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TITLE: UNCONDITIONALLY STABLE DIFFUSION-ACCELERATION OF THE TRANSPORT EQUATION

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UNCONDITIONALLY STABLE DIFFUSION-ACCELERATION OF THE TRANSPORT EQUATION

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The standard iterative procedure for solving fixed-source discrete-ordinates problems converges very slowly for problems in optically large regions with scattering ratios c near unity. The diffusion-synthetic acceleration method has been proposed to make use of the fact that for this class of problems, the diffusion equation is often an accurate approximation to the transport equation. However, stability difficulties have historically hampered the implementation of this method for general transport differencing schemes. In this article we discuss a recently developed procedure for obtaining unconditionally stable diffusion-synthetic acceleration methods for various transport differencing schemes. We motivate the analysis by first discussing the exact transport equation; then we illustrate the procedure by deriving a new stable acceleration method for the linear discontinuous transport differencing scheme. We also provide some numerical results.

UNCONDITIONALLY STABLE DIFFUSION-ACCELERATION OF THE TRANSPORT EQUATION

I. INTRODUCTION

The standard power method for iteratively solving the neutral particle transport equation has the following well-known physical interpretation. With a starting guess of zero, the n-th iterate is the flux consisting of all particles which have undergone up to n collisions. For transport problems in optically large regions with scattering ratios near unity, most of the particles undergo a large number of collisions and the power method converges very slowly. However, for this same class of problems, the transport solution is often well approximated by the solution of the standard diffusion equation. The "diffusion-synthetic" acceleration method[1-7] has been proposed to exploit this fact by alternating transport and diffusion calculations, but it is only fairly recently that numerical stability problems[2] have been overcome and that a common procedure for developing stable methods for fairly general transport differencing schemes has been formulated.[3-7]

In this article we discuss the diffusion-synthetic acceleration method, first from the point of view of the exact transport equation (Sec. II), next from the point of view of the discretized transport equation, with emphasis placed on a new and simpler acceleration method for the linear discontinuous spatial differencing scheme[8,9] (Sec. III), and then from the point of view of numerical results (Sec. IV). For simplicity we restrict our attention to fixed source problems for the one-group transport equation with isotropic scattering. We briefly discuss extensions to multigroup anisotropic transport in other geometries in Sec. V.

II. EXACT TRANSPORT EQUATION

We wish to solve the equation

$$\mu \frac{\partial \psi}{\partial x} + \psi = \frac{c}{2} \int_{-1}^{1} \psi \, d\mu' + S(x) \quad . \tag{2.1}$$

At this point we shall not specify the spatial domain or the boundary conditions. The standard power iteration method for solving Eq. (2.1) is ined by

$$\mu \frac{\partial \psi^{\ell+\frac{1}{2}}}{\partial x} + \psi^{\ell+\frac{1}{2}} = c\phi_0^{\ell} + S(x) \quad , \tag{2.2}$$

$$\phi_0^{\ell+1} = \frac{1}{2} \int_{-1}^{1} \psi^{\ell+\frac{1}{2}} \, d\mu' \quad , \tag{2.3}$$

where ϕ_0^0, the initial guess, is often chosen to be zero. To determine the convergence properties of this method we define

$$\psi^{\ell+\frac{1}{2}} = \psi^{\ell+\frac{1}{2}} - \psi^{\ell-\frac{1}{2}} \quad , \tag{2.4}$$

$$\phi^{\ell} = \phi^{\ell} - \phi^{\ell-1} \quad , \tag{2.5}$$

as the difference between successive iterates of Eqs. (2.2) and (2.3). The rate at which $\psi^{\ell+\frac{1}{2}}$ and ϕ^{ℓ} tend to zero is the rate of convergence of the power method (2.2), (2.3).

By subtracting two of the equation (2.2) and (2.3) for successive values of ℓ, we obtain

$$\mu \frac{\partial \psi^{\ell+\frac{1}{2}}}{\partial x} + \psi^{\ell+\frac{1}{2}} = c\phi^{\ell} \quad , \tag{2.6a}$$

$$\phi^{\ell+1} = \frac{1}{2} \int_{-1}^{1} \psi^{\ell+\frac{1}{2}} \, d\mu' \quad . \tag{2.6b}$$

To determine the convergence rate, we seek eigenvalues ω and eigenfunctions of this method of the form

$$\phi^{\ell} = (\omega)^{\ell} \, e^{i\lambda x} \quad , \qquad -\infty < \lambda > \infty \quad , \tag{2.7}$$

$$\psi^{\ell+\frac{1}{2}} = (\omega)^{\ell} \, f(\nu,\lambda) \, e^{i\lambda x} \quad , \tag{2.8}$$

for which Eqs. (2.6) become

$$f(\mu,\lambda)(i\lambda\mu + 1) = c \quad , \tag{2.9}$$

$$\omega = \frac{1}{2}\int_{-1}^{1} f \, d\mu' \quad . \tag{2.10}$$

Hence,

$$f(\mu,\lambda) = \frac{c}{1 + i\lambda\mu} \tag{2.11}$$

and

$$\omega = \frac{c}{2}\int_{-1}^{1} \frac{d\mu}{1 + \lambda^2\mu^2} \, d\mu \quad . \tag{2.12}$$

The spectral radius of the method is then

$$spr = \sup_{\lambda} \omega = c \quad , \tag{2.13}$$

which is attained for $\lambda = 0$. Thus, for $\lambda \sim 0$ and $c \sim 1$ (which corresponds physically to an optically large system with a scattering ratio near unity), the spectral radius is close to one, and the power iteration method converges very slowly.

To accelerate this iteration method, we shall keep Eq. (2.2) but replace Eq. (2.3) by a formula which treats the $\lambda \sim 0$ modes more accurately. To reformulate this idea, we rewrite Eqs. (2.8) and (2.11) as

$$\psi^{\ell+\frac{1}{2}} = (\omega)^{\ell} \, c[1 - i\lambda\mu + (i\lambda\mu)^2 \ \ldots \ ] \, e^{i\lambda x} \quad . \tag{2.14}$$

Thus if $P_m(\mu)$ is the m-th Legendre polynomial, we have

$$\frac{\partial}{\partial x}^{n} \int_{-1}^{1} P_m(\mu) \, \psi^{\ell+\frac{1}{2}}(x,\mu,\lambda) \, d\mu = O(\lambda^{n+m}) \quad . \tag{2.15}$$

In particular, $\psi^{\ell+\frac{1}{2}}$ is nearly a linear function of μ. Thus, to better treat the $\lambda \sim 0$ modes, we shall replace Eq. (2.3) by an equation which computes $\phi^{\ell+1}$ exactly if $\psi^{\ell+\frac{1}{2}}$ is a linear function of μ.

To do this, we take the zero-th and first spatial moments of Eq. (2.2) to obtain

$$\frac{d}{dx}\,\phi_1^{\ell+\frac{1}{2}} + \phi_0^{\ell+\frac{1}{2}} = c\phi_0^{\ell} + S \quad , \tag{2.16a}$$

$$\frac{2}{3}\,\frac{d}{dx}\,\phi_2^{\ell+\frac{1}{2}} + \frac{1}{3}\,\frac{d}{dx}\,\phi_0^{\ell+\frac{1}{2}} + \phi_1^{\ell+\frac{1}{2}} = 0 \quad , \tag{2.16b}$$

where

$$\phi_n = \frac{1}{2}\int_{-1}^{1} P_n(\mu)\,\psi(x,\mu)\,d\mu \quad . \tag{2.17}$$

Upon convergence, Eqs. (2.16) become

$$\frac{d}{dx}\,\phi_1 + (1 - c)\,\phi_0 = S \quad , \tag{2.18a}$$

$$\frac{2}{3}\,\frac{d}{dx}\,\phi_2 + \frac{1}{3}\,\frac{d}{dx}\,\phi_0 + \phi_1 = 0 \quad , \tag{2.18b}$$

where the converged quantities are indicated without iteration superscripts. Now let us <u>define</u> two equations for $\phi_0^{\ell+1}$ and $\phi_1^{\ell+1}$ as

$$\frac{d}{dx}\,\phi_1^{\ell+1} + (1 - c)\,\phi_0^{\ell+1} = S \quad , \tag{2.19a}$$

$$\frac{2}{3}\,\frac{d}{dx}\,\phi_2^{\ell+\frac{1}{2}} + \frac{1}{3}\,\frac{d}{dx}\,\phi_0^{\ell+1} + \phi_1^{\ell+1} = 0 \quad . \tag{2.19b}$$

We note that Eq. (2.19a) is the standard balance equation. For the eigenfunctions of this iteration scheme, the first (unaccelerated) term in Eq. (2.19b) is - by Eq. (2.15) - $0(\lambda^3)$, while the second and third (accelerated)

terms are $0(\lambda)$. Thus, Eqs. (2.19) can be expected to treat the $\lambda \sim 0$ modes very accurately. Additionally, we see that if $\psi^{\ell+\frac{1}{2}}$ is a linear function of μ, than $\phi_2^{\ell+\frac{1}{2}} = 0$ and Eqs. (2.19) can be solved for $\phi_0^{\ell+1}$ and $\phi_1^{\ell+1}$ exactly.

To proceed, we write

$$f_n^{\ell+1} = \phi_n^{\ell+1} - \phi_n^{\ell+\frac{1}{2}} \quad , \quad n = 0, 1 \tag{2.20}$$

and we subtract Eqs. (2.16) from (2.19) to get

$$\frac{d}{dx} f_1^{\ell+1} + (1 - c) f_0^{\ell+1} = c(\phi_0^{\ell+\frac{1}{2}} - \phi_0^{\ell}) \quad , \tag{2.21a}$$

$$\frac{1}{3} \frac{d}{dx} f_0^{\ell+1} + f_1^{\ell+1} = 0 \quad . \tag{2.21b}$$

Eliminating $f_1^{\ell+1}$, we get an equation only for $f_0^{\ell+1}$. The full iteration scheme, using this equation, is defined by

$$\mu \frac{\partial}{\partial x} \psi^{\ell+\frac{1}{2}} + \psi^{\ell+\frac{1}{2}} = c\phi_0^{\ell} + S(x) \quad , \tag{2.23a}$$

$$\phi_0^{\ell+\frac{1}{2}} = \frac{1}{2} \int_{-1}^{1} \psi^{\ell+\frac{1}{2}} \, d\mu' \quad , \tag{2.23b}$$

$$- \frac{1}{3} \frac{d^2}{dx^2} f_0^{\ell+1} + (1 - c) f_0^{\ell+1} + c(\phi_0^{\ell+1} - \phi_0^{\ell}) \quad , \tag{2.23c}$$

$$\phi_0^{\ell+1} = \phi_0^{\ell+\frac{1}{2}} + f_0^{\ell+1} \quad . \tag{2.23d}$$

The eigenvalues and eigenfunctions of this method can be computed just as before, with the result

$$\omega \leq c \left| \int_{-1}^{1} \frac{P_2(\mu)}{1 + \lambda^2\mu^2} \, d\mu \right| \quad , \qquad 0 \leq c \leq 1 \quad , \tag{2.24}$$

where equality holds for c = 1. A numerical search gives

$$\text{spr} \leq c\,(0.23) \quad , \tag{2.25}$$

and thus the spectral radius is less than 1/4 for all values of $c \leq 1$. For $c = 1$, the plots $\omega(\lambda)$ for the unaccelerated [Eq. (2.12)] and accelerated [Eq. (2.24)] methods are displayed in Figure 1. We see that the accelerated method treats not only the $\lambda = 0$ mode exactly, as it was designed to do, but in fact it treats all the modes, for $0 \leq \lambda \leq \infty$, more accurately than the unaccelerated method.

The diffusion-synthetic acceleration method of Eqs. (2.23) [together with its spectral radius (2.25)] has been known for some time, and was originally derived in a substantially different way.[1] The derivation of unconditionally stable discretized diffusion synthetic methods however was an unsolved problem for several years[2] and has only been accomplished recently.[3] The advantage of the analysis presented above is that, starting from the exact transport equation, we systematically derived the exact diffusion-synthetic acceleration method; in a similar manner, if we start with the discretized transport equation and follow the above procedure, basically line-for-line, we can derive a discretized diffusion-synthetic acceleration method which is, for all of the transport differencing schemes we have considered, unconditionally stable.[6,7] In the next section we carry out this procedure for the linear discontinuous differencing scheme.

III. LINEAR DISCONTINUOUS SCHEME

The linear discontinuous scheme for spatially discretizing the discrete-ordinates equations is based on a linear representation for the angular flux within each cell,

$$\psi_m(x) = \psi_{mk} + \frac{2}{h_k}\,(x - x_k)\,\xi_{mk} \quad . \tag{3.1}$$

This equation holds in the k-th spatial cell $x_{k-\frac{1}{2}} < x < x_{k+\frac{1}{2}}$, with midpoint $x_k = (x_{k-\frac{1}{2}} + x_{k+\frac{1}{2}})/2$ and width $h_k = x_{k+\frac{1}{2}} - x_{k-\frac{1}{2}}$. The subscript m refers to the discrete-ordinates direction μ_m; the corresponding weight is ω_m, normalized so that $\sum_1^n \omega_m = 1$. Equation (3.1) holds not only within the k-th cell, but also on the right edge for $\mu_m > 0$ and on the left edge for $\mu_m < 0$. Thus if $\psi_{m,k\pm\frac{1}{2}} = \psi_m(x_{k\pm\frac{1}{2}})$, then

$$\xi_{mk} = \begin{cases} \psi_{m,k+\frac{1}{2}} - \psi_{mk} & \mu_m > 0 \quad , \\ \psi_{mk} - \psi_{m,k-\frac{1}{2}} & \mu_m < 0 \quad . \end{cases}$$

For a constant source $S = S_k$, the linear discontinuous method is explicitly defined for the k-th cell by

$$\frac{\mu_m}{h_k} \left(\psi_{m,k+\frac{1}{2}}^{\ell+\frac{1}{2}} - \psi_{m,k-\frac{1}{2}}^{\ell+\frac{1}{2}}\right) + \sigma_{Tk}\psi_{mk}^{\ell+\frac{1}{2}} = \sigma_{Sk}\phi_{0k}^{\ell} + S_k \quad , \tag{3.2a}$$

$$\frac{3\mu_m}{h_k} \left(\psi_{m,k+\frac{1}{2}}^{\ell+\frac{1}{2}} + \psi_{m,k-\frac{1}{2}}^{\ell+\frac{1}{2}} - 2\,\psi_{mk}^{\ell+\frac{1}{2}}\right) + \sigma_{Tk}\xi_{mk}^{\ell+\frac{1}{2}} = \sigma_{Sk}\zeta_{0k}^{\ell} \quad , \tag{3.2b}$$

$$\psi_{mk}^{\ell+\frac{1}{2}} = \left(\frac{1 + \alpha_{mk}}{2}\right) \psi_{m,k+\frac{1}{2}}^{\ell+\frac{1}{2}} + \left(\frac{1 - \alpha_{mk}}{2}\right) \psi_{m,k-\frac{1}{2}}^{\ell-\frac{1}{2}} - \alpha_{mk} \frac{\sigma_{Sk}}{\sigma_{Tk}} \zeta_{0k}^{\ell} \quad . \tag{3.2c}$$

These are three equations for three unknowns, $\psi_{mk}^{\ell+\frac{1}{2}}$, $\xi_{mk}^{\ell+\frac{1}{2}}$, and either $\psi_{m,k+\frac{1}{2}}^{\ell+\frac{1}{2}}$ or $\psi_{m,k-\frac{1}{2}}^{\ell+\frac{1}{2}}$. Equations (3.2a) and (3.2b) are the zero-th and first order spatial balance equations, into which we have introduced Eq. (3.1). Equation (3.2c) follows from introducing

$$\xi_{mk}^{\ell+\frac{1}{2}} = \begin{cases} \psi_{m,k+\frac{1}{2}}^{\ell+\frac{1}{2}} - \psi_{mk}^{\ell+\frac{1}{2}} & , \quad \mu > 0 \quad , \\ \psi_{mk}^{\ell+\frac{1}{2}} - \psi_{m,k-\frac{1}{2}}^{\ell+\frac{1}{2}} & , \quad \mu < 0 \quad , \end{cases} \tag{3.3}$$

into Eq. (3.2b), rearranging, and defining

$$\alpha_{mk} = \frac{\sigma_T h_k/\mu_m}{3 + |\sigma_T h_k/\mu_m|} \quad . \tag{3.4}$$

Equations (3.2) constitute the discretized version of the transport equation (2.2), with the total and scattering cross sections σ_T and σ_S written explicitly. The unaccelerated method is based on the following discrete form of Eq. (2.3):

$$\phi_{0k}^{\ell+1} = \phi_{0k}^{\ell+\frac{1}{2}} \equiv \sum_{n=1}^{N} \psi_{nk}^{\ell+\frac{1}{2}} \mu_n \quad , \tag{3.5a}$$

$$\zeta_{0k}^{\ell+1} = \zeta_{0k}^{\ell+\frac{1}{2}} \equiv \sum_{n=1}^{N} \xi_{nk}^{\ell+\frac{1}{2}} \omega_n \quad . \tag{3.5b}$$

The spectral radius for this iteration method is found by determining eigenfunctions of the form $\sigma_0^{\ell} - \phi_{0k}^{\ell-1} = (\omega)^{\ell} e^{i\lambda x_k}$, $\zeta_{0k}^{\ell} - \zeta_{0k}^{\ell-1} = (\omega)^{\ell} u e^{i\lambda x_k}$ for systems in which σ_{Tk}, σ_{Sk}, and h_k are constants independent of k. The eigenvalue ω has a complicated form which (just as in Sec. II) equals $c = \sigma_S/\sigma_T$ for $\lambda = 0$ and monotonically tends to zero as $\lambda \to \infty$. Thus, as before, convergence will be very slow for $c \sim 1$ and $\lambda \sim 0$.

To derive the acceleration equations, which will replace Eqs. (3.5), we first define ρ_k, γ_{mk}, and β_{mk} as

$$\rho_k = \sum_{1}^{N} \mu_m \alpha_{mk} \omega_m \quad , \tag{3.6a}$$

$$\alpha_{mk} = 3 \rho_k \mu_m + \gamma_{mk} \quad , \tag{3.6b}$$

$$\mu_m \alpha_{mk} = \rho_k + \beta_{mk} \quad . \tag{3.6c}$$

Because α_{mk} is antisymmetric, i.e.,

$$\mu_m = - \mu_n \rightarrow \alpha_{mk} = - \alpha_{nk} \quad , \tag{3.7}$$

then γ_{mk} and β_{mk} have the properties

$$\sum_{m=1}^{N} P_n(\mu_m) \gamma_{mk} \omega_m = 0 \qquad , \qquad n = 0, 1, 2 \quad , \tag{3.8a}$$

$$\sum_{m=1}^{N} P_n(\mu_m) \beta_{mk} \omega_m = 0 \qquad , \qquad n = 0, 1 \quad . \tag{3.8b}$$

The procedure which we use is patterned directly on the method presented in Sec. II for deriving the acceleration equations (2.23) from the single equation (2.2). Our starting point here however is not Eq. (2.2), but rather Eqs. (3.2). We begin by taking the zero-th and first angular moments of Eqs. (3.2), i.e., by operating by $\sum_{m=1}^{N} (\cdot)\,\omega_m$ and $\sum_{m=1}^{N} \mu_m(\cdot)\,\omega_m$. This results in the following six equations:

$$\frac{1}{h_k}\left(\phi_{1,k+\frac{1}{2}}^{\ell+\frac{1}{2}} - \phi_{1,k-\frac{1}{2}}^{\ell+\frac{1}{2}}\right) + (\sigma_{Tk} - \sigma_{Sk})\,\phi_{0k}^{\ell+\frac{1}{2}} = \sigma_{Sk}\left(\phi_{0k}^{\ell} - \phi_{0k}^{\ell+\frac{1}{2}}\right) + S_k \quad , \tag{3.9a}$$

$$\frac{2}{3h_k}\left(\phi_{2,k+\frac{1}{2}}^{\ell+\frac{1}{2}} - \phi_{2,k-\frac{1}{2}}^{\ell+\frac{1}{2}}\right) + \frac{1}{3h_k}\left(\phi_{0,k+\frac{1}{2}}^{\ell+\frac{1}{2}} - \phi_{0,k-\frac{1}{2}}^{\ell+\frac{1}{2}}\right) + \sigma_{Tk}\phi_{1k}^{\ell+\frac{1}{2}} = 0 \quad , \tag{3.9b}$$

$$\frac{3}{h_k}\left(\phi_{1,k+\frac{1}{2}}^{\ell+\frac{1}{2}} + \phi_{1,k-\frac{1}{2}}^{\ell+\frac{1}{2}} - 2\phi_{1k}^{\ell+\frac{1}{2}}\right) + (\sigma_T - \sigma_{Sk})\,\zeta_{0k}^{\ell+\frac{1}{2}} = \sigma_{Sk}\left(\zeta_{0k}^{\ell} - \zeta_{0k}^{\ell+\frac{1}{2}}\right) \quad , \tag{3.9c}$$

$$\frac{2}{h_k}\left(\phi_{2,k+\frac{1}{2}}^{\ell+\frac{1}{2}} + \phi_{2,k-\frac{1}{2}}^{\ell+\frac{1}{2}} - 2\phi_{2k}^{\ell+\frac{1}{2}}\right) + \frac{1}{h_k}\left(\phi_{0,k+\frac{1}{2}}^{\ell+\frac{1}{2}} + \phi_{0,k-\frac{1}{2}}^{\ell+\frac{1}{2}} - 2\phi_{0k}^{\ell+\frac{1}{2}}\right) + \sigma_T\zeta_{1k}^{\ell+\frac{1}{2}} = 0 \quad , \tag{3.9d}$$

$$\phi_{0k}^{\ell+\frac{1}{2}} = \frac{1}{2}\left(\phi_{0,k+\frac{1}{2}}^{\ell+\frac{1}{2}} + \phi_{0,k-\frac{1}{2}}^{\ell+\frac{1}{2}}\right) + \frac{3}{2}\rho_k\left(\phi_{1,k+\frac{1}{2}}^{\ell+\frac{1}{2}} - \phi_{1,k-\frac{1}{2}}^{\ell+\frac{1}{2}}\right) + \frac{1}{2}L\gamma\left(\psi_{k+\frac{1}{2}}^{\ell+\frac{1}{2}} - \psi_{k-\frac{1}{2}}^{\ell+\frac{1}{2}}\right) \quad , \tag{3.9e}$$

$$\phi_{1k}^{\ell+\frac{1}{2}} = \frac{1}{2}\left(\phi_{1,k+\frac{1}{2}}^{\ell+\frac{1}{2}} + \phi_{1,k-\frac{1}{2}}^{\ell+\frac{1}{2}}\right) + \frac{1}{2}\rho_k\left(\phi_{0,k+\frac{1}{2}}^{\ell+\frac{1}{2}} - \phi_{0,k-\frac{1}{2}}^{\ell+\frac{1}{2}}\right) + \frac{1}{2}L\beta\left(\psi_{k+\frac{1}{2}}^{\ell+\frac{1}{2}} - \psi_{k-\frac{1}{2}}^{\ell+\frac{1}{2}}\right)$$

$$- \rho_k \frac{\sigma_{Sk}}{\sigma_{Tk}}\,\zeta_{0k}^{\ell} \quad . \tag{3.9f}$$

Here we have defined

$$\phi_{nk} = \sum_{m=1}^{N} P_n(\mu_m)\ \psi_{mk}\omega_m \quad , \tag{3.10a}$$

$$\zeta_{nk} = \sum_{m=1}^{N} P_n(\mu_m)\ \xi_{mk}\omega_m \quad , \tag{3.10b}$$

$$L\gamma\psi_k = \sum_{m=1}^{N} \gamma_{mk}\psi_{mk}\omega_m \quad , \tag{3.10c}$$

etc. Now we define acceleration equations in the following way:

$$\frac{1}{h_k}(\phi_{1,k+\frac{1}{2}}^{\ell+1} - \phi_{1,k-\frac{1}{2}}^{\ell+1}) + (\sigma_{Tk} - \sigma_{Sk})\ \phi_{0k}^{\ell+1} = S_k \quad , \tag{3.11a}$$

$$\frac{2}{3h_k}(\phi_{2,k+\frac{1}{2}}^{\ell+\frac{1}{2}} - \phi_{2,k-\frac{1}{2}}^{\ell+\frac{1}{2}}) + \frac{1}{3h_k}(\phi_{0,k+\frac{1}{2}}^{\ell+1} - \phi_{0,k-\frac{1}{2}}^{\ell+1}) + \sigma_{Tk}\phi_{1k}^{\ell+1} = 0 \quad , \tag{3.11b}$$

$$\frac{3}{h_k}(\phi_{1,k+\frac{1}{2}}^{\ell+1} + \phi_{1,k-\frac{1}{2}}^{\ell+1} - 2\phi_{1k}^{\ell+1}) + (\sigma_{Tk} - \sigma_{Sk})\ \zeta_{0k}^{\ell+1} = 0 \quad , \tag{3.11c}$$

$$\frac{2}{h_k}(\phi_{2,k+\frac{1}{2}}^{\ell+\frac{1}{2}} + \phi_{2,k-\frac{1}{2}}^{\ell+\frac{1}{2}} - 2\phi_{2k}^{\ell+\frac{1}{2}}) + \frac{1}{h_k}(\phi_{0,k+\frac{1}{2}}^{\ell+1} + \phi_{0,k-\frac{1}{2}}^{\ell+1} - 2\phi_{0k}^{\ell+1}) + \sigma_T\zeta_{1k}^{\ell+1} = 0 \quad , \tag{3.11d}$$

$$\phi_{0k}^{\ell+1} = \frac{1}{2}(\phi_{0,k+\frac{1}{2}}^{\ell+1} + \phi_{0,k+\frac{1}{2}}^{\ell+1}) + \frac{3}{2}\rho_k(\phi_{1,k+\frac{1}{2}}^{\ell+1} - \phi_{1,k-\frac{1}{2}}^{\ell+1}) + \frac{1}{2}L\gamma(\psi_{k+\frac{1}{2}}^{\ell+\frac{1}{2}} - \psi_{k-\frac{1}{2}}^{\ell+\frac{1}{2}}) \quad , \tag{3.11e}$$

$$\phi_{1k}^{\ell+1} = \frac{1}{2}(\phi_{1,k+\frac{1}{2}}^{\ell+1} + \phi_{1,k-\frac{1}{2}}^{\ell+1}) + \frac{1}{2}\rho_k(\phi_{0,k+\frac{1}{2}}^{\ell+1} - \phi_{0,k-\frac{1}{2}}^{\ell+1}) + \frac{1}{2} L\beta(\psi_{k+\frac{1}{2}}^{\ell+\frac{1}{2}} - \psi_{k-\frac{1}{2}}^{\ell+\frac{1}{2}})$$

$$- \rho_k \frac{\sigma_{Sk}}{\sigma_{Tk}} \zeta_{0k}^{\ell+1} \quad . \tag{3.11f}$$

These are six equations for the six quantities: $\phi_{nk}^{\ell+1}$, $\phi_{n,k+\frac{1}{2}}^{\ell+1}$, $\zeta_{nk}^{\ell+1}$, for $n = 0$ and 1. They were defined by altering the superscripts in Eqs. (3.9) in a manner that is consistent with Eqs. (2.15) and (3.8). Specifically, for the eigenfunctions of this iteration scheme and for small λ the accelerated terms in Eqs. (3.11b, d, e, and f) are respectively $0(\lambda)$, $0(\lambda^2)$, at worst $0(1)$, and $0(\lambda)$, while the unaccelerated terms are respectively $0(\lambda^3)$, $0(\lambda^3)$, $0(\lambda^2)$, and $0(\lambda^2)$. Thus in these four equations the unaccelerated terms are, for small λ, negligable compared to the accelerated terms. In Eqs. (3.11a and c), all of the terms are accelerated. In these two equations one cannot compare the magnitude of the various terms with respect to λ because $\sigma_{Tk} - \sigma_{Sk}$ and S_k can, in principle, have values which vary from zero to infinity.

Equations (3.11) satisfy the property, enuciated in Sec. II, that if ψ_m is linear function of μ_m then all of the terms with $\ell+\frac{1}{2}$ superscripts vanish and the six unknowns can be determined exactly. The acceleration method based on Eqs. (3.11) has been coded, tested, and reported elsewhere[6,7]; we shall refer to it as method A. In the following we discuss in detail a closely related method (referred to as method B) which (i) does not satisfy the above property, (ii) is computationally simpler than method A, and (iii) performs for most problems about as well as method A. In Sec. IV we present numerical results to compare the two methods.

Method B is based on the observation that if the eigenfunctions of any iteration scheme satisfy Eq. (2.15) for small λ, then the accelerated term on the left side of Eq. (3.11e') and the first accelerated term on the right side are $0(1)$, while the second accelerated term on the right side is $0(\lambda^2)$. Thus this latter term should be negligable when compared to the others for small λ, and one ought to be able to treat it as unaccelerated. In other words, one ought to be able to replace Eq. (3.11e) by

$$\phi_{0k}^{\ell+1} = \frac{1}{2}(\phi_{0,k+\frac{1}{2}}^{\ell+1} + \phi_{0,k-\frac{1}{2}}^{\ell+1}) + \frac{3}{2}\rho_k(\phi_{1,k+\frac{1}{2}}^{\ell+\frac{1}{2}} - \phi_{1,k-\frac{1}{2}}^{\ell+\frac{1}{2}}) + \frac{1}{2} L\gamma(\psi_{k+\frac{1}{2}}^{\ell+\frac{1}{2}} - \psi_{k-\frac{1}{2}}^{\ell+\frac{1}{2}}) \quad . \tag{3.11e'}$$

This method has been coded; we have found that for small spatial cells the spectral radius is (experimentally) identical to that of method A, but as the spatial cells increase in width, the spectral radius tends to c. Thus,

the new method is stable, but it does not accelerate effectively for large spatial cells. This unfortunate behavior of the spectral radius as a function of the cell width could not have been predicted from the analysis of the exact acceleration equations in Sec. II. However, it can be overcome by adopting the following strategy.

The purpose of any acceleration method is to obtain accelerated values of $\phi_{0k}^{\ell+1}$ and $\zeta_{0k}^{\ell+1}$. By Eqs. (3.11e) [or (3.11e')] and (3.11f), these quantities are given in terms of accelerated cell-edge scalar fluxes and currents. An acceleration method which accelerates effectively for all spatial cell widths is defined as follows. We take Eqs. (3.11a,b,c,d,e', and f) and solve these for the accelerated cell-edge scalar fluxes and currents; then we use these results in Eqs. (3.11e and f) to obtain the accelerated cell-average quantities $\phi_{0k}^{\ell+1}$ and $\zeta_{0k}^{\ell+1}$. In other words, we use Eq. (3.11e') in the first half of the calculation and Eq. (3.11) in the second half. If we follow this procedure, which we define as method B [or, if we use Eq. (3.11) in both halves, which is method A] we obtain an acceleration method which accelerates effectively for all cell widths. If we use Eq. (3.11e') in both halves, we obtain an acceleration method which only accelerates effectively for small cell widths. There is a computational simplification which occurs however in using Eq. (3.11e') rather than Eq. (3.11e) in the first half of the calculation, and this simplification may be crucial in multidimensional problems. In the following, we carry out the algebraic manipulations described above for method B so that it is recast in a computationally useful form. We point out, as a detail, that for method B, the symbol $\phi_{0k}^{\ell+1}$ in Eqs. (3.11a, d, and e') should be replaced by some other symbol, such as $\phi_{0k}^{\ell+3/4}$; however, for brevity, we shall not do this here.

The first step is to continue following the procedure in Sec. II and subtract Eqs. (3.9) from Eqs. (3.11a,b,c,d,e'. and f). Defining

$$f^{\ell+1} = \phi^{\ell+1} - \phi^{\ell+\frac{1}{2}} \quad , \tag{3.12a}$$

$$g^{\ell+1} = \zeta^{\ell+1} - \zeta^{\ell+\frac{1}{2}} \quad , \tag{3.12b}$$

we get

$$\frac{1}{h_k}(f_{1,k+}^{\ell+1} \quad {}^{\ell+1}_{1,k-\frac{1}{2}}) + (\sigma_{Tk} - \sigma_{Sk})\, f_{0k}^{\ell+1} = \sigma_{Sk}(\phi_{0k}^{\ell+\frac{1}{2}} - \phi_{0k}^{\ell}) \quad , \tag{3.13a}$$

$$\frac{1}{3h_k}\left(f^{\ell+1}_{0,k+\frac{1}{2}} - f^{\ell+1}_{0,k-\frac{1}{2}}\right) + \sigma_{Tk} f^{\ell+1}_{1k} = 0 \quad , \tag{3.13b}$$

$$\frac{3}{h_k}\left(f^{\ell+1}_{1,k+\frac{1}{2}} + f^{\ell+1}_{1,k-\frac{1}{2}} - 2f^{\ell+1}_{1k}\right) + (\sigma_{Tk} - \sigma_{Sk})\, g^{\ell+1}_{0k} = \sigma_{Sk}\left(\zeta^{\ell+\frac{1}{2}}_{0k} - \zeta^{\ell}_{0k}\right) \quad , \tag{3.13c}$$

$$\frac{1}{h_k}\left(f^{\ell+1}_{0,k+\frac{1}{2}} + f^{\ell+1}_{0,k-\frac{1}{2}} - 2f^{\ell+1}_{0k}\right) + \sigma_T g^{\ell+1}_{1k} = 0 \quad , \tag{3.13d}$$

$$f^{\ell+1}_{0k} = \frac{1}{2}\left(f^{\ell+1}_{0,k+\frac{1}{2}} + f^{\ell+1}_{0,k-\frac{1}{2}}\right) \quad , \tag{3.13e}$$

$$f^{\ell+1}_{1k} = \frac{1}{2}\left(f^{\ell+1}_{1,k+\frac{1}{2}} + f^{\ell+1}_{1,k-\frac{1}{2}}\right) + \frac{1}{2}\rho_k\left(f^{\ell+1}_{0,k+\frac{1}{2}} - f^{\ell+1}_{0,k-\frac{1}{2}}\right) - \rho_k \frac{\sigma_{Sk}}{\sigma_{Tk}}\left(g^{\ell+1}_{0k} + \zeta^{\ell+\frac{1}{2}}_{0k} - \zeta^{\ell}_{0k}\right) \quad . \tag{3.13f}$$

We note that for method A, Eq. (3.13e) would contain an extra term on the right side; this term would, in the ensuing manipulations, produce extra algebraic complications. Thus method B, the subject of this article, is algebraically simpler than method A.

To proceed, we solve Eqs. (3.13c) and (3.13f) for $f^{\ell+1}_{1k}$ and $g^{\ell+1}_{0k}$ in terms of the unknown cell-edge quantities and known cell-average quantities to obtain

$$f^{\ell+1}_{1k} = \frac{1}{2}\left(f^{\ell+1}_{1,k+\frac{1}{2}} + f^{\ell+1}_{1,k-\frac{1}{2}}\right) + \rho_k(\sigma_{Tk}h_k)\left[\frac{\frac{1}{2}(\sigma_{Tk} - \sigma_{Sk})\left(f^{\ell+1}_{0,k+\frac{1}{2}} - f^{\ell+1}_{0,k-\frac{1}{2}}\right) - \sigma_{Sk}\left(\zeta^{\ell+\frac{1}{2}}_{0k} - \zeta^{\ell}_{0k}\right)}{6\rho_k\sigma_{Sk} + (\sigma_{Tk}h_k)(\sigma_{Tk} - \sigma_{Sk})}\right] \tag{3.14}$$

$$\zeta^{\ell+1}_{0k} = \frac{3\rho_k\sigma_{Tk}\left(f^{\ell+1}_{0,k+\frac{1}{2}} - f^{\ell+1}_{0,k-\frac{1}{2}}\right) + \sigma_{Sk}(\sigma_{Tk}h_k - 6\rho_k)\left(\zeta^{\ell+\frac{1}{2}}_{0k} - \zeta^{\ell}_{0k}\right)}{6\rho_k\sigma_{Sk} + (\sigma_{Tk}h_k)(\sigma_{Tk} - \sigma_{Sk})} \quad . \tag{3.15}$$

Next, we use Eqs. (3.13e) and (3.14) to eliminate $f_{0k}^{\ell+1}$ and $f_{1k}^{\ell+1}$ from (3.13a and b). To simplify the notation, we define

$$D_k = \frac{1}{3\sigma_{Tk}} + \frac{\rho_k}{2}\left[\frac{h_k(\sigma_{Tk}h_k)(\sigma_{Tk} - \sigma_{Sk})}{6\rho_k\sigma_{Sk} + (\sigma_{Tk}h_k)(\sigma_{Tk} - \sigma_{Sk})}\right] , \tag{3.16a}$$

$$\sigma_{Rk} = \sigma_{Tk} - \sigma_{Sk} , \tag{3.16b}$$

$$R_k^{\ell+\frac{1}{2}} = \frac{\rho_k\sigma_{Sk}(\sigma_{Tk}h_k)(\zeta_{0k}^{\ell+\frac{1}{2}} - \zeta_{0k}^{\ell})}{6\rho_k\sigma_{Sk} + (\sigma_{Tk}h_k)(\sigma_{Tk} - \sigma_{Sk})} , \tag{3.16c}$$

$$P_k^{\ell+\frac{1}{2}} = \frac{1}{2}(\sigma_{Sk}h_k)(\phi_{0k}^{\ell+\frac{1}{2}} - \phi_{0k}^{\ell}) . \tag{3.16d}$$

Then we obtain

$$\frac{1}{2}(f_{1,k+\frac{1}{2}}^{\ell+1} + f_{1,k-\frac{1}{2}}^{\ell+1}) = -\frac{D_k}{h_k}(f_{0,k+\frac{1}{2}}^{\ell+1} - f_{0,k-\frac{1}{2}}^{\ell+1}) + R_k , \tag{3.17a}$$

$$\frac{1}{2}(f_{1,k-\frac{1}{2}}^{\ell+1} - f_{1,k+\frac{1}{2}}^{\ell+1}) = -\frac{1}{4}\sigma_{Rk}h_k(f_{0,k+\frac{1}{2}}^{\ell+1} + f_{0,k+\frac{1}{2}}^{\ell+1}) + P_k . \tag{3.18a}$$

Adding and subtracting these equations, we get

$$f_{1,k\pm\frac{1}{2}}^{\ell+1} = -\frac{D_k}{h_k}(f_{0,k+\frac{1}{2}}^{\ell+1} - f_{0,k-\frac{1}{2}}^{\ell+1}) \mp \frac{1}{4}\sigma_{Rk}h_k(f_{0,k+\frac{1}{2}}^{\ell+1} + f_{0,k-\frac{1}{2}}^{\ell+1}) + R_k \pm P_k . \tag{3.19}$$

Now we take the equation for $f_{1,k-\frac{1}{2}}^{\ell+1}$ and replace k by k+1 to obtain a second equations for $f_{1,k+\frac{1}{2}}^{\ell+1}$; equating these expressions and rearranging, we obtain, finally,

$$- \frac{D_{k+1}}{h_{k+1}} (f^{\ell+1}_{0,k+3/2} - f^{\ell+1}_{0,k+\frac{1}{2}}) + \frac{D_k}{h_k} (f^{\ell+1}_{0,k+\frac{1}{2}} - f^{\ell+1}_{0,k-\frac{1}{2}})$$

$$+ \frac{1}{4}[\sigma_{R,k+1} h_{k+1} (f^{\ell+1}_{0,k+3/2} + f^{\ell+1}_{0,k+\frac{1}{2}}) + \sigma_{Rk} h_k (f^{\ell+1}_{0,k+\frac{1}{2}} + f^{\ell+1}_{0,k-\frac{1}{2}})]$$

$$= (P_{k+1} + P_k) - (R_{k+1} - R_k) \quad , \tag{3.20}$$

which is a discretized diffusion equation, analogous to Eq. (2.23c).

To complete the iteration scheme, we must obtain expressions for $\phi^{\ell+1}_{0k}$ and $\zeta^{\ell+1}_{0k}$. Subtracting Eq. (3.9e) from Eq. (3.11e), and using Eqs. (3.12a) and (3.17a), we get

$$\phi^{\ell+1}_{0k} = \phi^{\ell+\frac{1}{2}}_{0k} + \frac{1}{2}(f^{\ell+1}_{0,k+\frac{1}{2}} + f^{\ell+1}_{0,k-\frac{1}{2}}) + \frac{3}{2} \rho_k (f^{\ell+1}_{1,k+\frac{1}{2}} - f^{\ell+1}_{1,k-\frac{1}{2}})$$

$$= \phi^{\ell+\frac{1}{2}}_{0k} + \left[\frac{1}{2} - \frac{3}{4} \rho_k (\sigma_{Rk} h_k)\right](f^{\ell+1}_{0,k+\frac{1}{2}} + f^{\ell+1}_{0,k-\frac{1}{2}}) + 3\rho_k P_k \tag{3.21a}$$

and from Eqs. (3.12b) and (3.15), we obtain

$$\zeta^{\ell+1}_{0k} = \zeta^{\ell+\frac{1}{2}}_{0k} + \frac{3\rho_k \sigma_{Tk} (f^{\ell+1}_{0,k+\frac{1}{2}} - f^{\ell+1}_{0,k-\frac{1}{2}}) + \sigma_{Sk} (\sigma_{Tk} h_k - 6\rho_k)(\zeta^{\ell+\frac{1}{2}}_{0k} - \zeta^{\ell}_{0k})}{6\rho_k \sigma_{Sk} + \sigma_{Tk} h_k (\sigma_{Tk} - \sigma_{Sk})} \tag{3.21b}$$

The derivation of the acceleration method is now basically complete. First, we perform the transport sweep of Eqs. (3.2). [This is analogous to solving Eq. (2.23a).] Next we introduce these results into Eqs. (3.5) to obtain $\phi^{\ell+\frac{1}{2}}_{0k}$ and $\zeta^{\ell+\frac{1}{2}}_{0k}$. [This is analogous to Eq. (2.23b).] Then we solve Eqs. (3.16) and (3.20). [This is analogous to solving Eq. (2.23c).] Finally, we obtain $\phi^{\ell+1}_{0k}$ and $\zeta^{\ell+1}_{0k}$ from Eqs. (3.21). [These equations are analogous to Eq. (2.23d).]

We have not analytically computed the spectral radius of this method for infinite medium problems. However, we have done this for method A and have obtained the upper bound

$$\text{spr} \leq c \quad (0.300) \quad . \tag{3.22}$$

Moreover, numerical results show that methods A and B generally require almost the same number of iterations to obtain any prescribed accuracy, and so we believe that the bound (3.22) gives a good approximation to the spectral radius for method B. Thus, the method is unconditionally stable and accelerates effectively for all size of spatial meshes.

Two subjects remain to be discussed before the acceleration method derived above can be implemented. First, we must derive boundary conditions for Eq. (3.20), and second we must describe how to select the initial values ϕ^0_{0k} and f^0_{0k}.

The subject of boundary conditions for Eq. (3.20) is important. In calculations, we have observed that with any improper choice the acceleration method becomes unstable for large spatial meshes, but with a correct choice the method remains unconditionally stable.[7] Let us suppose that at the left boundary, $x_{\frac{1}{2}}$, we have a prescribed incident flux, $x_{m,\frac{1}{2}}$ for $\mu_m > 0$. If, for the ℓ-th iteration, the full angular flux is a linear function of μ_m at this point, then we can write

$$\psi_{m,\frac{1}{2}} = \phi^{\ell+\frac{1}{2}}_{0,\frac{1}{2}} + 3\mu_m \phi^{\ell+\frac{1}{2}}_{1,\frac{1}{2}} \quad . \tag{3.23}$$

Taking the incoming partial current, we get

$$\sum_{\mu_m > 0} \mu_m \psi_{m,\frac{1}{2}} \omega_m = \sum_{\mu_m > 0} \mu_m \omega_m \phi^{\ell+\frac{1}{2}}_{0,\frac{1}{2}} + \frac{1}{2} \phi^{\ell+\frac{1}{2}}_{1,\frac{1}{2}} \quad . \tag{3.24}$$

We require accelerated flux and current to also satisfy this equation. Subtracting the two equations and using Eq. (3.12a), we obtain

$$0 = \left[\sum_{\mu_m > 0} \mu_m \omega_m \right] f^{\ell+1}_{0,\frac{1}{2}} + \frac{1}{2} f^{\ell+1}_{1,\frac{1}{2}} \quad . \tag{3.25}$$

Finally, we use Eq. (3.19) to eliminate $f^{\ell+1}_{1,\frac{1}{2}}$ from Eq. (3.25) and obtain a (boundary) condition explicitly relating $f^{\ell+1}_{0,\frac{1}{2}}$ and $f^{\ell+1}_{0,3/2}$. The boundary condition at the right edge of the system, as well as the treatment of reflecting and periodic boundary conditions, are all handled analogously.

The determination of initial values for ϕ^0_{0k} and ζ^0_{0k} is less crucial because the acceleration method is linear and its convergence rate is independent of the initial choice. Nevertheless, an accurate initial choice can obviously reduce the number of iterations for any given problem and thereby reduce the computational effort. Our experience has shown that the following procedure works very effectively. In Eqs. (3.11), delete all terms with "$\ell+\frac{1}{2}$" superscripts, and in the remaining terms set $\ell = -1$. This gives six equations which can be collapsed, as above, into a single (diffusion) equation for $\phi^0_{0,k+\frac{1}{2}}$ and auxilliary equations to determine ϕ^0_{0k} and ζ^0_{0k}. Boundary conditions for the diffusion equation are determined, for example, by setting $\ell+\frac{1}{2} = 0$ in Eq. (3.24). The details are straightforward and analogous to the manipulations described above.

IV. NUMERICAL RESULTS

Here we shall consider a model shielding problem to illustrate the statements, made in the previous section, regarding the estimated spectral radius and stability of methods A and B. The physical system consists of four regions. From left to right, the first region is 12 cm thick with $\sigma_T = 3.333$, $\sigma_S = 3.3136$, and $S = 1.0$; the second region is 3 cm thick with $\sigma_T = 3.333$, $\sigma_S = 3.3136$, and $S = 0.0$; the third region is 6 cm thick with $\sigma_T = 1.333$, $\sigma_S = 1.1077$, and $S = 0.0$; the fourth region is 9 cm thick with $\sigma_T = 3.333$, $\sigma_S = 3.3136$, and $S = 0.0$. (Dimensions of all cross sections are cm^{-1}.). The left boundary is reflecting, the right boundary is vacuum, and we use the standard S_4 and S_8 quadrature sets. The linear discontinuous method, accelerated by coarse-mesh rebalance as encoded in ONETRAN,[8] requires in excess of 440 iterations to converge to a 10^{-4} pointwise error for this problem, for any spatial mesh. The number of iterations required by methods A and B to converge to 10^{-4} and 10^{-8} pointwise errors for fine and coarse meshes are displayed in Table 1. The fine mesh consists of 40, 10, 8, and 30 equally-spaced cells in the four regions, while the coarse mesh consists of 1, 1, 2, and 1 cells in the four regions. We observe that for both methods, both spatial meshes, and both quadrature sets, the number of iterations required to decrease the pointwise error from 10^{-4} to 10^{-8} does not exceed six; this translates into a spectral radius of 0.215, which is well within the bound given by Eq. (3.22).

V. DISCUSSION

The full implementation of the acceleration method discussed above will require generalizations in several directions. First, the extension to anisotropic scattering must be made. This is straightforward, and one can use the fact that the acceleration method produces accelerated scalar fluxes and currents to accelerate the zero-th and first angular moments in an anisotropic scattering problem. (This procedure gives significant computational savings in problems for which the anisotropic scattering kernel is sharply peaked in the forward direction.[5-7]) Second, the inclusion

of a linearly-varying rather than constant source in each cell must be made; this also is straightforward.[6] Third, the extension to the multigroup arena must be made, together with a proper formulation for the ensuing inner and outer iteration strategies. This has been accomplished with the diamond difference scheme[3,10], and we see no conceptual difficulty with the linear discontinuous scheme.

The extension of this acceleration method to other geometries is another matter. One can certainly formulate equations such as (3.2) and then compute angular moments and derive a system of acceleration equations, such as (3.11), but it is not yet clear whether it is always possible, as it is in slab geometry, to reduce this system to a computationally manageable form. We plan to consider this difficulty in detail in our future research efforts.

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	Method A				Method B			
Quadrature Set	S_4		S_8		S_4		S_8	
Conv. Criterion	10^{-4}	10^{-8}	10^{-4}	10^{-8}	10^{-4}	10^{-8}	10^{-4}	10^{-8}
Fine Mesh	5	10	5	11	5	10	5	11
Coarse Mesh	7	12	8	14	6	10	7	12

Table 1: Number of Iterations Required by Methods A and B for Convergence of the Model Shielding Problem

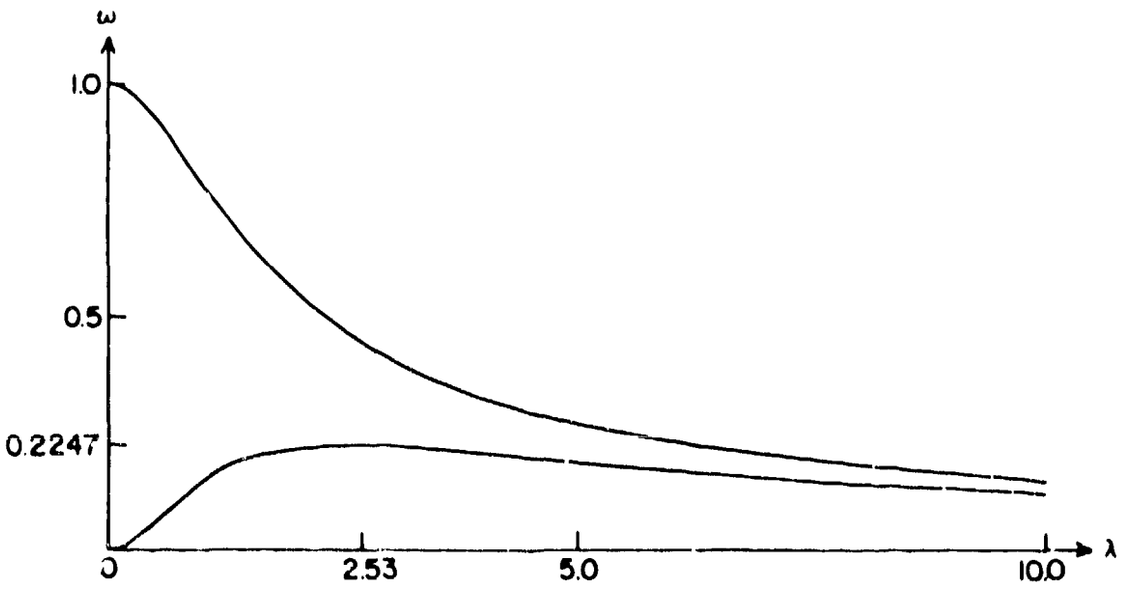

Figure 1: ω (unaccelerated and accelerated) versus λ for c = 1.