JOURNAL OF COMPUTATIONAL PHYSICS 92, 213–229 (1991)

Comment on the Discrete Ordinate Method in the Kinetic Theory of Gases

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Received April 25, 1989; revised November 21, 1989

The discrete ordinate (DO) method for solving the linear integro-differential equations of kinetic theory is investigated and other numerical methods for solving this type of problem are reviewed. It is pointed out that the DO method can be regarded as a special case of the method of weighted residuals. An efficient method for calculating the matrix D_{ij} representing the differential operator is described, and it is shown that the method does not necessarily require the use of the nodes of a Gaussian quadrature. © 1991 Academic Press, Inc.

1. INTRODUCTION

A considerable amount of research has gone into solving the linear, integro-differential Boltzmann equation that governs the motion of trace amounts of charged particles in a neutral gas under the influence of a uniform electrostatic field [1–3]. For light particles (electrons, positrons, muons) the Boltzmann equation can, to a good approximation, be decomposed into a chain of coupled differential equations whose solution can be sought through standard numerical procedures, furnishing the velocity distribution function at discrete points in the mesh chosen. In general, however, no such simplifications arise for ions, and the velocity distribution function is usually expanded in a series of known basis functions, of which the Burnett functions are perhaps the best known. In this case, the Boltzmann equation is thereby decomposed into an infinite set of algebraic equations for the expansion coefficients. This procedure has been successfully applied to both ions [4–6] and the lighter charged species [7–9] mentioned above. The question naturally arises as

0021-9991/91 $3.00

to the comparable efficiency of the two seemingly quite different approaches, providing respectively discrete and continuous values of the distribution function. It seems timely to address this question, given the considerable advances that have been made in recent times in both directions.

Of particular interest is the work of Shizgal and collaborators [10–17], who have developed a "discrete ordinate (DO) method" for application to a wide variety of physical problems, not just the kinetic theory of gases. Their work is based upon representation of the derivative operator on a discrete mesh of points generated by gaussian quadrature. It is pointed out in this paper that in this connection:

(i) Both the DO and expansion methods can be regarded as special cases of one general procedure—the method of weighted residuals (MWR);

(ii) The results of Shizgal *et al.* can be obtained directly from the Gaussian quadrature, without first proceeding through a representation in a polynomial basis. The numerical differentiation algorithm of the DO method is in any case subsumed by the well-known Lagrangian differentiation formula for unequally spaced abscissa.

(iii) The requirement that the nodes used in the DO method be the roots of an orthogonal polynomial is not essential. This allows a more general choice of nodes.

The first and third observations have both theoretical and practical implications, while the second is of some practical significance, for it facilitates more rapid computation than has hitherto been possible.

There are other numerical methods that attempt to solve the Boltzmann equation, such as the finite-difference techniques of Segur and co-workers [18–20] and the iterative methods of Kleban and Davis [21]. Some aspects of these methods could also be formulated in terms of the discussion given in Section 2, where we are concerned with procedures that involve an explicit expansion of the distribution function in terms of known functions. For example, Ref. [18] employs the method of weighted residuals with piecewise linear trial functions in velocity space. Such methods may be classified under the general heading of the method of weighted residuals [22].

2. Review of Some Standard Procedures

The prototype equation for our discussion is the one-dimensional operator equation

$$Lf(x) = g(x), \tag{1}$$

in which the function $g(x)$ and the linear operator L are defined for all x in some interval I, and f is the unknown function.

(a) *The Method of Weighted Residuals*

Solution of Eq. (1) by the MWR is based on two choices, as follows:

(i) Choose some trial functions $T_i(x)$, $0 \leqslant i \leqslant N-1$ and assume that they are sufficiently differentiable and well behaved, for all x contained in I, and that $f(x)$ is well approximated by the expansion

$$f(x) \simeq \sum_{i=0}^{N-1} f_i T_i(x). \tag{2}$$

The problem thus has become one of determining the expansion coefficients f_i such that

$$\sum_{i=0}^{N-1} f_i L T_i(x) \simeq g(x). \tag{3}$$

Some guidance as to what trial functions should be used can usually be obtained from a careful examination of the specific problem. For example, it may be convenient to choose the trial functions to be the eigenfunctions of L or the eigenfunctions of an operator similar to L. If L is a differential operator, then the trial functions should satisfy the same boundary conditions as $f(x)$. As another example, more suited to solution of the Boltzmann equation for gaseous ion transport, physical arguments about the behaviour of $f(x)$ throughout I may indicate some reasonable "zero-order" estimate of $f(x)$, $\bar{w}(x)$ say. Then we should construct the first N elements of the complete set of orthonormal polynomials $\phi_i(x)$ from the equation

$$\int \bar{w}(x)\, \phi_j(x)\, \phi_k(x)\, dx = \delta_{jk} \tag{4a}$$

and use

$$T_i(x) = \bar{w}(x)\, \phi_i(x), \tag{4b}$$

where the integral in (4a) is understood to be a definite integral over the interval I.

(ii) Choose some weight functions $A_j(x)$ and require that each of the weighted residuals

$$R_j = \int A_j(x) \left[\sum_{i=0}^{N-1} f_i L T_i(x) - g(x) \right] dx \tag{5}$$

be zero for $0 \leqslant j \leqslant N-1$. The problem thus has become one of determining the expansion coefficients f_i such that

$$\sum_{i=0}^{N-1} L_{ji} f_i = g_j, \qquad 0 \leqslant j \leqslant N-1 \tag{6}$$

where

$$L_{ji} = \int A_j(x)\, LT_i(x)\, dx = \int T_i(x)\, L^+ A_j(x)\, dx, \tag{7}$$

$$g_j = \int A_j(x)\, g(x)\, dx \tag{8}$$

and where Eq. (7) serves to define the adjoint operator L^+. The weight functions can be chosen in many ways, with each choice corresponding to a different method for using the MWR. Since different names are generally used for these different methods, their commonality is often overlooked by mathematical physicists. It is also often overlooked that "all comparisons of different methods indicate that similar results are achieved, especially for higher approximations" [22], which means higher values of N. References to such comparisons for solving differential equations are given in Ref. [22].

The *moment method* is a MWR in which

$$A_j(x) = x^j \tag{9}$$

and the T_i are given by (4). It has been advocated by Skullerud and co-workers [1, 23] for solving the Boltzmann equation for gaseous ion transport. Most other work [1–3] in this field has been based on the *Galerkin method*, a MWR in which

$$A_j(x) = \phi_j(x), \tag{10}$$

with (4) applying again. (The distinction between a moment method and a Galerkin method has not been made in most previous work.) Finally, we note that many other special forms of the MWR are known [22].

The present work is especially concerned with the collocation method, a MWR in which the weighting functions are Dirac delta functions,

$$A_j(x) = \delta(x - x_j), \qquad 0 \leqslant j \leqslant N-1, \tag{11}$$

where the x_j are N abscissas chosen to suit the particular problem. The delta function simplifies Eqs. (6)–(8), and the problem thus becomes one of determining the expansion coefficients f_i such that

$$\sum_{i=0}^{N-1} L_{ji} f_i = g(x_j), \qquad 0 \leqslant j \leqslant N-1 \tag{12}$$

and

$$L_{ji} = [LT_i(x)]_{x=x_j}. \tag{13}$$

Note that we are still free to choose the trial functions and the collocation points, as long as they are contained in I. When the collocation points x_j are chosen to be

the N roots of a particular orthogonal polynomial $\phi_N(x)$, of degree N, we speak of this MWR as being an orthogonal collocation method.

(b) *Gaussian Quadrature*

We now briefly review Gaussian quadrature [24]. Let $\bar{w}(x)$ be any positive-definite, infinitely-differentiable function on the interval I for which the quantities

$$\int \bar{w}(x)\, x^n\, dx \tag{14}$$

exist and are finite, positive numbers for all non-negative values of n. Let $\{\phi_i(x)\}$ be the corresponding, complete, unique set of orthonormal polynomials constructed such that

$$\int \bar{w}(x)\, \phi_j(x)\, \phi_k(x)\, dx = \delta_{jk} \tag{15}$$

and such that the highest power of x in $\phi_i(x)$ has a positive coefficient; these polynomials must satisfy a three-term recurrence relation, the Christoffel–Darboux identity, and Rodrigues' formula [24]. Further, let $\{x_i\}$ be the set of N real, distinct roots of $\phi_N(x)$ that are contained in I, i.e.,

$$\phi_N(x_i) = 0, \qquad 0 \leqslant i \leqslant N-1. \tag{16}$$

The set $\{x_i\}$ is also the set of eigenvalues of the Jacobi matrix formed from the coefficients in the three-term recurrence relation [24]. Then the weights of the corresponding Gaussian quadrature are

$$w_i = \left[\sum_{j=0}^{N-1} \phi_j^2(x_i) \right]^{-1}, \qquad 0 \leqslant i \leqslant N-1. \tag{17}$$

Thus for any function $f(x)$ defined in I we make the approximation that

$$\int \bar{w}(x) f(x)\, dx \simeq \sum_{i=0}^{N-1} w_i f(x_i). \tag{18}$$

This approximation is exact if $f(x) \in S^{2N-1}$ (S^N is the set of polynomials of degree less than or equal to N), and it becomes more accurate for any function as N increases [24]. We note in particular that for $j, k \leqslant N-1$, Eq. (15) is

$$\sum_{i=0}^{N-1} w_i \phi_j(x_i)\, \phi_k(x_i) = \delta_{jk}, \tag{19}$$

the discrete version of the orthogonality relation.

We now introduce a matrix T, important in the subsequent discussions concerning transformations, which is defined as

$$T_{ji} = T_{ij}^{+} = w_i^{1/2} \phi_j(x_i). \tag{20}$$

Then Eq. (19) becomes

$$\sum_{i=0}^{N-1} T_{ji} T_{ik}^{+} = \delta_{jk}, \tag{21}$$

indicating that T is a unitary matrix.

(c) *Numerical Differentiation—Finite Differences*

The derivative operator $D = d/dx$ is nonlocal, i.e., df/dx depends upon values of $f(x)$ at points other than the one under consideration. The discrete analogue of this is that the matrix D_{ij}, representing the operator, induces a linear transformation when it acts upon $f_j = f(x_j)$, as indicated in Eq. (23) below.

Perhaps the most commonly used numerical differentiation algorithms involve equally-spaced abscissas x_i, i.e., a mesh generated by

$$x_i = x_{i-1} + h, \qquad i = 1, 2, ..., N-1.$$

If f_i denote the corresponding ordinates, then one has, for example, the central difference formula

$$(Df)_i = \left(\frac{df}{dx}\right)_{x=x_i}$$

$$= \frac{f_{i+1} - f_{i-1}}{2h} + O(h^2), \tag{22}$$

or, in general,

$$(Df)_i = \sum_{j=0}^{N-1} D_{ij} f_j + E_i^{(N)}, \tag{23}$$

where D_{ij} denotes the appropriate matrix representation and $E_i^{(N)}$ is an error term. For the central differencing method,

$$D_{ij} = \frac{1}{2h} (\delta_{j,i+1} - \delta_{j,i-1}). \tag{24}$$

Forward and backward differencing methods have similar representations. There is, however, no need to restrict such analysis to equally-spaced abscissa and, in fact, in many problems in physics it may be highly undesirable to do so. Adaptive methods, for example, concentrate mesh points in regions of rapidly varying $f(x)$. We consider below the case where the x_i are the nodes of a Gaussian quadrature defined by (16).

(d) *Numerical Differentation and the Lagrangian Differentiation Formula*

Lagrange's interpolation formula for the set of points $\{(x_i, f(x_i)),\ i = 0, 1, 2, ... N-1\}$ is [40]

$$f(x) = \sum_{i=0}^{N-1} l_i(x) f(x_i) + R_N(x), \tag{25}$$

where the Lagrange polynomial

$$l_i(x)=\frac{(x-x_0)(x-x_1)\cdots(x-x_{i-1})(x-x_{i+1})\cdots(x-x_{N-1})}{(x_i-x_0)(x_i-x_1)\cdots(x_i-x_{i-1})(x_i-x_{i+1})\cdots(x_i-x_{N-1})} \tag{26}$$

is a polynomial of degree $N-1$ and has the property

$$l_i(x_j)=\delta_{ij}. \tag{27}$$

The $\{x_i\}$ may be any set of points on I, provided $x_i \neq x_j$ for $i \neq j$. Now if the x_i are roots of the polynomial $\phi_N(x)$, then

$$\phi_N(x)=k_N(x-x_0)(x-x_1)\cdots(x-x_{i-1})(x-x_i)(x-x_{i+1})\cdots(x-x_{N-1})$$

and

$$\phi'_N(x_i)=k_N(x_i-x_0)(x_i-x_1)\cdots(x_i-x_{i-1})(x_i-x_{i+1})\cdots(x_i-x_{N-1}),$$

where k_N is the coefficient of x^N.

Thus it follows that

$$l_i(x)=\frac{\phi_N(x)}{(x-x_i)\,\phi'_N(x_i)}. \tag{28}$$

The remainder term in (25) is [40]

$$R_N(x)=\frac{\phi_N(x)}{N!\,k_N}f^{(N)}(\xi), \tag{29}$$

where $x_0<\xi<x_{N-1}$ and $f^{(N)}$ denotes the Nth derivative of $f(x)$. If $f(x)\in S^{N-1}$, then $R_N(x)=0$.

Differentiating Eq. (25) w.r.t. x gives

$$f'(x)=\sum_{j=0}^{N-1} l'_j(x)f(x_j)+R'_N(x) \tag{30}$$

and, setting $x=x_i$, we have

$$(Df)_i=\sum_{j=0}^{N-1} l'_j(x_i)f(x_j)+R'_N(x_i). \tag{31}$$

Comparing with Eq. (23), it follows that

$$D_{ij}=l'_j(x_i),$$

and applying L'Hopital's rule to Eq. (28), we obtain

$$D_{ij} = l'_j(x_i) = \begin{cases} \dfrac{\phi''_N(x_i)}{2\phi'_N(x_i)} & i = j \\ \dfrac{\phi'_N(x_i)}{(x_i - x_j)\,\phi'_N(x_j)} & i \neq j \end{cases} \tag{32}$$

as the matrix representing d/dx on a mesh specified by the roots of $\phi_N(x)$.

The error term in Eq. (31) is

$$E_i^{(N)} = R'_N(x_i) = \frac{\phi'_N(x_i)}{N!\,k_N} f^{(N)}(\xi_i). \tag{33}$$

The value of ξ depends upon x and generally is not known. Hence the practical application of (33) is often difficult. However, (33) does show explicitly that $E_i^{(N)} = 0$, if $f(x) \in S^{N-1}$, i.e., the differential operation (31) will be exact for polynomials of degree $\leqslant N-1$.

Equation (32) is of primary importance, from both practical and analytical viewpoints. Calculations illustrating its computational advantages are given in Section 4 below. The explicit, general expression (32) of the differential operator in a DO representation defined by an arbitrary mesh $\{x_i\}$ has other equivalent counterparts in the literature [41]. However, all these, like (32), are subsumed by the well-known Lagrangian differentiation formula (Ref. [40], p. 882, Eq. (25.3.2)). Another part of the literature dealing with DO methods involves transformation from a polynomial basis. This is discussed in the next section.

3. The Discrete Ordinate Method

The DO method was developed initially as a technique to solve integral equations with the integral operator being replaced by a Gaussian quadrature formula and the resulting equation solved at the different quadrature points. The method appears to have been suggested by Wick [25], but was developed as a practical tool by Chandrasekhar [26] who used it to solve radiative transfer problems. In the context of kinetic theory a DO method may simply be viewed as an analysis of the Boltzmann equation at discrete points in velocity space. The same may be said of finite-difference methods. However, due to the piecewise nature of the latter we choose to exclude them from the DO classification in the present work.

Some early applications in kinetic theory, primarily in the field of rarefied gas dynamics are discussed in Ref. [27, 28]. In Ref. 28 it is shown that in low-order approximation the DO method gave results in excellent agreement with half-range "moment" methods for the linearized steady Couette flow problem. In subsequent work, Huang and Giddens [29] and others [30, 31] used the DO method for one-dimensional operator equations obtained from the BGK kinetic equation. An

extension of the method to solve the non-linear Boltzmann equation for "pseudo-shock" relaxation is discussed by Wachman and Hamel [32]. The method is used extensively in neutron transport problems [25].

The DO method has also been used to study problems that arise in quantum mechanics [33–38]. Here it is referred to as a "discrete variable representation," and its connection to the Galerkin method (referred to as "finite basis representation" in these papers) has been noted [36–38]. The more recent studies in quantum mechanics [36–38] have shown the advantage of remaining completely in the DO representation, the (surmountable) difficulties associated with extending the method to multi-dimensional operator equations, and the good agreement between DO results of order N and results obtained by Galerkin methods of the same order.

Following the extension of the DO method to include differential operators [13, 39], Shizgal and co-workers have made extensive use of the method to solve the Boltzmann equation for a wide range of problems [10–17]. In this work and also in Ref. [36–38], the DO method is viewed as an approximation to the Galerkin method, where the DO representation of an operator is obtained by a unitary transformation of an orthogonal polynomial (Galerkin) representation.

We believe that it is more efficient to interpret the DO method as a collocation method. In fact, the collocation method outlined in Section 2 encompasses all DO methods, with Eq. (13) defining a DO representation of the operator L. In particular, a DO method chosen such that the ordinates coincide with the nodes of a Gaussian quadrature, such as that of Shizgal and co-workers [10–17] is an orthogonal collocation method with suitably chosen trial functions. This is what most usage of the term "discrete ordinate method" in the literature refers to. Both the Galerkin and collocation aspects of the DO method are considered in this section.

(a) *Transformation between Polynomial and DO Basis*

The set of polynomials $\{\phi_i(x)\}$ is complete on I and hence any function $f(x)$ on I can be expanded as follows:

$$f(x) \simeq \sum_{i=0}^{N-1} f_i^{(e)} \phi_i(x), \tag{34}$$

where

$$f_i^{(e)} = \int \bar{w}(x)\, \phi_i(x) f(x)\, dx \tag{35a}$$

$$\simeq \sum_{j=0}^{N-1} w_j \phi_i(x_j) f(x_j) = \sum_{j=0}^{N-1} T_{ij} w_j^{1/2} f(x_j) \tag{35b}$$

and T_{ij} is defined by Eq. (20). Hence if we define [13]

$$f_i^{(f)} = \sum_{j=0}^{N-1} T_{ji} f_j^{(e)}; \tag{36}$$

that is,

$$\mathbf{f}^{(f)} = \mathbf{T}^{+} \cdot \mathbf{f}^{(e)}, \tag{37}$$

then Eq. (35) shows that

$$f_i^{(f)} \simeq w_i^{1/2} f(x_i). \tag{38}$$

The matrix $\mathbf{T}$ can be interpreted as defining a transformation [13] between an "e basis" and "f basis." Equations (35b) and (38) become exact when $f(x) \in S^{N-1}$.

Using expansion (34) in Equation (1) and choosing $A_i(x) = \bar{w}(x)\,\phi_i(x)$ as our weight function, we have from Eq. (5)

$$R_i = \int \bar{w}(x)\,\phi_i(x) \left[\sum_{j=0}^{N-1} f_j^{(e)} L\phi_j(x) - g(x) \right] dx. \tag{39}$$

These will be zero if

$$\mathbf{L}^{(e)} \cdot \mathbf{f}^{(e)} = \mathbf{g}^{(e)}, \tag{40}$$

where

$$L_{ij}^{(e)} = \int \bar{w}(x)\,\phi_i(x)\,L\phi_j(x)\,dx \tag{41}$$

and

$$g_i^{(e)} = \int \bar{w}(x)\,\phi_i(x)\,g(x)\,dx. \tag{42}$$

From Eq. (37) it follows that

$$\mathbf{f}^{(e)} = \mathbf{T} \cdot \mathbf{f}^{(f)} \tag{43a}$$

and, similarly,

$$\mathbf{g}^{(e)} = \mathbf{T} \cdot \mathbf{g}^{(f)}. \tag{43b}$$

Substituting for $\mathbf{f}^{(e)}$ and $\mathbf{g}^{(e)}$ into Eq. (40), we obtain

$$\mathbf{L}^{(f)} \cdot \mathbf{f}^{(f)} = \mathbf{g}^{(f)}, \tag{44}$$

where

$$\mathbf{L}^{(f)} = \mathbf{T}^{+} \cdot \mathbf{L}^{(e)} \cdot \mathbf{T}. \tag{45}$$

Equation (45) defines the DO representation of L used by Shizgal and Blackmore [13] in terms of the polynomial representation $L^{(e)}$. Thus we see that the DO

method as presented by Shizgal and Blackmore [13] is a Galerkin method with the choices $T_i(x) = \phi_i(x)$ and $A_i(x) = \bar{w}(x)\,\phi_i(x)$, followed by a unitary transformation using the matrix T defined in Eq. (20). It is thus possible to calculate $L_{ij}^{(f)}$ from a knowledge of $L_{ij}^{(e)}$, as Shizgal and co-workers [10–17] do for the differential operator, but as will be pointed out in the next section, this is neither necessary nor desirable in general.

(b) *Orthogonal Collocation and the DO method*

Suppose Eq. (1) is to be solved by an orthogonal collocation method with the collocation points being the roots of the polynomial $\phi_N(x)$. Then it follows from Eq. (2) and (25) that a suitable choice of trial functions is given by Eq. (28); i.e.,

$$T_i(x) = l_i(x) = \frac{\phi_N(x)}{(x - x_i)\,\phi_N'(x_i)}. \tag{46}$$

For this choice, the representation of the operator L is, from Eq. (13),

$$L_{ij} = (Ll_j(x))_{x = x_i} \tag{47}$$

with $\{x_i,\ i = 0, 1, ..., N-1\}$ being the roots of $\phi_N(x)$. Equation (47) is our definition of the discrete ordinate representation of the operator L.

If we consider the general linear differential operator

$$L = \sum_m H_m(x) \frac{d^m}{dx^m}, \tag{48}$$

then it follows from Eq. (47) and the properties of $l_i(x)$ given in Section 2(d), that the DO representation of (48) is

$$\mathbf{L} = \sum_m \mathbf{H}_m \mathbf{D}^m, \tag{49}$$

where

$$(H_m)_{ij} = H_m(x_i)\,\delta_{ij} \tag{50}$$

and $(D^m)_{ij}$ is the matrix resulting from m applications of the matrix D_{ij}, defined by Eq. (32) ($\mathbf{D}^0 = \mathbf{I}$).

As another example, consider the integral operator,

$$Lf = \int K(x, y) f(y)\, dy, \tag{51}$$

where K denotes some kernel and the integral is over the interval I. For this operator, Eq. (18), (47), and (27) yield

$$L_{ij} \simeq \frac{w_j K(x_i, x_j)}{w(x_j)}. \tag{52}$$

To see how L_{ij} is related to $L_{ij}^{(f)}$ we use Eq. (25) to write $\phi_j(x)$ as

$$\phi_j(x) = \sum_{k=0}^{N-1} l_k(x)\, \phi_j(x_k). \tag{53}$$

Note that there is no remainder term as $\phi_j(x) \in S^{N-1}$. Substituting for $\phi_j(x)$ from (53) into equation (41), replacing the integral by a sum and using equation (45), we see that the method of Section 3(a) for finding the DO representation of an operator is in general related to orthogonal collocation, through the relation

$$L_{ij}^{(f)} \simeq \sqrt{\frac{w_i}{w_j}}\, L_{ij}. \tag{54}$$

For the particular case of the differential operator, however, the relationship is *exact*,

$$D_{ij}^{(f)} = \sqrt{\frac{w_i}{w_j}}\, D_{ij}. \tag{55}$$

Thus Eq. (23) may be written as

$$(Df^{(f)})_i \simeq \sum_{j=0}^{N-1} D_{ij}^{(f)} f_j^{(f)}. \tag{56}$$

It is interesting that in the collocation approach to the DO method there has been no direct reference to the polynomials $\phi_i(x)$ $(0 \leqslant i \leqslant N-1)$ that are orthogonal on I with respect to $w(x)$, though the roots of the polynomial $\phi_N(x)$ are used as the nodes.

4. Numerical Calculations and Discussion

Equation (32) of Section 2(d) is exact and offers a means of calculating D_{ij} (or $D_{ij}^{(f)}$) directly from the polynomial nodes chosen. On the other hand, Shizgal and Blackmore [13] use the theory of Section 3(a) to calculate $D_{ij}^{(f)}$ indirectly, by first using Eq. (41) to calculate $D_{ij}^{(e)}$ and then making the transformation (45). Table I

TABLE I

Comparison of Computer Times in Minutes and Seconds for the Calculation of $D_{ij}^{(f)}$ on VAX-11/750 in the Case Where $\phi_i(x)$ Are the "Speed" Polynomials ($\bar{w}(x) = x^2 e^{-x^2}$, $I = (0, \infty)$)

N	10	20	40	60	80	100
Eq. (45)	2.82	4.67	14.10	37.06	1:19.25	2:25.96
Eq. (32)	1.53	2.52	6.07	11.82	19.79	29.54

shows the saving in computer time in the case where $\phi_i(x)$ are the speed polynomials [11, 12] ($\bar{w}(x) = x^2 e^{-x^2}$, $I = (0, \infty)$). We see that as N increases from 10 to 100, direct calculation of $D_{ij}^{(f)}$ goes from being approximately twice to five times faster than the indirect method of Shizgal and Blackmore [13, 42].

Shizgal *et al.* [10–17] consider the DO representation of the derivative operator to be the cornerstone of the DO method. Our view is that it is subsumed by the well-known Lagrangian interpolation formula for unequally-spaced abscissas.

The choice of the abscissas to coincide with the nodes of a Gaussian quadrature appears to generate highly accurate values of the derivatives and the practical implications of the work of Shizgal *et al.* are indeed significant. However, the practice of choosing the nodes to be the roots of an orthogonal polynomial may in some instances be a disadvantage. In cases where boundary values are to be matched, it is often desirable to include the end points of the interval as nodes. In addition, depending on the expected properties of the solution, it may be desirable to choose the nodes according to some other criterion. The properties of $l_i(x)$ in part (a) suggest this is possible. Furthermore, with the choice $A_j(x) = \delta(x - x_j)$, Eq. (6) may be regarded as an approximation to Eq. (1) at the point $x = x_j$. The accuracy of the method then depends on how accurately $\sum_{i=0}^{N-1} L_{ji} f_i$ approximates $(Lf)_{x=x_j}$. Shizgal and Blackmore [13] have given a striking example of the accuracy of this approximation when $L = d^2/dx^2$ by using their method of determining $D_{ij}^{(f)}$ to calculate the second derivative of the function

$$f(x) = \sin[3(\sinh(x) + (1+x)^2)], \qquad (0 \leqslant x \leqslant 1). \tag{57}$$

The nodes chosen were those of the 30-point Gauss–Legendre quadrature formula. Similar accuracy can be obtained with other choices of nodes. As indicated in Table II, even when the nodes are chosen to be equally spaced, high accuracy may be obtained, except near the ends of the interval. This is to be expected, since the error term given by Eq. (33) can be written as

$$E_i^{(N)} = \frac{f^{(N)}(\xi_i)}{N!} \prod_{\substack{j=0 \\ j \neq i}}^{N-1} (x_i - x_j). \tag{58}$$

The factor $\prod_{j \neq i} (x_i - x_j)$ indicates that if the nodes are evenly spaced, the error will in general be small for points near the middle of the interval, but not so small for points close to the ends. If possible, the nodes should be chosen so that $\prod_{j \neq i} (x_i - x_j)$ is small for each i. The above example was repeated using the roots of the 28th degree Chebyshev polynomial (appropriately scaled) together with the end points and we show the results in Table III. Although these nodes are not those of a Gaussian quadrature on the interval (0, 1), the errors obtained are comparable with those of Shizgal and Blackmore's 30-point Gauss–Legendre results. Thus it may not be necessary to restrict the choice of nodes to those of a Gaussian quadrature formula to obtain a high degree of accuracy.

The question of nodes differing from Gaussian quadrature points has been

TABLE II

Accuracy of Numerical Differentiation for 30 Equally Spaced Nodes on (0, 1), for $f(x)$ Defined by (57)

x	f(x)	f"(x)[a]	Error[b]
0.00000d+00	0.14112d+00	-0.17371d+02	0.16d-04
0.34483d-01	-0.17149d+00	0.85291d+01	-0.39d-06
0.68966d-01	-0.47374d+00	0.36580d+02	0.24d-07
0.10345d+00	-0.73258d+00	0.63737d+02	-0.26d-08
0.13793d+00	-0.91607d+00	0.86418d+02	0.42d-09
0.17241d+00	-0.99763d+00	0.10090d+03	-0.68d-10
0.20690d+00	-0.96035d+00	0.10385d+03	0.15d-10
0.24138d+00	-0.80098d+00	0.92946d+02	-0.48d-11
0.27586d+00	-0.53253d+00	0.67558d+02	0.96d-12
0.31034d+00	-0.18505d+00	0.29249d+02	-0.23d-12
0.34483d+00	0.19632d+00	-0.17925d+02	-0.34d-12
0.37931d+00	0.55613d+00	-0.67520d+02	0.28d-12
0.41379d+00	0.83622d+00	-0.11133d+03	-0.22d-12
0.44828d+00	0.98539d+00	-0.14055d+03	0.23d-12
0.48276d+00	0.96967d+00	-0.14742d+03	-0.35d-12
0.51724d+00	0.78138d+00	-0.12712d+03	0.56d-12
0.55172d+00	0.44467d+00	-0.79544d+02	-0.53d-12
0.58621d+00	0.15533d-01	-0.10505d+02	0.64d-12
0.62069d+00	-0.42511d+00	0.68206d+02	-0.37d-12
0.65517d+00	-0.78531d+00	0.14019d+03	-0.47d-12
0.68966d+00	-0.98127d+00	0.18746d+03	0.76d-12
0.72414d+00	-0.95833d+00	0.19471d+03	-0.19d-11
0.75862d+00	-0.70867d+00	0.15412d+03	0.44d-11
0.79310d+00	-0.28020d+00	0.69273d+02	-0.15d-10
0.82759d+00	0.22785d+00	-0.43084d+02	0.76d-10
0.86207d+00	0.68469d+00	-0.15500d+03	-0.40d-09
0.89655d+00	0.96058d+00	-0.23329d+03	0.29d-08
0.93103d+00	0.96536d+00	-0.24901d+03	-0.25d-07
0.96552d+00	0.68175d+00	-0.18807d+03	0.39d-06
0.10000d+01	0.18135d+00	-0.59517d+02	-0.17d-04

[a] Analytic value.

[b] Analytic value minus numerical value from Eq. (32).

TABLE III

Accuracy of Numerical Differentiation, Choosing the Nodes to Be the (Scaled) Roots of the 28th Degree Chebyshev Polynomial Plus $x=0$ and $x=1$, for the Same Case as Table II

x	f(x)	f"(x)[a]	Error[b]
0.00000d+00	0.14112d+00	-0.17371d+02	-0.92d-10
0.78659d-03	0.13411d+00	-0.16822d+02	-0.47d-10
0.70645d-02	0.77784d-01	-0.12363d+02	0.15d-10
0.19541d-01	-0.35421d-01	-0.31101d+01	-0.84d-11
0.38060d-01	-0.20388d+00	0.11386d+02	0.49d-11
0.62388d-01	-0.41842d+00	0.31196d+02	-0.38d-11
0.92220d-01	-0.65508d+00	0.55204d+02	0.24d-11
0.12718d+00	-0.86870d+00	0.80053d+02	-0.15d-11
0.16683d+00	-0.99218d+00	0.99258d+02	0.14d-11
0.21066d+00	-0.94879d+00	0.10336d+03	-0.92d-12
0.25814d+00	-0.68265d+00	0.82375d+02	0.24d-12
0.30866d+00	-0.20325d+00	0.31371d+02	0.24d-12
0.36158d+00	0.37748d+00	-0.42197d+02	-0.56d-12
0.41625d+00	0.85169d+00	-0.11399d+03	0.75d-12
0.47196d+00	0.99338d+00	-0.14804d+03	-0.10d-11
0.52804d+00	0.68990d+00	-0.11501d+03	0.10d-11
0.58375d+00	0.47508d-01	-0.15908d+02	-0.85d-12
0.63842d+00	-0.62606d+00	0.10720d+03	0.12d-11
0.69134d+00	-0.98551d+00	0.18885d+03	-0.15d-11
0.74186d+00	-0.85665d+00	0.17990d+03	0.13d-11
0.78934d+00	-0.33304d+00	0.80293d+02	-0.17d-11
0.83317d+00	0.30897d+00	-0.62099d+02	0.72d-12
0.87282d+00	0.79550d+00	-0.18456d+03	-0.71d-12
0.90778d+00	0.99447d+00	-0.24636d+03	-0.15d-12
0.93761d+00	0.93257d+00	-0.24339d+03	0.11d-11
0.96194d+00	0.72319d+00	-0.19790d+03	-0.31d-11
0.98046d+00	0.48425d+00	-0.13920d+03	0.51d-11
0.99294d+00	0.29514d+00	-0.90027d+02	-0.14d-10
0.99921d+00	0.19420d+00	-0.62994d+02	0.17d-09
0.10000d+01	0.18135d+00	-0.59517d+02	0.24d-09

[a,b] As in Table II.

addressed by several authors, for example, by Kourganoff [43] in connection with the integral equation of the Milne problem. Our remarks are of wider generality, applying to differential and integro-differential equations as well. Note that in certain radiative transfer problems [44] the use of Gaussian quadrature may be desirable to ensure that the angular scattering cross section accurately sums to the total cross section.

5. Conclusion

We have surveyed methods for numerical solution of linear operator equations and have shown that the discrete ordinate method is intimately related to the method of collocation. Expressions (32) give the general representation of the derivative operator, which avoids the unnecessary transformation from the polynomial basis employed elsewhere. The nodes of the mesh need not be the roots of an orthogonal polynomial set and can be chosen according to some other criteria.

We intend to apply these results to a wide variety of physical problems in the near future, including turbulent dispersion in the atmosphere, gaseous discharges, plasma stability, and wave functions for quarks and relativistic electrons.

Acknowledgments

We gratefully acknowledge the support of the Australian Research Council, the Australian-American Education Foundation, and U.S. National Science Foundation (Grant CHE-8814963). We thank Dr. B. Shizgal for constructive criticism of the manuscript.

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