

A NEW VERSION OF THE DISCRETE-ORDINATES METHOD

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Abstract. A discussion of a modern version of the discrete-ordinates method is given, and in order to demonstrate well some aspects of the method, a very basic transport model is used to solve the elementary critical problem for a bare slab and for a bare cylinder. In addition to numerical results for these basic applications, various extensions of the method made to more challenging problems are noted.

Keywords: discrete ordinates, critical problems.

1. Introduction. Most of the credit, in our opinion, for the introduction and development of the discrete-ordinates method in the general area of particle transport theory should go to Chandrasekhar (1950), who in his fundamental work on radiative transfer did much to define the method as an effective computational tool. The method as used by Chandrasekhar had, however, one difficult computational aspect that kept the approach from being used effectively past a certain order. This practical limitation is due to the fact that the required “separation constants” are defined in terms of the zeros of a certain polynomial. Here we do not intend to review the numerous works devoted, in general, to discrete-ordinates methods, but some particularly important computational improvements to Chandrasekhar’s original formulation should be mentioned. We know from, for example, Barichello and Siewert (1998) that under certain restrictions on the quadrature scheme, the discrete-ordinates method is equivalent to the spherical-harmonics method (often used in radiative transfer and neutron transport theory). For these special quadrature schemes, where the equivalence holds between the spherical-harmonics method and the discrete-ordinates method, the separation constants can be computed as the eigenvalues of a tridiagonal matrix – a much easier task than finding zeros of polynomials. A second improvement we mention here has to do with a scaling of the discrete-ordinates solution so as to avoid all positive exponentials that cause unnecessary “overflows” in numerical calculations and have lead many formulations to fail. Finally, we believe the use of “half-range” quadrature schemes, as used in this work, have made the discrete-ordinates method a much more powerful technique, since boundary conditions in transport applications are typically of the half-range type. To complement Chandrasekhar’s version of the method, the discrete-ordinates method has been combined with finite-difference techniques (Lewis and Miller, 1984) that are useful when the spatial dependence of the problem can not be treated analytically.

Here we use what we consider to be a modern analytical version (Barichello and Siewert, 1999a) of the discrete-ordinates method that (i) does not depend on any special properties of the quadrature scheme and (ii) for many applications, such as the case of isotropic scattering considered here, has the separation constants defined as the eigenvalues of a matrix with special properties (diagonal matrix plus a rank-one update) so that the basic eigenvalue computation is of a type generally considered even easier than the one for a tridiagonal matrix.

Our first paper (Barichello and Siewert, 1999a) concerning the version of the discrete-ordinates method we use here was developed in the context of non-coherent scattering for applications related to stellar atmospheres, and so in order to demonstrate the development of the method for reactor-physics applications, we now discuss our analytical discrete-ordinates solution in a much simpler setting. We start with the steady-state, one-speed transport equation relevant to isotropic scattering written as

$$\mu \frac{\partial}{\partial x} \psi(x, \mu) + \psi(x, \mu) = \frac{c}{2} \int_0^1 [\psi(x, \mu') + \psi(x, -\mu')] d\mu', \quad (1.1)$$

for $x \in (-x_0, x_0)$ and $\mu \in [-1, 1]$. Here $\psi(x, \mu)$ is the angular flux, x is the spatial variable measured in mean-free paths, μ is the direction cosine (as measured from the positive x axis) of the propagating

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neutrons, and c is the mean number of secondary neutrons (fission and scattering) per collision. In addition to Eq. (1.1) we consider boundary conditions written as

$$\psi(-x_0, \mu) = L(\mu), \quad \mu \in (0, 1], \quad (1.2a)$$

and

$$\psi(x_0, -\mu) = R(\mu), \quad \mu \in (0, 1], \quad (1.2b)$$

where $L(\mu)$ and $R(\mu)$ are specified.

2. A Solution. Seeking exponential solutions of Eq. (1.1), we substitute

$$\psi(x, \mu) = \phi(\nu, \mu)e^{-x/\nu} \quad (2.1)$$

into the Eq. (1.1) to find

$$(\nu - \mu)\phi(\nu, \mu) = \frac{c\nu}{2} \int_0^1 [\phi(\nu, \mu') + \phi(\nu, -\mu')] d\mu'. \quad (2.2)$$

Since it is Eq. (2.2) that we wish to solve with the discrete-ordinates approximation, we introduce a quadrature scheme (at this point, arbitrary) and rewrite the equation as

$$(\nu - \mu)\phi(\nu, \mu) = \frac{c\nu}{2} \sum_{k=1}^N w_k [\phi(\nu, \mu_k) + \phi(\nu, -\mu_k)], \quad (2.3)$$

where the N weights and nodes $\{w_k, \mu_k\}$ are defined for use on the integration interval $[0,1]$. If we now evaluate Eq. (2.3) at $\mu = \pm\mu_i$, we can write

$$(\nu \mp \mu_i)\phi(\nu, \pm\mu_i) = \frac{c\nu}{2} \sum_{k=1}^N w_k [\phi(\nu, \mu_k) + \phi(\nu, -\mu_k)], \quad (2.4)$$

which can be rewritten as

$$\frac{1}{\nu} \mathbf{M} \Phi_+(\nu) = (\mathbf{I} - \mathbf{W}) \Phi_+(\nu) - \mathbf{W} \Phi_-(\nu) \quad (2.5a)$$

and

$$-\frac{1}{\nu} \mathbf{M} \Phi_-(\nu) = (\mathbf{I} - \mathbf{W}) \Phi_-(\nu) - \mathbf{W} \Phi_+(\nu), \quad (2.5b)$$

where \mathbf{I} is the $N \times N$ identity matrix,

$$\Phi_{\pm}(\nu) = [\phi(\nu, \pm\mu_1) \quad \phi(\nu, \pm\mu_2) \quad \dots \quad \phi(\nu, \pm\mu_N)]^T, \quad (2.6)$$

the superscript T denotes the transpose operation, the elements of the matrix \mathbf{W} are

$$(\mathbf{W})_{i,j} = \frac{c}{2} w_j, \quad (2.7)$$

and

$$\mathbf{M} = \text{diag}\{\mu_1, \mu_2, \dots, \mu_N\}. \quad (2.8)$$

If we now let

$$\mathbf{U}(\nu) = \Phi_+(\nu) + \Phi_-(\nu), \quad (2.9)$$

then we can eliminate between the sum and the difference of Eqs. (2.5) to find

$$(\mathbf{D} - 2\mathbf{M}^{-1}\mathbf{W}\mathbf{M}^{-1})\mathbf{M}\mathbf{U}(\nu) = \frac{1}{\nu^2}\mathbf{M}\mathbf{U}(\nu), \quad (2.10)$$

where

$$\mathbf{D} = \text{diag}\{\mu_1^{-2}, \mu_2^{-2}, \dots, \mu_N^{-2}\}. \quad (2.11)$$

Multiplying Eq. (2.10) by a diagonal matrix \mathbf{T} , we find

$$(\mathbf{D} - 2\mathbf{V})\mathbf{X}(\nu) = \frac{1}{\nu^2}\mathbf{X}(\nu), \quad (2.12)$$

where

$$\mathbf{V} = \mathbf{M}^{-1}\mathbf{T}\mathbf{W}\mathbf{T}^{-1}\mathbf{M}^{-1} \quad (2.13)$$

and

$$\mathbf{X}(\nu) = \mathbf{T}\mathbf{M}\mathbf{U}(\nu). \quad (2.14)$$

We can define (Barichello and Siewert, 1999a) the elements t_1, t_2, \dots, t_N of \mathbf{T} so as to make \mathbf{V} symmetric; and therefore, since \mathbf{V} is a symmetric, rank one matrix, we can write our eigenvalue problem in the form

$$(\mathbf{D} - \mathbf{c}\mathbf{z}\mathbf{z}^T)\mathbf{X}(\nu) = \lambda\mathbf{X}(\nu), \quad (2.15)$$

where $\lambda = 1/\nu^2$ and

$$\mathbf{z} = [(1/\mu_1)w_1^{1/2} \quad (1/\mu_2)w_2^{1/2} \quad \dots \quad (1/\mu_N)w_N^{1/2}]^T. \quad (2.16)$$

We note that the eigenvalue problem defined by Eq. (2.15) is of a form that is encountered when the so-called ‘‘divide and conquer’’ method (Datta, 1995) is used to find the eigenvalues of tridiagonal matrices. While a general subroutine from some existing mathematical software package can be used to find the eigenvalues defined by Eq. (2.15), the special package DZPACK (Siewert and Wright, 1999) that makes use of the special structure of Eq. (2.15) can also be used to advantage here.

Considering that we have found the required eigenvalues from Eq. (2.15), we impose the normalization condition

$$\sum_{k=1}^N w_k [\phi(\nu, \mu_k) + \phi(\nu, -\mu_k)] = 1 \quad (2.17)$$

so that we can write our discrete-ordinates solution as

$$\psi(x, \pm\mu_i) = \sum_{j=1}^N [A_j\phi(\nu_j, \pm\mu_i)e^{-(x_0+x)/\nu_j} + B_j\phi(\nu_j, \mp\mu_i)e^{-(x_0-x)/\nu_j}], \quad (2.18)$$

where

$$\phi(\nu_j, \mu_i) = \frac{c\nu_j}{2} \frac{1}{\nu_j - \mu_i}. \quad (2.19)$$

Here the arbitrary constants $\{A_j\}$ and $\{B_j\}$ are to be determined from the boundary conditions and the separation constants $\{\nu_j\}$ are the reciprocals of the positive square roots of the eigenvalues defined by Eq. (2.15).

Now we can substitute Eq. (2.18) into discrete versions (we assume here that neither $L(\mu)$ nor $R(\mu)$ contain generalized functions) of Eqs. (1.2), *viz.*

$$\psi(-x_0, \mu_i) = L(\mu_i) \quad (2.20a)$$

and

$$\psi(x_0, -\mu_i) = R(\mu_i), \quad (2.20b)$$

for $i = 1, 2, \dots, N$, to define a linear algebraic system we can solve to find the required constants $\{A_j\}$ and $\{B_j\}$. And so our solution is established. Since the angular flux is available, we can use Eqs. (2.17)–(2.19) to express the flux and current,

$$\rho(x) = \int_0^1 [\psi(x, \mu) + \psi(x, -\mu)] d\mu \quad (2.21)$$

and

$$j(x) = \int_0^1 [\psi(x, \mu) - \psi(x, -\mu)] \mu d\mu, \quad (2.22)$$

as

$$\rho(x) = \sum_{j=1}^N [A_j e^{-(x_0+x)/\nu_j} + B_j e^{-(x_0-x)/\nu_j}] \quad (2.23)$$

and

$$j(x) = (1 - c) \sum_{j=1}^N \nu_j [A_j e^{-(x_0+x)/\nu_j} - B_j e^{-(x_0-x)/\nu_j}]. \quad (2.24)$$

To conclude this section, we note that while Eq. (2.18) is a discrete-ordinates expression for the angular flux, a better result can be obtained (Barichello and Siewert, 1999a). In fact, we can use Eq. (2.23) to rewrite Eq. (1.1) as

$$\mu \frac{\partial}{\partial x} \psi(x, \mu) + \psi(x, \mu) = \frac{c}{2} \sum_{j=1}^N [A_j e^{-(x_0+x)/\nu_j} + B_j e^{-(x_0-x)/\nu_j}] \quad (2.25)$$

which we can solve, after noting Eqs. (1.2), to find

$$\psi(x, \mu) = \psi_0(x, \mu) + \frac{c}{2} \sum_{j=1}^N \nu_j [A_j C(x_0 + x : \nu_j, \mu) + B_j e^{-(x_0-x)/\nu_j} S(x_0 + x : \nu_j, \mu)] \quad (2.26a)$$

and

$$\psi(x, -\mu) = \psi_0(x, -\mu) + \frac{c}{2} \sum_{j=1}^N \nu_j [A_j e^{-(x_0-x)/\nu_j} S(x_0 - x : \nu_j, \mu) + B_j C(x_0 - x : \nu_j, \mu)], \quad (2.26b)$$

for $\mu \in (0, 1]$. Here the uncollided components are

$$\psi_0(x, \mu) = L(\mu) e^{-(x_0+x)/\mu} \quad (2.27a)$$

and

$$\psi_0(x, -\mu) = R(\mu) e^{-(x_0-x)/\mu}. \quad (2.27b)$$

In addition, the S and C functions are given by

$$S(\tau : x, y) = \frac{1 - e^{-\tau/x} e^{-\tau/y}}{x + y} \quad (2.28a)$$

and

$$C(\tau : x, y) = \frac{e^{-\tau/x} - e^{-\tau/y}}{x - y}. \quad (2.28b)$$

Although our analysis is based on a quadrature approximation, we note that our final results for the flux, the current and the angular flux are continuous functions of the independent variables.

3. Two Typical Calculations. While our version of the discrete-ordinates method was used (Siewert, 2001b) recently to solve the critical problem for a model with a scattering law that is highly anisotropic, we use this problem, for the case of isotropic scattering, to illustrate a typical calculation. To supplement this calculation, in this work we extend our analysis to solve the critical problem for a cylinder.

For the plane-parallel case we consider that $c > 1$ is given and we seek the critical half thickness x_0 so that there exists a physically meaningful solution of Eq. (1.1) subject to Eqs. (1.2) with both $L(\mu)$ and $R(\mu)$ equal to zero. We therefore rewrite Eq. (2.18) as

$$\Psi_{\pm}(x) = \sum_{j=1}^N A_j [\Phi_{\pm}(\nu_j) e^{-(x_0+x)/\nu_j} + \Phi_{\mp}(\nu_j) e^{-(x_0-x)/\nu_j}]. \quad (3.1)$$

Here $\Psi_{\pm}(x)$ are vectors whose N components are the angular fluxes evaluated at $\pm\mu_k$ and the elementary vectors $\Phi_{\pm}(\nu_j)$ have components given by Eq. (2.19). In writing Eq. (3.1), we have made use of the symmetry condition $\psi(-x, -\mu) = \psi(x, \mu)$. In this notation the boundary condition can be written as

$$\Psi_+(-x_0) = \mathbf{0}, \quad (3.2)$$

and so we use Eq. (3.1) to obtain the condition

$$\sum_{j=1}^N A_j [\Phi_+(\nu_j) + \Phi_-(\nu_j) e^{-2x_0/\nu_j}] = \mathbf{0}. \quad (3.3)$$

It is known (Case and Zweifel, 1967) from exact theory (isotropic scattering) that there is only one “discrete eigenvalue” that is imaginary (for $c > 1$), and since we have found in our computations only one imaginary separation constant, say ν_1 , we let $\nu_1 = i\eta$ and rewrite Eq. (3.3) as

$$\sin(x_0/\eta)\Phi_I + \cos(x_0/\eta)\Phi_R + \sum_{j=2}^N A_j [\Phi_+(\nu_j) + \Phi_-(\nu_j) e^{-2x_0/\nu_j}] = \mathbf{0}. \quad (3.4)$$

Noting that Eq. (3.3) is homogeneous, we have, in obtaining Eq. (3.4), introduced the normalization

$$A_1 = (1/2)e^{x_0/\nu_1}, \quad (3.5)$$

and we have let Φ_R and Φ_I denote respectively the real and imaginary parts of the elementary vector $\Phi_+(\nu_1)$. We can now divide Eq. (3.4) by $\cos(x_0/\eta)$ and rewrite that equation as

$$\hat{A}_1 \Phi_I + \sum_{j=2}^N \hat{A}_j [\Phi_+(\nu_j) + \Phi_-(\nu_j) e^{-2x_0/\nu_j}] = -\Phi_R, \quad (3.6)$$

where

$$\hat{A}_1 = \tan(x_0/\eta). \quad (3.7)$$

If we consider that x_0 is known then Eq. (3.6) is a system of N linear algebraic equations for the constants \hat{A}_j , $j = 1, 2, \dots, N$. And so we use an iterative approach to find x_0 . We start our calculation with some assumed value of x_0 , we then solve the linear system defined by Eq. (3.6) and obtain an improved value for x_0 from Eq. (3.7). Continuing this process, we found the numerical results given in Table 1.

To be clear, we note that Eq. (3.7) does not have a unique solution x_0 when values of \hat{A}_1 and η are given. However, for all the cases in Table 1 and for various selected cases (including the extreme cases) of $c \in [1.00000001, 500]$ we found good results by writing Eq. (3.7) as

$$x_0 = \eta \arctan(\hat{A}_1), \quad (3.8)$$

using the principal branch of the arctan function and starting the calculation with $x_0 = 1$.

Turning now to the cylindrical case, we note (Thomas, Southers and Siewert, 1983) that this critical problem can be expressed in terms of a pseudo problem originally defined by Mitsis (1963). We omit the

Table 1. The Critical Half Thickness

$c = 1.1$	$c = 1.5$	$c = 2.0$	$c = 2.5$	$c = 3.0$	$c = 3.5$	$c = 4.0$
2.113310	6.050565(-1)	3.110259(-1)	2.032464(-1)	1.482194(-1)	1.152581(-1)	9.351064(-2)

derivation of this pseudo problem and note simply that we seek, for $c > 1$, the critical radius R (measured in mean-free-paths) such that there exists a solution to

$$\left[\mu^2 \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r} \frac{\partial}{\partial r} \right) - 1 \right] F(r, \mu) + c \int_0^1 F(r, \mu') d\mu' = 0, \quad (3.9)$$

for $r \in (0, R)$ and $\mu \in (0, 1]$, with

$$F(R, \mu) + \mu \Upsilon(\mu) \frac{\partial}{\partial r} F(r, \mu) \Big|_{r=R} = 0, \quad \mu \in (0, 1]. \quad (3.10)$$

Here

$$\Upsilon(\mu) = \frac{K_0(R/\mu)}{K_1(R/\mu)}, \quad (3.11)$$

where $K_0(z)$ and $K_1(z)$ are modified Bessel functions. In analogy with the slab case, we find we can write our discrete-ordinates solution of Eq. (3.9) as

$$F(r, \mu_i) = \sum_{j=1}^N A_j \phi(\nu_j, \mu_i) \widehat{I}_0(r/\nu_j) e^{-(R-r)/\nu_j} \quad (3.12)$$

for $i = 1, 2, \dots, N$. Here $I_0(z)$ is also a modified Bessel function and, in general, we use

$$\widehat{I}_n(z) = I_n(z) e^{-z} \quad \text{and} \quad \widehat{K}_n(z) = K_n(z) e^z. \quad (3.13a,b)$$

We note that the separation constants $\{\nu_j\}$ are the same for both the slab case and the cylindrical case, and so we can write the elementary functions in Eq. (3.12) as

$$\phi(\nu_j, \mu_i) = \frac{c\nu_j^2}{\nu_j^2 - \mu_i^2}, \quad (3.14)$$

where we have imposed the (arbitrary) normalization

$$\sum_{i=1}^N w_i \phi(\nu_j, \mu_i) = 1, \quad (3.15)$$

for all j . Continuing, we let $\nu_1 = i\eta$ and

$$A_1 e^{iR/\eta} = 1 \quad (3.16)$$

so that we can substitute Eq. (3.12) into Eq. (3.10) evaluated at the quadrature points to obtain

$$\widehat{A}_1 f(\eta, \mu_i) + \sum_{j=2}^N \widehat{A}_j \phi(\nu_j, \mu_i) \Xi_j(R, \mu_i) = f(\eta, \mu_i) (\mu_i/\eta) \Upsilon(\mu_i) J_1(R/\eta), \quad (3.17)$$

for $i = 1, 2, \dots, N$. Here

$$\Xi_j(R, \mu_i) = \widehat{I}_0(R/\nu_j) + (\mu_i/\nu_j) \Upsilon(\mu_i) \widehat{I}_1(R/\nu_j), \quad (3.18)$$

Table 2. The Critical Radius

$c = 1.1$	$c = 1.5$	$c = 2.0$	$c = 2.5$	$c = 3.0$	$c = 3.5$	$c = 4.0$
3.577391	1.178341	6.686129(-1)	4.679233(-1)	3.596731(-1)	2.918644(-1)	2.454069(-1)

$$f(\eta, \mu_i) = \frac{c\eta^2}{\eta^2 + \mu_i^2}, \quad (3.19)$$

$\hat{A}_j = A_j$, for $j = 2, 3, \dots, N$, and

$$\hat{A}_1 = J_0(R/\eta). \quad (3.20)$$

And so if, in analogy with the plane case, we consider that R is known, then Eq. (3.17) is a system of N linear algebraic equations for the constants \hat{A}_j , $j = 1, 2, \dots, N$. We therefore use an iterative approach to find R . We start our calculation with some assumed value of R , we then solve the linear system defined by Eq. (3.17) and obtain an improved value for R from Eq. (3.20). Continuing this process, we found the numerical results given in Table 2. Since Eq. (3.20) can have more than one solution, some care must be exercised in solving that equation for R when values of \hat{A}_1 and η are given. Here we use Newton's method of iteration to solve Eq. (3.20), and we have used

$$R = 12\eta/5 - 3/(4c) \quad (3.21)$$

as a starting value for the iterative process. This scheme worked well for all the cases listed in Table 2 and for various selected cases (including the extreme cases) of $c \in [1.00000001, 10]$.

In order to clarify still a couple of issues, we note that we have typically used $N = 40$ in our calculations, for both the plane case and the cylindrical case, and that such computations (implemented in FORTRAN) required less than a second on a 400 MHz PC. And while we have no convergence proof for the iterative procedure used to find the critical dimensions reported in our tables, we did find stability in the results as the number of iterations was increased and as the order of the discrete-ordinates approximation was increased. And so to conclude this section, we note that the results reported in Tables 1 and 2 confirm previously reported computations (Thomas, Southers and Siewert, 1983; Mitsis, 1963; Siewert, 2001b) and are thought to be correct to all figures given.

4. Concluding Remarks. In this work, in order to demonstrate in a simple setting the development of our analytical discrete-ordinates method, we have discussed two simple, but basic, problems related to the nuclear field, and so now in order to complete this work, we note briefly the various problems that have been solved using this version of the method. These remarks are noted just to indicate how the analytical version of the method discussed here has been used for problems considerable more challenging than the specific problems used here to illustrate the method. First of all in regard to other applications in the nuclear field, we note that solutions basic to fully-coupled multigroup neutron transport theory are reported by Siewert (2000b), and another recent paper (Garcia and Siewert, 2000) concerns the transport of neutral hydrogen atoms in a hydrogen plasma. Continuing, we can point out that references (Siewert, 1999a, 2000a, 2000c; Barichello and Siewert, 1999a, 1999b, 2000a; Barichello et al., 2001c) are devoted to radiative transfer (grey and non grey models, one and multidimensional applications, scalar and vector problems, and with and without the inclusion of polarization effects) in atmospheric sciences, and references (Siewert, 1999b, 2000d, 2001a, 2001c, 2001d; Barichello and Siewert, 1999c, 2000b; Barichello et al., 2001a, 2001b; Siewert and Valougeorgis, 2001a, 2001b) all report solutions to classical problems in the area of rarefied gas dynamics. In solving this broad class of problems, we have found it very convenient to make use of quadrature schemes defined specifically for the considered application. In this way we have made use of a fundamental aspect of our discrete-ordinates method, and so we have been able to deal efficiently with problems defined by difficult characteristic functions and with boundary conditions that are not continuous. To conclude, we note that in implementing our algorithms for the considered problems, we have found the analytical discrete-ordinates method to be concise, easy to implement and especially accurate.

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