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A Discrete Ordinate Method of Solution of Linear Boundary Value and Eigenvalue Problems

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A discrete ordinate method is developed for the solution of linear differential equations. The method is based on a Gaussian quadrature procedure and is an extension of a discrete ordinate method used for the solution of integral equations. The present method is based on a representation of the derivative operator in a discrete ordinate basis. The method is applied to a number of problems with known solutions and is found to work extremely well.

1. INTRODUCTION

In a recent paper, Shizgal [1] introduced a new Gaussian quadrature procedure in the solution of the Boltzmann equation of kinetic theory. The method was based on the replacement of the integration in the integral operator by a sum involving the points and weights of the quadrature procedure. Many problems in kinetic theory have been treated efficiently with this and similar discrete ordinate methods. These include the calculation of the eigenvalues of the Boltzmann collision operator [2, 3], radiative transfer problems [4, 5] hot atom reaction rates [6], and non Maxwellian effects in planetary atmospheres [7]. In addition discrete ordinate methods have been used in neutron transport problems [8].

The authors are presently involved in the solution of the Boltzmann equation which has the form [9],

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla f + \mathbf{F} \cdot \nabla_v^f = J[f], \tag{1}$$

where

$$J[f] = \int K(\mathbf{v}, \mathbf{v}') f(\mathbf{v}', \mathbf{r}, t)\, d\mathbf{v}' - f(\mathbf{v}, \mathbf{r}, t) \int K(\mathbf{v}', \mathbf{v})\, d\mathbf{v}' \tag{2}$$

is the integral collision operator and $K(\mathbf{v}, \mathbf{v}')$ is the scattering kernel [9]. The quantity $\mathbf{F}$ in Eq. (1) is the external force per unit mass which may include electric, magnetic, and gravitational forces. Work is in progress on the solution of the Boltzmann equation with regard to an extension of the earlier work on the escape of planetary atmospheres [7]. The initial objective was to develop a discrete ordinate method that

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would be applicable to both the integral and differential portions of the Boltzmann equation. The purpose of the present paper is to describe such a method and to illustrate its utility in the application to a number of solved problems.

The application of the discrete ordinate method to the integral operator in Eq. (1) has been discussed elsewhere [1–3]. The action of the spherical component of the kernel in Eq. (2) on some function $f(v')$, that is,

$$g(v) = \int_0^\infty k_0(v, v')\, v'^2 f(v')\, dv' \tag{3}$$

can be approximated by

$$g(x_i) \cong \sum_{j=0}^{N-1} k_0(x_i, x_j)\, w_j x_j^2 f(x_j), \tag{4}$$

where $\{x_i\}$ and $\{w_i\}$ are a set of quadrature points and weights [1]. This may be written as a matrix equation.

$$\mathbf{g} \cong \mathbf{K}_0 \cdot \mathbf{f}, \tag{5}$$

where $\mathbf{g}$ and $\mathbf{f}$ are N dimensional vectors whose elements are $g(x_i)$, and $f(x_i)$, respectively. The $N \times N$ matrix $\mathbf{K}_0$ is the discrete ordinate representation of the kernel in Eq. (3).

An arbitrary differential equation may be written as

$$g = Lf, \tag{6}$$

where

$$L = \sum_m H_m(x) \frac{d^m}{dx^m}. \tag{7}$$

The main objective of the present paper is to treat this operator in a manner analogous to the numerical treatment of the integral collision operator in Eqs. (4) and (5). We are interested in a discrete ordinate approximation for L such that, Eq. (6) can be written in the form

$$\mathbf{g} \cong \mathbf{L} \cdot \mathbf{f}, \tag{8}$$

where $\mathbf{g}$ and $\mathbf{f}$ are as defined previously and $\mathbf{L}$ is the N dimensional discrete ordinate representation of the differential operator.

Once this approximate representation of the operator L has been found, a differential equation may be solved by inverting the matrix $\mathbf{L}$ in Eq. (8), subject to appropriate boundary conditions. Similarly the eigenvalues of the differential operator may be approximated by the eigenvalues of the matrix $\mathbf{L}$. The method for finding the matrix approximation of L with an arbitrary set of quadrature points and weights is discussed in the next section. The subsequent section describes several applications of the new method.

2. Discrete Ordinate Method

The discrete ordinate representation of the differential operator, Eq. (7), is based on the transformation between the representation of a function in a polynomial basis set and the corresponding discrete ordinate representation. We develop the discrete ordinate representation of the derivative operator, d/dx, from its finite matrix representation in some polynomial basis. The representation of the differential operator, L in Eq. (7) is then easily written. We begin the development with a series of definitions.

2.1. *Definitions*

A set of polynomials $R_n(x)$, orthonormal with respect to the weight function $w(x)$ on the interval $[a, b]$, form a complete basis of the $L^2[a, b]$ Hilbert space [10]. If $R_n(x)$ is a polynomial of degree n, then the set is fully specified and unique [10]. The first N of these polynomials form a subspace of this Hilbert space which is isomorphic with the $\mathbb{R}^N$ Euclidean space. The elements of the basis vectors of this polynomial basis, referred to as the e-basis, are defined by,

$$e_i^{(n)} = \int_a^b w(x) R_n(x) R_i(x) \, dx = \delta_{in}, \tag{9}$$

where $e_i^{(n)}$ is the ith element of the nth basis vector. The e basis will be referred to as the polynomial basis.

Let S^M be the set of all polynomials of degree less than or equal to M. The inner product between two vectors in this subspace will be denoted by the dot product between the two vectors. It will be assumed throughout the paper that all vectors and operators are in the N dimensional space $\mathbb{R}^N$.

Since $\{R_n(x)\}$ is a set of orthonormal polynomials, it is possible to find a set of weights $\{w_i, i = 0, 1, 2,..., N-1\}$ such that

$$\sum_{i=0}^{N-1} w_i \, g(x_i) = \int_a^b w(x) \, g(x) \, dx, \tag{10}$$

provided $g \in S^{2N-1}$ and $\{x_j\}$ are the roots of $R_N(x)$ [11]. With the use of Eq. (10), it is possible to define a unitary transformation which will allow a change to the discrete ordinate basis of the $\mathbb{R}^N$ Euclidean space.

The matrix T, whose elements are given by

$$T_{ij} = R_i(x_j) \sqrt{w_j} \tag{11}$$

is a unitary matrix, that is,

$$(\mathbf{T}\cdot\mathbf{T}^{\dagger})_{ij}=\sum_{k=0}^{N-1} R_i(x_k)\,R_j(x_k)w_k=\delta_{ij}, \tag{12}$$

since $R_iR_j \in S^{2N-2}$ and R_i is orthonormal to R_j. Hence $\mathbf{T}^{\dagger}$ is a matrix that defines a new basis referred to as the f basis. The nth vector, $\mathbf{f}^{(n)}$, of this basis, satisfies

$$\mathbf{f}^{(n)}\cdot\mathbf{e}^{(m)}=\sqrt{w_n}\,R_m(x_n), \tag{13}$$

where the rhs of Eq. (13) is $(T^{+})_{nm}\equiv T_{mn}$.

This new basis will be referred to as the discrete ordinate (DO) basis. An arbitrary function $g\in S^{N-1}$ may be represented exactly in this basis by a vector $\mathbf{g}^{(f)}$ with the elements

$$g_k^{(f)}=\sum_{i=0}^{N-1} T_{ki}^{\dagger}\,g_i^{(e)}, \tag{14a}$$

where

$$g_i^{(e)}=\int_a^b w(x)\,R_i(x)\,g(x)\,dx.$$

With Eq. (10) and the definition Eq. (11), we find that

$$g_k^{(f)}=\sum_{i=0}^{N-1}\sum_{j=0}^{N-1} T_{ki}^{\dagger}T_{ij}\sqrt{w_j}\,g(x_j)=\sqrt{w_k}\,g(x_k), \tag{14b}$$

where Eq. (12) has been used to perform the sum over i. This result is the working definition of the representation of functions in the DO basis.

Now it is only necessary to express arbitrary differential operators in this basis so that differential equations of the form of Eq. (6) can be solved. To do this we will first find the polynomial representation of the derivative operator and then transform it to DO representation. The matrix elements of the derivative operator in the polynomial basis are given by

$$D_{ij}^{(e)}=\int_a^b w(x)\,R_i(x)\,R_j'(x)\,dx. \tag{15}$$

This matrix is upper triangular since for $i\geqslant j$, $R_i(x)$ is orthogonal to $R_j'(x)$. The representation of this operator in the DO basis is given by

$$\mathbf{D}^{(f)}=\mathbf{T}^{\dagger}\cdot\mathbf{D}^{(e)}\cdot\mathbf{T}. \tag{16}$$

If $g\in S^{N-1}$ then the differentiation operation in the discrete ordinate basis is given simply by,

$$\mathbf{g}'^{(f)}=\mathbf{D}^{(f)}\cdot\mathbf{g}^{(f)}. \tag{17}$$

The approximate DO representation of the functions $H(x)$ in the differential operator L of Eq. (7) considered as multiplicative operators, is given by the diagonal matrix with the elements,

$$H_{ij}^{(f)} = H(x_i)\delta_{ij}, \tag{18}$$

where the m index has been omitted.

The discrete ordinate differential approximation of the operator in Eq. (7) is now written in the form,

$$\mathbf{L}^{(f)} \cong \sum_m [\mathbf{H}^{(f)}]_m \cdot [\mathbf{D}^{(f)}]^m, \tag{19}$$

where $[\mathbf{D}^{(f)}]^0$ is the unit matrix. This is not an exact representation of the differential operator in the DO basis. However, if all the $H_m(x)$ functions in Eq. (7) are polynomials of degree $m+1$ or less, then it may be shown that the DO representation is equivalent to the truncated polynomial representation of the same order.

2.2. *Discrete Ordinate Representation of Differential Operators*

The basic procedure involves the determination $D_{ij}^{(e)}$ defined by Eq. (15) and performing the transformation given by Eq. (16). A polynomial basis set must be chosen and this choice depends on the problem to be considered. The methods developed here are applicable to any basis set although the present paper considers the Legendre polynomials $P_l(x)$, orthogonal on the interval $[-1, 1]$ with unit weight function and the new speed polynomials $B_n(x)$ [1], orthogonal on $[0, \infty]$ with the weight function $w(x) = x^2 e^{-x^2}$.

The matrix elements $D_{ij}^{(e)}$, may be readily evaluated from Eq. (15) with an integration by parts, that is,

$$\begin{aligned} D_{ij}^{(e)} &= 0, && i > j, \\ &= w(x)\, R_i(x)\, R_j(x)\big|_a^b - \int_a^b w(x)\, R_i(x)\, R_j(x) \frac{w'(x)}{w(x)}\, dx, && i < j. \end{aligned} \tag{20}$$

In the case of normalized Legendre polynomials $P_l(x)$, this reduces to

$$\begin{aligned} D_{nm}^{(e)} &= (\sqrt{(2m+1)(2n+1)}, && m > n, m+n \text{ odd} \\ &= 0, && \text{otherwise.} \end{aligned} \tag{21}$$

This polynomial representation was transformed into the DO representation using the appropriately defined transformation operator. Many of the applications in the next section will be based on the differential operator defined with the Gauss–Legendre quadrature.

For the speed polynomials it was convenient to proceed in an alternate way. The B_n polynomials may be generated by the three term recurrence relation [1],

$$\sqrt{\beta_{n+1}}\, B_{n+1}(x) = (x - \alpha_n)\, B_n(x) - \sqrt{\beta_n}\, B_{n-1}(x), \tag{22}$$

where the calculation of α and β is discussed in [1]. The matrix representative of the derivative operator in the polynomial basis may be found by the use of the confluent form of the Christoffel–Darboux identity [11],

$$\sum_{k=0}^{N-1} (B_k(x))^2 = \sqrt{\beta_n}\, [B_n'(x)\, B_{n-1}(x) - B_n(x)\, B_{n-1}'(x)]. \tag{23}$$

If Eq. (23) is multiplied by $x^2 e^{-x^2}$ and integrated over $[0, \infty]$ we find that,

$$D_{n-1,n}^{(e)} = n/\sqrt{\beta_n}. \tag{24}$$

Similarly the multiplication of Eq. (23) by $x^3 e^{-x^2}$ and the use of the recurrence relation Eq. (22), followed by integration over x, yields,

$$\sum_{k=0}^{N-1} \alpha_k = \sqrt{\beta_n}\, \alpha_{n-1} D_{n-1,n}^{(e)} + \sqrt{\beta_n \beta_{n-1}}\, D_{n-2,n}^{(e)}. \tag{25}$$

This equation may be rearranged with the use of Eq. (24) to give

$$D_{n-2,n}^{(e)} = \left[\sum_{k=0}^{n-1} \alpha_k - n\alpha_{n-1} \right] / \sqrt{\beta_n \beta_{n-1}}. \tag{26}$$

The remaining matrix elements may be found by multiplication of the recurrence relation (22) by $x^2 e^{-x^2} B_n'(x)$ followed by integration. This yields

$$D_{k-1,n}^{(e)} = \left[\int_0^{\infty} B_k(x)\, x^3 e^{-x^2} B_n'(x)\, dx - \beta_{k+1} D_{k+1,n}^{(e)} - \alpha_k D_{k,n}^{(e)} \right] / \sqrt{\beta_k}. \tag{27}$$

The integral in Eq. (27) may be evaluated by integration by parts and hence rewritten as

$$D_{k-1,n}^{(e)} = [2\sqrt{\beta_{k+1}\beta_{k+2}}\, \delta_{k+2,n} - \sqrt{\beta_{k+1}}\, D_{k+1,n}^{(e)} - \alpha_k D_{k,n}^{(e)}] / \sqrt{\beta_k} \tag{28}$$

provided $k + 2 < n$. Thus all of the nonzero matrix elements are evaluated by recursion. The method outlined above is applicable for weight functions of the form $x^p e^{-x^2}$ as used in [1]. As before this operator is transformed into the corresponding DO basis. The DO representation of the differential operator has now been generated in the Gauss–Legendre quadrature and the B_n quadrature.

As an illustration of the usefulness of this representation of the derivative operator, we consider the differentiation of the oscillatory function $f(x) = \sin[3(\sinh(x) + (1 + x)^2)]$, chosen arbitrarily. Since we are considering the interval $[0, 1]$, Gauss–Legendre quadrature points are employed. The second derivative of this

TABLE I

Comparison of Numerical Differentiation

x	f(x)	f"(x) [a]	E [b]	f"(x) [c]	E [b]
0.00155326	0.12726007	- 16.28527098	0.76E-12	- 16.28527098	0.60E-09
0.00816594	0.06784673	- 11.56632236	-0.58E-09	- 11.56632237	-0.17E-07
0.01998907	-0.03950136	- 2.76935530	0.60E-10	- 2.76935532	-0.16E-07
0.03689998	-0.19339086	10.45676067	-0.15E-10	10.45676083	0.16E-06
0.05871973	-0.38695791	28.18794863	0.51E-10	28.18794863	0.78E-09
0.08521712	-0.60315987	49.70003239	-0.38E-11	49.70003239	0.28E-08
0.11611128	-0.81028462	72.78496383	0.33E-11	72.78496379	-0.41E-07
0.15107475	-0.96035612	93.10145744	-0.24E-11	93.10145736	-0.86E-07
0.18973691	-0.99431669	103.99807283	0.19E-11	103.99807280	-0.30E-07
0.23168793	-0.85766993	97.48245360	-0.21E-11	97.48245353	-0.66E-07
0.27648312	-0.52685871	66.97435252	0.32E-11	66.97435250	-0.22E-07
0.32364764	-0.03906356	11.79600346	-0.26E-11	11.79600335	-0.11E-06
0.37268154	0.49138963	- 58.16487063	0.17E-11	- 58.16487070	-0.74E-07
0.42306504	0.89100469	-120.97517431	-0.56E-12	-120.97517431	-0.16E-08
0.47426408	0.98977657	-148.12752992	-0.54E-12	-148.12752990	0.20E-07
0.52573592	0.71055940	-117.80989495	-0.89E-13	-117.80989491	0.43E-07
0.57693496	0.13575281	- 30.60966056	0.36E-13	- 30.60966045	0.11E-06
0.62731846	-0.50342574	83.12313611	-0.24E-12	83.12313602	-0.89E-07
0.67635236	-0.92948994	173.24524007	0.16E-11	173.24524008	0.32E-08
0.72351688	-0.96080670	194.99796879	-0.13E-11	194.99796866	-0.13E-06
0.76831207	-0.60287125	134.26194964	0.22E-11	134.26194954	-0.96E-07
0.81026309	-0.02957128	15.26821907	-0.24E-11	15.26821888	-0.18E-06
0.84892525	0.52532054	-114.48439921	0.12E-11	-114.48439945	-0.23E-06
0.88388872	0.88728264	-210.48866829	0.94E-12	-210.48866828	0.88E-08
0.91478288	0.99998511	-250.76022160	-0.60E-11	-250.76022161	-0.20E-08
0.94128027	0.90969816	-238.99727696	0.12E-10	-238.99727675	0.21E-06
0.96310002	0.72002361	-194.79292701	-0.80E-11	-194.79292677	0.24E-06
0.98001093	0.49067637	-140.83294025	-0.42E-10	-140.83293976	0.49E-06
0.99183406	0.31251156	- 94.62706369	-0.27E-09	- 94.62706375	-0.61E-07
0.99844674	0.20667729	- 66.36410768	-0.22E-08	- 66.36410798	-0.30E-06

[a] Discrete ordinate method based on a Gauss–Legendre quadrature procedure, $N = 30$.
[b] Error, E = analytic-numerical.
[c] Finite difference method, Eq. (29).

function was determined numerically by repeated application of Eq. (17) with $\mathbf{D}^{(f)}$ constructed as described above. For comparison, the fourth order finite difference approximation of the second derivative, that is,

$$f''(x) = [-f(x-2h) + 16f(x-h) - 30f(x) + 16f(x+h) - f(x-2h)]/12h^2 + O(h^4) \tag{29}$$

was also calculated. The result of this comparison with $N = 30$ and $h = 0.0001$ together with $f(x)$ are shown in Table I. To generate a matrix derivative operator based on finite differences that even approached the accuracy of the DO operator, it would be necessary to use a matrix of order 300 times that of the DO matrix. In the next section the solution of some model problems is presented.

3. Applications

The linear equations to be considered in this paper are of the form

$$Lu = f \tag{30}$$

together with appropriate boundary conditions. Table II lists the equations to be considered, the boundary conditions and the analytic solution. In the first three examples, a linear variable change, $x' = mx + b$ was employed to change the domain from x from $[0, 1]$ to $[-1, 1]$ so that Gauss–Legendre quadrature points can be employed. For example D in Table II, the quadrature rule of [1] is employed, without a variable change. All the operators in the equations in Table II are approximated with the discrete ordinate representation and it is understood that $L_{ij} = L_{ij}^{(f)}$ and similarly for the other quantities. Thus Eq. (30) may be rewritten as

$$\sum_{j=0}^{N-1} L_{ij} u(x_j) \sqrt{w_j} = f(x_i) \sqrt{w_i}. \tag{31}$$

The linear boundary conditions in Table II may be studied in their most general form for second order problems, as given by

$$\gamma_{1k} u(a) + \gamma_{2k} u'(a) + \gamma_{3k} u(b) + \gamma_{4k} u'(b) = \gamma_{5k}, \qquad k = 1, 2, \tag{32}$$

where γ_{ik} are arbitrary constants. If the quadrature points are scaled as discussed previously so that the first and last quadrature points can be made to coincide with a and b, respectively, then Eq. (32) may be written as

$$\sum_{j=0}^{N-1} [(\gamma_{1k}\delta_{0j} + \gamma_{2k} D_{0j})/\sqrt{w_0} + (\gamma_{3k}\delta_{N-1,j} + \gamma_{4k} D_{N-1,j})/\sqrt{w_{N-1}}] \sqrt{w_j}\, u(x_j) = \gamma_{5k}, \qquad k = 1, 2. \tag{33}$$

Equations (31) and (33) completely specify the second order differential equations. However, there are $N + 2$ equations and N unknowns, and the problem would appear to be over specified. However, if the first and last equations of Eq. (31) are replaced by Eq. (33), then we have N equations in N unknowns and the problem is well defined. It is possible to calculate the solution at points other than the quadrature points by transforming the solution vector into the polynomial basis, that is,

$$\mathbf{u}^{(e)} = \mathbf{T} \cdot \mathbf{u}^{(f)}. \tag{34}$$

The specific examples in Table II will now be considered.

TABLE II

Linear Differential and Integral Operators

	Operator L	Source F	Domain	Boundary Conditions	Exact Solution
A	$\frac{d^2}{dx^2}+\frac{2(\sin 2x-1)}{\cos 2x}\frac{d}{dx}+\frac{(3-\sin 2x)}{1+\sin 2x}$	$-2(\sin x+\cos x)$	$x\in[0,\pi]$	$y(0)=y(\pi)$ $y'(0)=y'(\pi)$	$y(x)=x(\pi-x)[\sin x+\cos x]$
B	$\frac{\partial}{\partial x}-\int_0^1 d\tau e^{(x-\tau)}$	$\sin x$	$x\in[0,1]$	$y(x_0)=1$	$y(x)=\left[\frac{\sqrt{2}\sin(4-\pi/4)+e}{2(e-1)e^{x_0}}+\frac{\cos x_0-1}{e^{x_0}}\right](e^x-1)$ $+\cos x+\cos x_0+1$
C	$\frac{1}{x}\frac{d}{dx}x^3\frac{d}{dx}-\lambda$	0	$x\in[1,e]$	$y(1)=y(e)=0$	$y_n(x)=\sin(n\pi \ln x)/x$ $\lambda_n=(n\pi)^2+1$
D	$x\frac{d^2}{dx^2}+(3-2x^2)\frac{d}{dx}-\lambda$	0	$x\in[0,\infty]$	$y(0)=y(\infty)=0$	[12]

3.1. *Periodic Boundary Value Problem*

Example A was devised to illustrate the ease of application of the present method. The solution of this equation by integrating from one end point to the other is difficult with periodic boundary conditions. Also, there is a regular singular point at $x = 3\pi/4$.

The solution with the discrete ordinate method with $N = 20$ was obtained as described earlier. The comparison with the analytic solution at intervals of $\pi/20$ is shown in Table III and the agreement is excellent. If the functions multiplying the derivatives in L are changed, that is the functions $H_m(x)$, there is essentially no modification to the basic method involved. This is one of the major features of the present method.

3.2. *Integro-Differential Problem*

As mentioned in the Introduction, the authors have developed this method with the objective of applying it to transport problems which involve the solution of the

TABLE III

Example A

X	Numerical [a]	Analytic
0.0	-0.0000000002	0.0
0.1570796327	0.5363718750	0.5363718752
0.3141592654	1.1192784358	1.1192784360
0.4712388980	1.6925100396	1.6925100397
0.6283185307	2.2057416961	2.2057416962
0.7853981634	2.6170740748	2.6170740749
0.9424777961	2.8950359762	2.8950359762
1.0995574288	3.0199688944	3.0199688944
1.2566370614	2.9847424960	2.9847424960
1.4137166941	2.7947797708	2.7947797708
1.5707963268	2.4674011003	2.4674011003
1.7278759595	2.0305263600	2.0305263599
1.8849555922	1.5208022620	1.5208022619
2.0420352248	0.9812473759	0.9812473758
2.1991148575	0.4585286529	0.4585286528
2.3561944902	-0.0000000000	0.0000000000
2.5132741229	-0.3493551641	-0.3493551641
2.6703537556	-0.5499298481	-0.5499298480
2.8274333882	-0.5703008484	-0.5703008482
2.9845130209	-0.3896969784	-0.3896969782
3.1415926536	-0.0000000002	0.0

[a] $N = 20$.

integro-differential Boltzmann equation. With this in mind, we considered the following problem defined by,

$$\frac{dy}{dx} - \int_{x_0}^{1} e^{(x-\tau)} y(\tau)\, d\tau = \sin x \tag{35}$$

subject to the initial condition $y(x_0) = 1$.

In the discrete space, Eq. (35) may be approximated by

$$\sum_{j=0}^{N-1} [D_{ij} - K_{ij}] \sqrt{w_j}\, y(x_j) = \sin(x_i) \sqrt{w_i}, \tag{36}$$

where

$$K_{ij} = e^{(x_i - x_j)} \sqrt{w_i w_j} \tag{37}$$

and x_i and w_i are the Gauss–Legendre quadrature points and weights, respectively.

The set of equations (36) was solved together with the initial condition and the results for $N = 20$ are shown in Table IV. The agreement with the exact solution is good although somewhat lower than for the other examples studied.

TABLE IV

Example B

X	Analytic	Numerical [a]	Error
0.003435	1.0000000	1.0000000	
0.018014	1.0127462	1.0127464	0.17E-06
0.043882	1.0353092	1.0353097	0.49E-06
0.080441	1.0671042	1.0671051	0.94E-06
0.126834	1.1073666	1.1073682	0.16E-05
0.181973	1.1552360	1.1552383	0.23E-05
0.244566	1.2098367	1.2098399	0.32E-05
0.313146	1.2703411	1.2703454	0.43E-05
0.386107	1.3359967	1.3360022	0.55E-05
0.461736	1.4061019	1.4061088	0.69E-05
0.538263	1.4799250	1.4799333	0.83E-05
0.613892	1.5565761	1.5565860	0.99E-05
0.686853	1.6348555	1.6348671	0.12E-04
0.755433	1.7131174	1.7131307	0.13E-04
0.818026	1.7891927	1.7892076	0.15E-04
0.873165	1.8604100	1.8604263	0.16E-04
0.919558	1.9237369	1.9237546	0.18E-04
0.956117	1.9760371	1.9760559	0.19E-04
0.981985	2.0144095	2.0144291	0.20E-04
0.996564	2.0365562	2.0365762	0.20E-04

[a] $N = 20$.

TABLE V
Example C

n	$\lambda_n{}^a$	$\lambda_n{}^b$
1	10.8696044015	10.8696044011
2	40.4784175928	40.4784176044
3	89.8264365475	89.8264396098
4	158.9137074948	158.9136704174
5	247.7401505683	247.7401100272
6	356.3178629772	356.3057584392
7	484.5163020440	484.6106156534
8	632.9205561547	632.6546816697
9	797.3395103782	800.4379564882
10	966.1809546573	987.9604401989

[a] $N = 15$.
[b] $\lambda_n = (n\pi)^2 + 1$.

3.3. *A Sturm–Liouville Problem*

A Sturm–Liouville eigenvalue problem of the form

$$\frac{1}{x}\frac{d}{dx}\left(x^3\frac{dy}{dx}\right) = \lambda y, \qquad x \in [1, e] \tag{38}$$

with boundary conditions $y(1) = y(e) = 0$, where e is the base of natural logarithms, was also considered.

In the discrete ordinate approximation the eigenvalues are calculated by first determining the matrix representation of the lhs of Eq. (38) denoted by $\mathbf{L}$. The boundary conditions are imposed by removing the first and last columns of the matrix $\mathbf{L}$ since these elements are multiplied by the first and last elements of the eigenvector, which are zero. The first and last rows of $\mathbf{L}$ define the equations for $y(x_0)$ and $y(x_{N-1})$, hence these rows should be removed. The resulting matrix of dimension $(N-2) \times (N-2)$ was diagonalized numerically. A comparison of these eigenvalues with the exact eigenvalues is shown in Table V. The lower order eigenvalues have converged remarkably well and even some of the higher eigenvalues are determined with reasonable accuracy considering that a very small number of points ($N = 15$) was used. The higher order oscillatory eigenfunctions require more points for their accurate calculation.

3.4. *Eigenvalues of the Fokker–Planck Operator*

In electron thermalization, the Fokker–Planck equation gives the change in the electron distribution function as a result of collisions with the moderator [13]. For a hard sphere cross section the Fokker–Planck operator is given by

$$L_{\mathrm{FP}} = x\frac{d^2\psi}{dx^2} + (3 - 2x^2)\frac{d\psi}{dx}, \tag{39}$$

TABLE VI
Example D

n	$\lambda_n{}^a$	$\lambda_n{}^b$
1	− 4.68339516	− 4.68339516
2	−10.11251880	−10.11251880
3	−16.42968416	−16.42968416
4	−23.57185079	−23.57185079
5	−31.46625300	−31.46625300
6	−40.05237885	−40.05237855
7	−49.28102526	−49.28101338
8	−59.11193192	−59.11162283
9	−69.51550758	−69.51024024
10	−80.50507473	−80.44793669

[a] Discrete ordinate method, $N = 20$.
[b] Polynomial method, $N = 90$ [12].

where x is the reduced velocity of the electron and $x^2 e^{-x^2}\psi(x)$ is the electron distribution function. The eigenvalues of the operator have previously been found [12] by diagonalization of the truncated operator in the B polynomial representation.

The diagonalization of this operator in DO space, based on the quadrature derived from the B_n polynomials is carried out as in the previous example with $N = 20$. In this case it is not necessary to impose any boundary conditions since the weight function, $x^2 e^{-x^2}$ ensures that the distribution function will approach zero as $x \to 0$ and $x \to \infty$. Table VI gives the first 20 numerical and exact eigenvalues and these eigenvalues are identical to the ones obtained by direct diagonalization of the matrix in the B_n representation. As discussed before the DO and polynomial representations will be identical if the polynomials multiplying the derivative operators are polynomials of small enough degree.

4. Summary

A discrete ordinate method for the solution of linear differential equations has been developed. The main advantages include a high order algorithm in the numerical calculation of derivatives. Also, boundary conditions are imposed in a natural and simple fashion. In the applications discussed in this paper, no more than 20 discrete points were employed in the solution of boundary value and eigenvalue problems.

In instances where a differential equation can be written as a set of coupled first order differential equations, the usual procedure is to employ a direct numerical integration. For this purpose there are a number of algorithms to choose from [14]. A detailed comparison of these methods has recently appeared [15, 16]. Although we have not compared the present results with results obtained by a direct numerical integration, it is anticipated that the DO method will prove efficient for a variety of applied problems owing to the small number of quadrature points required to obtain accurate solutions. The present method can easily incorporate two point boundary value problems (Example A) whereas direct numerical integration methods are more involved.

Green's function methods [17] which involve the calculation of the inverse of the operator can also be used. As with the present method, boundary conditions are incorporated into Green's function. However, Green's functions are often not easily determined and their use is sometimes made difficult by the presence of singularities.

Finite difference methods are also often used in the solution of differential equations [18], and in neutron transport [15, 19]. The present DO derivative matrix was shown to be superior to finite difference approximations in the calculation of derivatives. This suggests that it may be possible to represent differential operators more accurately with a DO approximation than with a finite difference approximation.

The DO approximation also has the advantage of being, like the collocation method [16], a nonlocal method. That is the solution is known at all points and not just at the quadrature points. The collocation method is similar to the present method in that the solution is found at a set of quadrature points. The collocation method differs from the present method in that it generates a set of nonorthogonal functions, satisfying the boundary condition, which are superimposed to yield a solution. The present method requires the superposition of a set of othogonal functions which satisfy the boundary conditions.

Since the DO method is an approximation to polynomial methods, it is basis dependent. However, it has two advantages over using polynomials. First, once the derivative operator has been generated the approximation of any linear differential operator is easily and accurately computed. Second, it is a very simple matter to impose boundary conditions in this representation.

Advantages of this present method include high accuracy with relatively few quadrature points, a solution defined at all points of the domain and the ease with which boundary conditions may be imposed. A wide variety of problems may be treated with discrete ordinates.

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