c - 1) > 4/3$, the expression on the right side of Eq. (30b) exceeds one, and this iterative method is unstable.

Equations (30) provide an interesting contrast to the SI eigenvalue given by Eq. (16):

$$\omega(0) = c \quad , \tag{31a}$$

$$\omega\left(\frac{\pi}{h}\right) = 0 \quad . \tag{31b}$$

Here the most rapidly convergent modes correspond to $\lambda = \pi/h$, while the most poorly convergent modes correspond to $\lambda = 0$; this is just the opposite of Reed's method [Eqs. (30)]. We infer that in one important sense, Reed's numerical discretization of Eqs. (25b,c,d) succeeds: it does make the $\lambda \simeq 0$ modes converge more quickly, as it was designed to do. However, in another more critical sense it fails because the oscillatory modes, which converge very rapidly for the SI method, now converge more slowly or even diverge.

After Reed's results were published, it became clear that while Eqs. (25) were potentially useful as a basis for a practical acceleration method (because they did, even for the discretized case, cause a more rapid convergence of the $\lambda \simeq 0$ modes), the following essential question remained to be answered: for a specific discretization of the transport equation [Eq. (25a)], does there exist a discretization of the remaining equations [Eqs. (25b,c,d)] such that the resulting method is stable for all h, and if so, how can one determine it?

Alcouffe[7,10,13,14] answered this question in the affirmative for the diamond-difference scheme. His logic (paraphrased, so as to make sense in the present context) was as follows. If the cause of the instability is an improper spatial differencing of Eqs. (25b,c,d), then this difficulty might be removed by making the differencing of these equations more consistent with that of Eq. (25a). To accomplish this, suppose we have a direct algebraic procedure which, starting with the analytic Eq. (25a), allows us to derive the analytic Eqs. (25b,c,d). Let us then apply this same algebraic procedure, starting with the discretized Eq. (25a), and attempt to derive discretized forms of Eqs. (25b,c,d). If such a procedure is possible, there is no a priori guarantee that it will produce a stable method. However, it will at least produce spatial discretizations which are as consistent as possible with the discretized Eq. (25a).

Actually, Alcouffe worked with a set of acceleration equations that were different from, but algebraically equivalent to, Eqs. (25). However, the logic is the same for both sets of equations.

A direct four-step procedure for deriving Eqs. (25b,c,d), developed by Larsen,[25] is described by Eqs. (19)-(24). We shall now apply this procedure to the diamond-differenced discrete-ordinates equations [Eqs. (10a,b)].

[1] To begin, we take the zeroth and first (discrete) Legendre moments of Eqs. (10a,b). This produces the following four equations:

$$\frac{1}{h}\left(\varphi_{1,k+1/2}^{(\ell+1/2)} - \varphi_{1,k-1/2}^{(\ell+1/2)}\right) + \varphi_{0k}^{(\ell+1/2)} = c\,\phi_{0k}^{(\ell)} + Q_k \quad , \tag{32a}$$

$$\frac{2}{3h}\left(\varphi_{2,k+1/2}^{(\ell+1/2)} - \varphi_{2,k-1/2}^{(\ell+1/2)}\right) + \frac{1}{3h}\left(\varphi_{0,k+1/2}^{(\ell+1/2)} - \varphi_{0,k-1/2}^{(\ell+1/2)}\right) + \varphi_{1k}^{(\ell+1/2)} = 0 \quad , \tag{32b}$$

$$\phi_{nk}^{(\ell+1/2)} = \frac{1}{2}\left(\varphi_{n,k+1/2}^{(\ell+1/2)} + \varphi_{n,k-1/2}^{(\ell+1/2)}\right) \quad , \qquad n = 0,\ 1 \quad . \tag{32c}$$

Here we have defined

$$\phi_{nk}^{(\ell+1/2)} = \sum_{m=1}^{N} P_n(\mu_m)\,\psi_{mk}^{(\ell+1/2)}\,w_m \quad , \tag{33}$$

etc. This step parallels the derivation of Eqs. (20) from Eq. (19).

[2] Next we define acceleration equations as

$$\frac{1}{h}\left(\varphi_{1,k+1/2}^{(\ell+1)} - \varphi_{1,k-1/2}^{(\ell+1)}\right) + (1-c)\,\phi_{0k}^{(\ell+1)} = Q_k \quad , \tag{34a}$$

$$\frac{2}{3h}\left(\varphi_{2,k+1/2}^{(\ell+1/2)} - \varphi_{2,k-1/2}^{(\ell+1/2)}\right) + \frac{1}{3h}\left(\varphi_{0,k+1/2}^{(\ell+1)} - \varphi_{0,k-1/2}^{(\ell+1)}\right) + \varphi_{1k}^{(\ell+1)} = 0 \quad , \tag{34b}$$

$$\phi_{nk}^{(\ell+1)} = \frac{1}{2}\left(\varphi_{n,k+1/2}^{(\ell+1)} + \varphi_{n,k-1/2}^{(\ell+1)}\right) \qquad n = 0,1 \quad . \tag{34c}$$

This step parallels the derivation of Eqs. (21) from Eqs. (20).

[3] Now we subtract Eqs. (32) from Eqs. (34) to obtain

$$\frac{1}{h}\left(f_{1,k+1/2}^{(\ell+1)} - f_{1,k-1/2}^{(\ell+1)}\right) + (1-c)\,f_{0k}^{(\ell+1)} = c\left(\phi_{0k}^{(\ell+1/2)} - \phi_{0k}^{(\ell)}\right) \quad , \tag{35a}$$

$$\frac{1}{3h}\left(f_{0,k+1/2}^{(\ell+1)} - f_{0,k-1/2}^{(\ell+1)}\right) + f_{1k}^{(\ell+1)} = 0 \quad , \tag{35b}$$

$$f_{nk}^{(\ell+1)} = \frac{1}{2}\left(f_{n,k+1/2}^{(\ell+1)} + f_{n,k-1/2}^{(\ell+1)}\right) \quad , \qquad n = 0,\ 1 \quad , \tag{35c}$$

where

$$f_{nk}^{(\ell+1)} = \phi_{nk}^{(\ell+1)} - \phi_{nk}^{(\ell+1/2)} \quad , \tag{36}$$

etc. This step parallels the derivation of Eqs. (22) and (23) from Eqs. (21). We note that Eqs. (34) and (35) are a discretized form of the P_1 equations.

[4] Finally, we rearrange Eqs. (35) to obtain a single equation for $f_{0,k+1/2}^{(\ell+1)}$. To do this, we use Eqs. (35c) to eliminate the cell-averaged unknowns in Eqs. (35a,b) and then manipulate the resulting equations over two adjacent cells, obtaining

$$-\frac{1}{3h^2}\left(f_{0,k+3/2}^{(\ell+1)} - 2f_{0,k+1/2}^{(\ell+1)} + f_{0,k-1/2}^{(\ell+1)}\right)$$

$$+\frac{1-c}{4}\left(f_{0,k+3/2}^{(\ell+1)} + 2f_{0,k+1/2}^{(\ell+1)} + f_{0,k-1/2}^{(\ell+1)}\right)$$

$$= \frac{c}{2}\left[\left(\phi_{0,k+1}^{(\ell+1/2)} + \phi_{0k}^{(\ell+1/2)}\right) - \left(\phi_{0,k+1}^{(\ell)} + \phi_{0k}^{(\ell)}\right)\right] \quad , \tag{37a}$$

$$f_{0k}^{(\ell+1)} = \frac{1}{2}\left(f_{0,k+1/2}^{(\ell+1)} + f_{0,k-1/2}^{(\ell+1)}\right) \quad , \tag{37b}$$

$$f_{1k}^{(\ell+1)} = -\frac{1}{3h}\left(f_{0,k+1/2}^{(\ell+1)} - f_{0,k-1/2}^{(\ell+1)}\right) \quad . \tag{37c}$$

This step parallels the derivation of Eqs. (24) from Eqs. (22).

The fully discretized method now consists of Eqs. (10a,b), (33) with $n = 0$, (37a,b), and (36) with $n = 0$. An algebraically equivalent form of this method was first derived by Alcouffe[14]; the form presented here was first derived by Aull[17,18,20]. For this method we obtain, as in Sec. II,

$$\omega = c\left[\frac{\left(\frac{2}{h}\tan\frac{\lambda h}{2}\right)^2}{\left(\frac{2}{h}\tan\frac{\lambda h}{2}\right)^2 + 3(1-c)}\right]\sum_{m=1}^{N}\frac{1-3\mu_m^2}{1+\mu_m^2\left(\frac{2}{h}\tan\frac{\lambda h}{2}\right)^2}w_m \quad .$$

Therefore,

$$|\omega| \le c\left|\sum_{m=1}^{N}\frac{1-3\mu_m^2}{1+\mu_m^2\left(\frac{2}{h}\tan\frac{\lambda h}{2}\right)^2}w_m\right| \le (0.2247)\,c \quad .$$

(The bound on the sum was obtained numerically, and holds for all λ, h, and N.) Thus, the correctly discretized method is unconditionally stable (i.e., $\rho < 1$ for all $0 \leq c \leq 1$ and all h).

The above four-step method has been successfully applied to a number of spatial differencing schemes for the discrete-ordinates equations in slab geometry[25,26]. In other geometries a difficulty for non-diamond transport differencing schemes can arise; we discuss this in the next section (see item 8).

To summarize, the DSA method in both its analytic and its correctly discretized form produces more rapidly convergent discrete-ordinates solutions than the standard SI method for all spatial meshes. The difference between the convergence rates for the two methods is most dramatic for diffusion-like problems, for which the error in the SI method can decrease arbitrarily slowly from one iteration to the next, whereas the DSA method has the property that for all problems at most 1.54 iterations are required to reduce the error by a full order of magnitude. (We refer the reader to references 14, 21, 22, and 26 for numerical results which confirm these theoretical predictions.)

IV. DISCUSSION

Here we discuss some additional topics concerning DSA.

1. In the preceeding sections we have described the DSA method as a device for speeding up the convergence of the $\lambda = 0$ (or, nearly linear-in-angle) modes. However, there is another way to view the method. It can easily be shown that the standard SI method [Eqs. (10)] leads to a numerical solution which satisfies the particle balance equation only upon full convergence, and never at the end of each iteration. [See Eq. (10a).] However, the DSA method has the property that at the end of each iteration, the angularly integrated balance equation is satisfied in every cell. [See Eq. (34a).] Thus, the DSA method can be viewed as a linear fine-mesh rebalance method. Miller[12,15] and Rhoades and Tomlinson[19] have given a more complete discussion.

2. In the earlier sections we have discussed neither the derivation of boundary conditions to go with the diffusion equation that has to be solved in each DSA iteration, nor how to determine the initial scalar flux $\phi_0^{(0)}$. The derivation of these equations, however, is straightforward and is described in Reference 25. The guiding principle is, as above: organize the diffusion part of the iteration so that the scalar flux is computed exactly in one iteration if the angular flux is linear in angle.

3. Morel[24] has shown that for highly anisotropic-scattering problems, the DSA method can be significantly improved if one accelerates both the zeroth and

first angular moments of ψ from one iteration to the next. This can be done with very little extra work; for example, see Eqs. (37c) and (36) with n = 1. A discussion is also given in Reference 25. Currently, an effort is being made to determine the benefits of accelerating more than only the zeroth and first angular moments of ψ for such problems.

4. The lesson which arises from the work of Reed[3] and Alcouffe[14] is that for the DSA method to attain unconditional stability, the differenced forms of the transport and diffusion equations must be consistent. In Sec. III we derived the differenced form of the diffusion equation [Eq. (37a)] from the differenced form of the transport equation [Eqs. (10a,b)]; these equations are consistent only if both of Eqs. (10a) and (10b) hold for every direction in every cell. However, if negative flux fixups are included in the transport part of the calculation, then Eq. (10b) is not used for those values of k and m for which the fixup is invoked and Eqs. (37a) and (10a,b) are no longer fully consistent. If too many fixups are used, the DSA method can destabilize, just as can happen with the unaccelerated SI method. An important open problem concerns the elimination of this type of instability; a full discussion is given in Reference 26.

5. In the preceeding sections we have only discussed linear acceleration methods. Nonlinear methods have also been proposed and implemented[4,8,11,12,14,15,21], but these methods typically become inoperative if spatial meshes are large enough that negative scalar fluxes arise. To cure this, a negative flux fixup could be used in the transport part of the iteration, but then the accuracy of integral quantities may suffer and other stability problems can arise (see the above paragraph). However, nonlinear methods can possess certain advantages; we refer the reader to References 14, 15, and 21. Also, we note that a fair amount of work on nonlinear "quasi-diffusion" acceleration methods has appeared in the Russian literature[32-35]. However, these methods are not acceleration methods in our sense of the word because the numerically generated scalar fluxes from the transport and diffusion calculations do not generally agree upon convergence, and neither of these generally agrees with scalar flux obtained by solving the unaccelerated transport equation. (This is because the spatial differencing of the transport and diffusion equations is not required to be consistent.) However, all three results do converge to the correct answer in the limit of arbitrarily small meshes. Reference 32 provides the simplest description of the method, which is equivalent to the Variable Eddington Factor method discussed by Miller[15]. The issue of numerical stability is not discussed in References 32 through 35.

6. Linear and nonlinear versions of DSA have been applied to eigenvalue problems with success; for details, see References 14 and 23. Work on the linear DSA method for eigenvalue problems in two-dimensional geometries is currently under way.

7. The four-step procedure for deriving discretized acceleration equations, outlined above, has been successfully applied to numerous standard forms of the spatially discretized discrete-ordinates equations[25]. However, there do exist nonstandard forms for which this procedure is unsuccessful, in that it does not lead to an unconditionally stable method. For example, standard weighted diamond methods are defined by Eqs. (10), with Eq. (10b) replaced by

$$\psi_{mk}^{(\ell+1/2)} = \frac{1+\alpha_m}{2}\psi_{m,k+1/2}^{(\ell+1/2)} + \frac{1-\alpha_m}{2}\psi_{m,k-1/2}^{(\ell+1/2)} ,$$

where $0 \leq \mu_m\alpha_m \leq |\mu_m|$ and $\mu_m = -\mu_m$ implies $\alpha_m = -\alpha_n$. This latter constraint on the α's requires them to be antisymmetric in the same sense as the μ's; thus, the numerical solution is invariant if the system is rotated 180°. Such methods are amenable to the four-step procedure described above, and the resulting acceleration methods are unconditionally stable[25]. However, if one abandons the symmetry condition on the α's, then the acceleration method resulting from the four-step procedure may no longer be unconditionally stable. For example, if one sets $\alpha_m = 1$ for $\mu_m > 0$ and $\alpha_m = 0$ for $\mu_m < 0$, then the acceleration method resulting from the four-step procedure becomes unstable for spatial cells larger than 10.5 mean free paths, for the S_4 quadrature set. An open question is: do there exist conditions guaranteeing that a given transport spatial discretization will lead to an unconditionally stable acceleration algorithm when the four-step procedure is applied to it, and if so, then what are they?

8. In slab geometry, the four-step procedure for deriving stable DSA equations is workable and has led to unconditionally stable DSA methods for numerous discrete-ordinates differencing schemes[25]. In other geometries, however, it is possible that only the first three steps of this procedure can be carried out; the algebraic complexity of the system of P_1 acceleration equations resulting from step [3] can be such that collapse down to a single diffusion equation, as in step [4], is impossible. For example, in x,y-geometry, the step [3] system of P_1 acceleration equations arising from the diamond-differenced discrete-ordinates equations can be collapsed down to a single nine-point diffusion equation differenced on cell vertices, but this is <u>not</u> true in general for weighted diamond schemes. Stability analyses, however,

have shown that if one could solve the P_1 system of acceleration equations in place of the single diffusion equation, then one would have a stable and effective acceleration method. In this situation, two approaches are possible: (1) develop efficient ways to solve the P_1 system of equations, or (2) attempt to simplify the P_1 system without sacrificing stability, so that it can be collapsed. [It has been shown possible in slab geometry to weaken the requirement that the scalar flux be computed exactly, in the acceleration part of the iteration, if the angular flux is linear in μ. This leads to a simpler set of P_1 equations, and with the same stability properties as before[27]. Unfortunately, this idea has not yet been successfully extended to two-dimensional geometries.]

However, even in situations where collapse of the P_1 equations to a single diffusion equation is possible, it turns out that a much larger proportion of the computing effort goes into the diffusion part of the iteration in two-dimensional geometries than in one-dimensional geometries, and special techniques have to be used to minimize the cost of performing the diffusion calculations[36,37]. Therefore, whether the "acceleration" part of the iteration is a single discretized diffusion equation or a system of discretized P_1 equations, the central question for two-dimensional geometries is: for general problems, can the acceleration equations be solved economically enough to make the resulting DSA method a significant improvement over the standard SI method? The main research efforts currently under way are focused on this question, and the outcome of this research will determine whether the DSA method fulfills its potential as a generally superior and more economical iterative method than the standard SI method for practical two-dimensional problems.

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Received: November 16, 1983
Revised: January 14, 1984