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PREFACE

The following articles represent the contributed and invited lectures given at the Symposium on Constructive and Computational Methods for Differential and Integral Equations held at Indiana University, Bloomington, Indiana, from February 17-20, 1974. The Symposium was organized through the Research Center for Applied Science at Indiana University under the sponsorship of the Air Force Office of Scientific Research Grant No. 74-2674.

One of the main objects of this Symposium was to collect together those mathematicians working in the general area of constructive and computational methods for solving differential and integral equations in order to prepare a survey of recent developments in this important area of applied mathematical research. Such a survey would have the aim of not only coordinating the work of the active researchers in this area, but would also supply a means through which applied mathematicians and engineers could become more acquainted with the new methods now available for solving problems they may be presently grappling with unsuccessfully. The following collection of addresses therefore contains both reviews and discussions of current problems and it is hoped they will provide a beginning towards accomplishing the long range objectives of the Symposium.

It was decided by the Editors that it also would be interesting to hear if the new generation of computers such as the ILLIAC IV would pose new techniques and perhaps introduce new mathematical problems in the study of the numerical solution of differential and integral equations. As it is apparent from the lecture by Robert Wilhelmson, parallel computation is still somewhat in its infancy and even though it shows great promise, it is difficult to assess at this time how much it will influence the development of numerical methods for solving differential and integral equations.

The organizers take this opportunity of thanking the Air Force Office of Scientific Research for making the Symposium possible. They would also like to gratefully acknowledge the assistance of many members of the Systems Analysis Institute and Computer Science Department of Indiana University whose help contributed immeasurably to the success of the Symposium.

David L. Colton
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Editors

CONTENTS

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Convergence of the Discrete Ordinates Method for the Transport Equation

P. M. Anselone* and A. G. Gibbs**

1. Introduction

The transport equation (transfer equation, linear Boltzmann equation) governs the distribution of neutrons in a nuclear reactor or of radiation in a stellar or planetary atmosphere. It is an integro-differential equation of some complexity in its more general forms. Primary independent variables are position and direction, speed (alternatively energy, frequency or wavelength), plus possibly time. The differential operator in the equation describes attenuation due to both absorption and scattering away from a particular direction. The integral operator describes scattering into a particular direction from other directions and production by fission. Source terms may be present. On any boundary surface there are boundary conditions corresponding to incoming directions. For time-dependent problems there are initial conditions.

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Since the transport equation can be solved explicitly only in a few very special cases, approximation methods are commonly used. The discrete ordinates method involves the replacement of the integral operator by a numerical integral operator in order to obtain differential equations for approximate solutions. Empirically, this method yields very satisfactory results for a large class of transport problems. However, a complete and rigorous convergence and error analysis is presently available only in some rather idealized cases.

The discrete ordinates method was first applied by Wick [18] and by Chandrasekhar [7, 8] to particular steady-state problems from astrophysics with homogeneous media bounded by single planes or parallel planes (half-spaces or slabs), usually under conditions of isotropic scattering and isotropic sources. Convergence theorems for the approximations were obtained for various problems of this type with isotropic scattering by Anselone [1-5], Kofink [13], Keller [10, 11] and Wendroff [17]. Subsequently, convergence theorems have been obtained for certain transport problems involving anisotropic scattering, other geometries, and time-dependence, by Keller [12], Nestell [16], Madsen [14] and Wilson [20].

We shall survey these contributions from an abstract and unifying point of view in order to isolate what is essential to the convergence of the discrete ordinates approximations. In the process, methods of analysis will be developed which appear to be applicable to very general transport problems and to other integro-differential equations. The discussion is in terms of a sequence of model problems of increasing complexity. All functions considered will be real. For mathematical convenience and physical relevence specified functions are continuous and usually nonnegative. We remark that the problems surveyed here involve discrete ordinates approximations only for the angular integrals, and thus do not represent the most general case of discretization as practiced, say, in many nuclear reactor applications today, where the spatial variable is also discretized. However, as noted below, the powerful analytical tools developed in applications to angular discrete ordinates approximations also show promise for investigations of the more general case.

2a. An Isotropic Transport Problem in a Finite Slab

Consider the problem for $\phi(x, \mu)$ with $a \leq x \leq b$, $-1 \leq \mu \leq 1$, given by

$$\mu \frac{\partial\phi(x, \mu)}{\partial x} + \phi(x, \mu) = \frac{c}{2}\int_{-1}^{1} \phi(x, \mu')d\mu' + g(x),$$

(2.1)

$$\phi(a, \mu) = 0 \quad \text{for} \quad \mu > 0, \quad \phi(b, \mu) = 0 \quad \text{for} \quad \mu < 0,$$

where $\phi(x, \mu)$ is the one-speed angular flux at depth x in a homogeneous slab in a direction making an angle $\theta = \cos^{-1}\mu$ with the positive x-axis. The positive number c is of order 1 and represents the mean number of secondary neutrons per collision. In the above equation, distance has been measured in units of neutron mean free paths, i.e., $x = \sigma\tau$, where σ is the total cross section and τ is the actual distance.

The boundary conditions correspond to a situation with no reflection of neutrons at the surface and no incident neutrons. Actually, a non-zero incident flux boundary condition could have been assumed. However, such a problem can be reduced to (2.1) for $\phi_1 = \phi - \phi_0$, where ϕ_0 satisfies the homogeneous equation

$$\mu \frac{\partial \phi_0(x, \mu)}{\partial x} + \phi_0(x, \mu) = 0$$

and the given boundary conditions. If this reduction is not made, then an unnecessary approximation is introduced for ϕ_0, which can be found explicitly. For the same reason, zero boundary conditions can and should be assumed also in applications of the discrete ordinates method to more general transport problems.

To proceed, assume a numerical integration rule such that, for any continuous function $h(\mu)$, $-1 \leq \mu \leq 1$,

$$\sum_{j=\pm 1}^{\pm n} w_{nj}\, h(\mu_{nj}) \to \int_{-1}^{1} h(\mu)\, d\mu, \quad n \to \infty,$$

$$w_{n,-j} = w_{n,j} > 0, \quad \mu_{n,-j} = -\mu_{n,j},$$

$$0 < \mu_{n1} < \mu_{n2} \cdots < \mu_{nn} \leq 1.$$

The Gauss quadrature formula is an example. The symmetry conditions on the w_{nj} and μ_{nj} are a convenience rather than a necessity.

Discrete ordinates approximations $\phi_n(x, \mu)$, $n = 1, 2, \ldots,$ satisfy

$$\mu \frac{\partial \phi_n(x, \mu)}{\partial x} + \phi_n(x, \mu) = \frac{c}{2} \sum_{j=\pm 1}^{\pm n} w_{nj}\, \phi_n(x, \mu_{nj}) + g(x),$$

(2.2)

$$\phi_n(a, \mu) = 0 \quad \text{for} \quad \mu > 0, \ \phi_n(b, \mu) = 0 \quad \text{for} \quad \mu < 0.$$

For $\mu = \mu_{ni}$, $i = \pm 1, \ldots, \pm n$, this is a system of ordinary differential equations for $\phi_n(x, \mu_{ni})$. Then (2.2) yields $\phi_n(x, \mu)$.

The problems for ϕ and ϕ_n have equivalent integral equation formulations which are more convenient for the convergence analysis. Let

$$f(x) = \frac{c}{2} \int_{-1}^{1} \phi(x, \mu)\, d\mu + g(x), \tag{2.3}$$

$$f_n(x) = \frac{c}{2} \sum_{j=\pm 1}^{\pm n} w_{nj}\, \phi(x, \mu_{nj}) + g(x). \tag{2.4}$$

From (2.1) and (2.3), it follows that

$$\phi(x, 0) = f(x),$$

(2.5)

$$\phi(x, \mu) = \frac{1}{\mu} \int_z^x e^{(y - x)/\mu} f(y)\, dy, \quad \begin{matrix} z = a, \ \mu > 0, \\ z = b, \ \mu < 0. \end{matrix}$$

The equations for ϕ_n in terms of f_n are identical. From (2.3) and (2.5),

$$(2.6) \qquad f(x) - \frac{c}{2} \int_a^b E_1(|x - y|)\, f(y)dy = g(x),$$

where E_1 is the exponential integral function of order one,

$$(2.7) \qquad E_1(s) = \int_0^1 e^{-s/\mu} \mu^{-1}\, d\mu, \quad s > 0,$$

which has a logarithmic singularity at $s = 0$. Similarly,

$$(2.8) \qquad f_n(x) - \frac{c}{2} \int_a^b E_{n1}(|x - y|)\, f_n(y)dy = g(x),$$

where E_{n1} is a numerical integration approximation to E_1:

$$(2.9) \qquad E_{n1}(s) = \sum_{j=1}^{n} w_{nj} \frac{e^{-s/\mu_{nj}}}{\mu_{nj}}, \quad s \geq 0,$$

$$(2.10) \qquad E_{n1}(s) \to E_1(s) \quad \text{uniformly for} \quad s \geq \varepsilon \quad \text{as} \quad n \to \infty$$

for each $\varepsilon > 0$. Thus, the discrete ordinates method is seen to be equivalent to the approximation of the integral operator in (2.6) by the integral operator in (2.8).

Express (2.6) and (2.8) in operator form

$$(2.11) \qquad (I - K)\, f = g, \qquad (I - K_n) f_n = g$$

on the space $C[a, b]$ with the max norm. Then K and K_n are Fredholm integral operators with kernels

$$k(x, y) = \frac{c}{2} E_1(|x - y|), \qquad k_n(x, y) = \frac{c}{2} E_{n1}(|x - y|).$$

These are bounded linear operators on $C[a, b]$ and for c not too large (the case of a subcritical medium, assumed here) we have

$$\|K\| = \max_x \int_a^b k(x, y)dy < 1.$$

Hence, $(I - K)^{-1}$ exists,

$$\|(I - K)^{-1}\| \leq (1 - \|K\|)^{-1},$$

and f and ϕ are uniquely determined.

From (2.10),

$$\|K_n - K\| \to 0, \qquad \|K_n\| \to \|K\| \quad \text{as} \quad n \to \infty.$$

Thus, we are in the realm of standard operator approximation theory. For n sufficiently large, $\|K_n\| < 1$, $(I - K_n)^{-1}$ exists and is bounded uniformly in n, and

(2.12) $$(I-K_n)^{-1} - (I-K)^{-1} = (I-K_n)^{-1}(K_n-K)(I-K)^{-1},$$

(2.13) $$\|(I-K_n)^{-1} - (I-K)^{-1}\| \leq \|(I-K_n)^{-1}\| \, \|K_n-K\| \, \|(I-K)^{-1}\|,$$

(2.14) $$\|(I-K_n)^{-1} - (I-K)^{-1}\| \leq \frac{\|(I-K)^{-1}\|^2 \, \|K_n-K\|}{1 - \|(I-K)^{-1}\| \, \|K_n-K\|},$$

(2.15) $$\|(I-K_n)^{-1} - (I-K)^{-1}\| \leq \frac{\|(I-K_n)^{-1}\|^2 \, \|K_n-K\|}{1 - \|(I-K_n)^{-1}\| \, \|K_n-K\|},$$

(2.16) $$\|(I-K_n)^{-1} - (I-K)^{-1}\| \to 0 \quad \text{as} \quad n \to \infty.$$

The error bound in (2.14) is "theoretical" in the sense that it involves $(I - K)^{-1}$, whereas (2.15) is "practical" because it depends on $(I - K_n)^{-1}$, and can thus be computed. The bound (2.13) is of mixed type. It follows from (2.16) and (2.5)ff that $f_n \to f$ and $\phi_n \to \phi$ uniformly as $n \to \infty$.

This is essentially the path followed by Anselone [4, 5] and by Keller [11], although Keller's analysis was less abstract and he defined the discrete ordinates approximations only at the quadrature points. Previously, Keller [10] and Wendroff [17] treated the differential operators directly without inverting them. The results were less satisfactory: L^2 convergence on quadrature points, and uniform convergence on quadrature points under a restrictive assumption. Kofink [13] established L^2 convergence on quadrature points by exploiting an equivalence between the discrete ordinates method and the spherical harmonics method.

2b. An Isotropic Transport Problem in a Half Space

Anselone [1-4] also derived uniform convergence theorems for isotropic transport problems in the case of semi-infinite slabs $(0 \leq x \leq \infty)$. In particular, the classical Milne problem leads to the homogeneous equation $(I - K)f = 0$, where K is the same integral operator as above. The Wiener-Hopf method, based on Fourier transforms, was devised originally to solve this equation.

A more direct method, which anticipated later theories of positive and monotone operators, was given by Hopf [9] for the case $c = 1$. It involves a change of variable $f(x) = x + q(x)$. Then q satisfies the inhomogeneous equation $(I - K)q = E_3$, where E_3 is the exponential integral function of order 3,

$$E_3(s) = \int_0^1 e^{-s/\mu}\, \mu d\mu, \quad s \geqq 0.$$

A nonnegative solution q is sought in the space of bounded continuous functions on $[0, \infty)$. Although now $\|K\| = 1$, monotonicity considerations yield a unique solution q given by the uniformly convergent Neumann series

$$q = \sum_{m=0}^{\infty} K^m E_3.$$

The discrete ordinates approximation problem can be recast in the form $(I - K_n)f_n = 0$. Let $f_n(x) = x + q_n(x)$. Then $(I - K_n)q_n = E_{n3}$, where E_{n3} is a numerical integration approximation to E_3, and q_n is given by

$$q_n = \sum_{m=0}^{\infty} K_n^{\,m} E_{n3}.$$

A detailed term by term analysis yields $q_n \to q$ uniformly as $n \to \infty$. It follows that $f_n \to f$ and $\phi_n \to \phi$ uniformly.

3a. An Anisotropic Transport Problem in a Finite Slab

Consider the problem for $\phi(x, \mu)$ with $a \leq x \leq b$, $-1 \leq \mu \leq 1$, given by

$$\mu \frac{\partial \phi(x, \mu)}{\partial x} + \phi(x, \mu) = \frac{1}{2} \int_{-1}^{1} p(x,\mu,\mu')\phi(x,\mu')d\mu' + g(x,\mu), \tag{3.1}$$

$$\phi(a, \mu) = 0 \quad \text{for} \quad \mu > 0, \quad \phi(b, \mu) = 0 \quad \text{for} \quad \mu < 0.$$

Here, x represents the optical depth measured from the plane of the origin, i.e.,

$$x(\tau) = \int_{0}^{\tau} \sigma(\tau')d\tau',$$

with $\sigma(\tau)$ the total cross section at position τ, and τ the distance measured from 0. The differential kernel $p(x, \mu, \mu')d\mu$ represents the average number of neutrons emerging with direction cosines in $d\mu$, following a collision by a neutron with direction cosine μ' at position x. The function g represents sources within the slab. We assume here that both p and g are continuous functions of x and μ.

Let

$$f(x, \mu) = \frac{1}{2} \int_{-1}^{1} p(x, \mu, \mu')\phi(x, \mu')d\mu'. \tag{3.2}$$

Then the problem is expressed in operator form as

$$D\phi = f, \qquad f = L\phi + g, \tag{3.3}$$

where $f,g \in C(X)$ with $X = [a, b] \times [-1, 1]$. Under reasonable conditions on ϕ, $M = D^{-1}$ exists as an operator on $C(X)$, and $\phi = Mf = D^{-1}f$ is given by

$$\phi(x, 0) = f(x, 0),$$

(3.4)

$$\phi(x, \mu) = \frac{1}{\mu}\int_z^x e^{(x' - x)/\mu} f(x', \mu)\,dx', \qquad \begin{array}{ll} z = a & \text{for } \mu > 0, \\ z = b & \text{for } \mu < 0. \end{array}$$

Therefore, an equivalent formulation of the problem is

(3.5) $$\phi = Mf, \qquad (I - K)f = g, \qquad K = LM.$$

It can be shown that K is a bounded integral operator which maps $C(X)$ into $C(X)$. Since K has a non-negative kernel

$$\|K\| = \|Ke\|, \qquad e \in C(X), \qquad e \equiv 1.$$

If p is not too large, then $\|K\| < 1$, which we assume in what follows. Then $(I - K)^{-1}$ exists as a bounded operator on $C(X)$, and f, ϕ are uniquely determined.

Assume a convergent, positive quadrature rule:

$$\sum_{j=1}^{n} w_{nj}\, h(\mu_{nj}) \to \int_0^1 h(\mu)\,d\mu \quad \text{as} \quad n \to \infty, \qquad h \in C[-1, 1],$$

$$w_{nj} > 0, \qquad 1 \le j \le n, \qquad n = 1, 2, \ldots \, .$$

In particular, for $h = e \equiv 1$,

$$\sum_{j=1}^{n} w_{nj} \to 1 \quad \text{as} \quad n \to \infty.$$

Hence, there exists $B < \infty$ such that

$$\sum_{j=1}^{n} w_{nj} \le B, \qquad n = 1, 2, \ldots \, .$$

The discrete ordinates approximations ϕ_n satisfy

$$\mu \frac{\partial\phi_n(x,\mu)}{\partial x} + \phi_n(x,\mu) = \frac{1}{2}\sum_{j=1}^{n} w_{nj}\ p(x,\mu,\mu_{nj})\phi(x,\mu_{nj}) + g(x,\mu),$$

(3.6)

$$\phi_n(a,\mu) = 0 \quad \text{for} \quad \mu > 0, \qquad \phi_n(b,\mu) = 0 \quad \text{for} \quad \mu < 0.$$

Equivalent formulations are

(3.7) $\quad D\phi_n = f_n, \qquad f_n = L_n\phi_n + g,$

(3.8) $\quad \phi_n = Mf_n, \qquad (I - K_n)f_n = g, \qquad K_n = L_nM,$

where K_n is a bounded linear operator on $C(X)$.
Since the "kernel" of K_n is positive, $\|K_n\| = \|K_ne\|$, where $e \equiv 1$.

It follows from (3.5) that $K_n \to K$, i.e., $\|K_nh - Kh\| \to 0$ as $n \to \infty$ for each $h \in C(X)$. However, $\|K_n - K\| \not\to 0$ in the anisotropic case, so the standard operator approximation theory used in Section 2 above is not applicable. An alternative course of action is pursued here.

It follows from $K_n \to K$, $\|K\| = \|Ke\|$ and $\|K_n\| = \|K_ne\|$ that $\|K_n\| \to \|K\|$. Recall that $\|K\| < 1$. Hence, for n sufficiently large, $\|K_n\| < 1$, $(I - K_n)^{-1}$ exists and is bounded uniformly in n, and

(3.9) $\quad (I - K_n)^{-1} - (I - K)^{-1} = (I - K_n)^{-1}(K_n - K)(I - K)^{-1},$

(3.10) $\quad f_n - f = (I - K_n)^{-1}(K_nf - Kf),$

(3.11) $$\|f_n - f\| \leq \|(I - K_n)^{-1}\| \ \|K_n f - Kf\| .$$

It follows that $f_n \to f$ and $\phi_n \to \phi$ uniformly as $n \to \infty$. The error bound in (3.11) is of mixed type, neither purely theoretical nor purely practical.

The fact that K and K_n are positive operators is essential to the foregoing analysis, which is an abstract version of that carried out by Keller [12] in a more classical spirit.

3b. An Anisotropic Transport Problem in a Half Space

We remark that the case of anisotropic scattering problems in a half-space was treated by Nestell [16] by an adaptation of the positive operator theory of Hopf. That work is an extension of the isotropic scattering problem discussed in Section 2b above.

4. Collectively Compact Operator Approximation Theory

We shall consider the same problem as in 3 from another point of view, which yields both theoretical and practical (computable) error bounds. The analysis is based on collectively compact operator approximation theory (cf. Anselone [6]).

It can be shown that the operator K in (3.4) is compact: $\{Kh : \|h\| \leq 1\}$ is relatively compact or, equivalently, bounded and equicontinuous. The sequence $\{K_n : n \geq 1\}$ is collectively compact: $\{K_n h : \|h\| \leq 1, n \geq 1\}$ is relatively compact. Thus, we have