JOURNAL OF COMPUTATIONAL PHYSICS 2, 245-256 (1967)

Invariant Imbedding and Radiative Transfer in Spherical Shells

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ABSTRACT

The invariant imbedding equation for the reflection function of a spherical shell, in which absorption and isotropic multiple scattering processes take place, is a nonlinear, partial differential integral equation. Two methods for its numerical solution are sketched, and the results of some numerical experiments are presented.

1. INTRODUCTION

The theory of radiative transfer has attracted a great deal of attention from mathematicians over the last 50 years, with the result that a number of distinguished names are attached to various parts of the theory: Ambarzumian, Busbridge, Chandrasekhar, Hopf, Milne, Sobolev, and Wiener, to name a few. In recent years, the linear Boltzmann equation, which plays an important position in the mathematical formulation, has been approached by means of such sophisticated techniques as the theory of distributions, singular integral equations, and operator theory; see Lehner-Wing [1] for this last.

Elegant and interesting as much of this work has been, and continues to be, it nevertheless possesses serious drawbacks as far as the scientist is concerned. To begin with, a quite high level of mathematical training and analytical expertise is required both to absorb and apply a number of the techniques that have been developed. What is even more serious is that the majority of mathematical models are tailored more to the analytical techniques that are available than to the day-to-day needs of the engineer and physicist. Thus, we see an undue emphasis upon isotropic, time-independent processes in homogeneous, plane-parallel media to the exclusion of anisotropic, time-dependent processes in inhomogeneous, cylindrical, and spherical media. Results obtained under idealized assumptions are not easily applied to the interpretation of experimental results.

These self-imposed limitations were completely understandable, and indeed unavoidable, in the world of the desk calculator. With the electronic digital computers now available, not to mention those contemplated 5 and 10 years hence, a new look at these problems, and indeed most of the problems of mathematical physics, is in order. There is every hope that the power and versatility of modern digital computers will enable the scientist in many classical fields simultaneously to treat quite realistic models of physical processes and to eliminate completely the mathematical middle-man. Multiple scattering is a simple process conceptually; it should be capable of a simple numerical treatment at a time when we can carry out a million multiplications a second. What we are asserting is a "principle of balance," requiring that the mathematical complexity of the treatment of a physical process be of no higher order than that of the underlying physical process [2].

To illustrate our ideas, we shall discuss a problem of some interest in a number of fields: that of diffuse reflection by a medium with a spherical geometry. Our aim is to show that a combination of simple analytic ideas, quadrature, series expansion, and the ability of the digital computer to handle large systems of ordinary differential equations with initial conditions permits us to treat the quite complicated nonlinear partial differential-integral equation governing reflection in a straightforward fashion. Nothing we do is beyond the level of a first-year graduate student, or, indeed, of a well-trained undergraduate junior.

Rather than deal with the boundary-value problem for the transport equation, we use invariant imbedding [3–5] to obtain an initial-value problem for the reflection function. The equation is

$$\begin{aligned}\frac{\partial S(z, v, u)}{\partial z} + \frac{1 - v^2}{vz}\frac{\partial S}{\partial v} + \frac{1 - u^2}{uz}\frac{\partial S}{\partial u} + \left(\frac{1}{v} + \frac{1}{u}\right)S - \frac{v^2 + u^2}{v^2u^2}\frac{S}{z} \\ = \lambda\left[1 + \frac{1}{2}\int_0^1 S(z, v, u')\frac{du'}{u'}\right]\left[1 + \frac{1}{2}\int_0^1 S(z, v', u)\frac{du'}{u'}\right], z > a,\end{aligned} \tag{1.1}$$

subject to the initial condition $S(a, v, u) = 0$ for $0 < v, u \leq 1$. This equation is obtained via invariant imbedding (see Bailey [3]).

Of course, it is true that digital computers and the numerical solution of approximating systems of differential equations have played an important role in the study of the transport equation for the last 25 years. Not sufficient attention, however, has been devoted to constructing new approaches specifically designed to exploit the properties of the contemporary computer. Our work constitutes a step in this direction.

To orient the reader, we begin with a brief account of the methods we have used to treat the plane-parallel case [4, 5]. Following this, we present a perturbation technique which enables us to apply the methods just described to the case of a thin spherical shell. Next we introduce a different approach, a "quadrature" technique for partial derivatives, which once again allows us to use the methods of the plane-parallel case. The agreement between the numerical results obtained using the two different methods is excellent. In order to compare our results with those previously obtained for the plane-parallel case, we carried out the calculations for homogeneous shells.

2. The Plane-Parallel Case

Let us consider a plane-parallel slab backed up by a semi-infinite slab which is a perfect absorber (see Fig. 1). Let $r(z, v, u)$ denote the intensity of diffusely re-

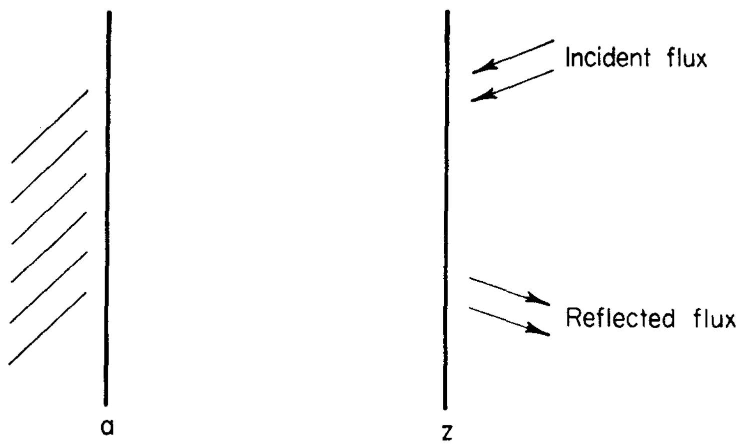

Fig. 1

flected radiation in the direction arc cos v due to incident flux with direction arc cos u. Then, setting $S(z, v, u) = 4vr(z, v, u)$ (in order to obtain a symmetric function in v and u), we obtain the integro-differential equation

$$\frac{\partial S}{\partial z} + \left(\frac{1}{u} + \frac{1}{v}\right)S = \lambda\left[1 + \frac{1}{2}\int_0^1 S(z, v', u)\frac{dv'}{v'}\right]\left[1 + \frac{1}{2}\int_0^1 S(z, v, u')\frac{du'}{u'}\right], \tag{2.1}$$

$z \geq a$, with the initial condition $S(a, v, u) = 0$. Here λ is the albedo for single scattering. For the derivation of this equation employing invariant imbedding, see [4], where a detailed discussion of what follows, together with extensive numerical tables, may be found.

To obtain a numerical solution to this equation, we employ Gaussian quadrature. Write

$$\begin{aligned} \int_0^1 S(z, v', u)\frac{dv'}{v'} &\cong \sum_{i=1}^{N} \frac{w_i S(z, v_i, u)}{v_i}, \\ \int_0^1 S(z, v, u')\frac{du'}{u'} &\cong \sum_{j=1}^{N} \frac{w_j S(z, v, u_j)}{u_j}, \end{aligned} \tag{2.2}$$

and then

$$S(z, v_i, u_j) = S_{ij}(z). \tag{2.3}$$

Then Eq. (1) becomes a finite set of ordinary differential equations,

$$\begin{aligned} &\frac{dS_{ij}}{dz} + \left(\frac{1}{u_j} + \frac{1}{v_i}\right)S_{ij} \\ &= \lambda\left[1 + \frac{1}{2}\sum_{k=1}^{N}\frac{w_k}{v_k}S_{kj}\right]\left[1 + \frac{1}{2}\sum_{k=1}^{N}\frac{w_k}{v_k}S_{ik}\right], \end{aligned} \tag{2.4}$$

$S_{ij}(0) = 0, \ i, j = 1, 2, \ldots, N.$

Excellent results are obtained by using $N = 7$, with no appreciable difference between the numbers obtained for $N = 7, 9, 11$. Usable results are obtained for $N = 5$. The calculation of the solution of 49, 81, 121 equations of this type on a modern digital computer for z in an interval $[a, b]$ consumes only a few minutes. We can use the symmetry relation $S_{ij} = S_{ji}$ either to reduce the number of equations or as an internal check on the computations.

3. Spherical Shell

Let us now consider a spherical shell, $a \leq z \leq b$, with a core, $0 \leq z \leq a$, that is a perfect absorber, subject to conical incident flux. Then the equation for the S-function is now that given in Eq. (1). In order to obtain a numerical solution, we use a power series expansion technique which transforms (1) into a set of equations similar to that considered in Section 1.

The interesting point about this procedure is that it illustrates the important fact that the digital computer enables us to reduce a single formidable problem to a large set of less formidable problems. The ability of the computer to handle large systems of several hundred differential equations with given initial conditions permits us to use this simple technique; see [6] for a similar discussion.

Write $x = z - a$, assume that $x/a \ll 1$, and set

$$S = S_0 + \frac{S_1}{a} + \frac{S_2}{a^2} + \cdots, \tag{3.1}$$

where $S_0, S_1, S_2, \ldots$ are independent of a. Substituting in (1.1) and equating coefficients, we obtain the following equations:

$$\begin{aligned}(S_0)_x &+ \left(\frac{1}{u} + \frac{1}{v}\right)S_0 \\ &= \lambda\left[1 + \frac{1}{2}\int_0^1 S_0(x, v', u)\frac{dv'}{v'}\right]\left[1 + \frac{1}{2}\int_0^1 S_0(x, v, u')\frac{du'}{u'}\right],\end{aligned} \tag{3.2}$$

$$\begin{aligned}(S_1)_x &+ \left(\frac{1-v^2}{v}\right)(S_0)_v + \left(\frac{1-u^2}{u}\right)(S_0)_u + \left(\frac{1}{u} + \frac{1}{v}\right)S_1 - \frac{u^2+v^2}{u^2v^2}S_0 \\ &= \lambda\left[1 + \frac{1}{2}\int_0^1 S_0(x, v, u')\frac{du'}{u'}\right]\left[\frac{1}{2}\int_0^1 S_1(x, v', u)\frac{dv'}{v'}\right] \\ &+ \lambda\left[1 + \frac{1}{2}\int_0^1 S_0(x, v', u)\frac{dv'}{v'}\right]\left[\frac{1}{2}\int_0^1 S_1(x, v, u')\frac{du'}{u'}\right].\end{aligned} \tag{3.3}$$

Using the quadrature techniques described above, we reduce these equations to a system of ordinary differential equations with initial conditions and readily obtain numerical solutions. In Section 7, we shall compare computational results obtained in different fashions.

4. Acceleration of Convergence

If the thickness of the shell is small compared with the inner radius, we can expect this perturbation technique to provide excellent results. If $x \geq a$, we face divergence.

There are several ways of overcoming this difficulty. One method is to do the calculation in parts. First, we carry it out for $x/a \leq 0.1$, say. Then we consider a new problem in which the inner radius is $(1.1)a$. This replaces the complete absorber by an inhomogeneous reflecting material, but this is not a matter of any difficulty. It merely yields a new initial condition. We can proceed in this fashion step by step until we obtain the desired shell thickness.

Another approach is based upon the observation that the divergence of the power series for $|x| \geq a$:

$$\frac{1}{a+x} = \frac{1}{a}\left[1 - \frac{x}{a} + \frac{x^2}{a^2} - \dots\right] \tag{4.1}$$

is due to the singularity at $x = -a$. However, we are interested only in $x \geq 0$. Let us then set

$$y = \frac{x}{x+K}, \quad x = \frac{Ky}{1-y} \tag{4.2}$$

for some suitably chosen K and expand in powers of y. Thus,

$$\frac{1}{a+x} = \frac{1}{a + Ky/1-y} = \frac{1-y}{a+(K-a)y}. \tag{4.3}$$

A convenient choice is $K = a$. Although we do not know the analyticity properties of S as a function of x, we do know that the function exists for $x \geq 0$ and that $0 \leq y \leq 1$ for $x \geq 0$. A detailed discussion of this device for analytic continuation with further references and applications will be found in [7].

5. Numerical Estimation of Derivatives

In Section 2, we indicated the use of quadrature techniques in the approximation of (2.1) by a system of ordinary differential equations. It is interesting to see if an analogous technique can be applied directly to (1.1). We wish to eliminate the derivatives by using linear combinations of the values of the functions at other points in the interval.

Let $x_1 < x_2 < \cdots < x_N$ be N points in an x-interval, and suppose that we wish to approximate the derivatives of a function $f(x)$ at the points x_1 by linear combinations of the values of $f(x)$ at the x_i, $i = 1, 2, \dots, N$,

$$f'(x_i) \cong \sum_{j=1}^{N} \alpha_j^{(i)} f(x_j). \tag{5.1}$$

Let us determine the coefficients, by analogy with the quadrature case, by the condition that the equations be exact for all polynomials of degree $N-1$ or less. Using the trial functions $f(x) = x^k$, $k = 0, 1, \ldots, N-1$, we obtain a system of linear algebraic equations

$$\sum_{j=1}^{N} x_j^{k-1}\alpha_j^{(i)} = (k-1)x_i^{k-2}, \quad k = 1, 2, \ldots, N. \tag{5.2}$$

If we choose the x_i to be the N roots of the shifted Legendre polynomial of degree N, $\varphi_N(x)$, we can readily invert the coefficient matrix, a Vandermonde matrix [5].

Alternatively, we can obtain the $\alpha_j^{(i)}$ explicitly by using the N test functions [8],

$$f_i(x) = \frac{\varphi_N(x)}{x - x_i}. \tag{5.3}$$

The matrices $(\alpha_j^{(i)})$ for $N = 7$ and 9 are given in Tables I and II.

TABLE I

THE COEFFICIENTS $\alpha_j^{(i)}$ FOR $N = 7$

$i = 1$			
− 0.19136364E 02	0.30166068E 02	− 0.18345136E 02	0.12020668E 02
− 0.73554054E 01	0.37037909E 01	− 0.10536210E 01	
$i = 2$			
− 0.30774001E 01	− 0.32947313E 01	0.94826608E 01	− 0.49141384E 01
0.27743267E 01	0.13485609E 01	0.37784329E–00	
$i = 3$			
0.73878691E 00	− 0.37433740E 01	− 0.97174703E 00	0.56413488E 01
− 0.24639939E 01	0.10951929E 01	− 0.29621352E–00	
$i = 4$			
− 0.36940283E–00	0.14803137E 01	− 0.43048331E 01	− 0.99475983E–13
0.43048331E 01	− 0.14803137E 01	0.36940283E–00	
$i = 5$			
0.29621352E–00	− 0.10951929E 01	0.24639939E 01	− 0.56413488E 01
0.97174703E 00	0.37433740E 01	− 0.73878691E 00	
$i = 6$			
− 0.37784329E–00	0.13485609E 01	− 0.27743267E 01	0.49141384E 01
− 0.94826608E 01	0.32947313E 01	0.30774001E 01	
$i = 7$			
0.10536210E 01	− 0.37037909E 01	0.73554054E 01	− 0.12020668E 02
0.18345136E 02	− 0.30166068E 02	0.19136364E 02	

TABLE II

THE COEFFICIENTS $\alpha_j^{(i)}$ FOR $N = 9$

$i = 1$			
− 0.30899183E 02	0.49462602E 02	− 0.31847722E 02	0.23009713E 02
− 0.16634325E 02	0.11463908E 02	− 0.71444862E 01	0.36223711E 01
− 0.10328869E 01			
$i = 2$			
− 0.46321847E 01	− 0.55540647E 01	0.15529632E 02	− 0.88594615E 01
0.58950087E 01	− 0.39077266E 01	0.23856884E 01	− 0.11961277E 01
0.33923594E–00			
0.33923594E–00			
$i = 3$			
0.99779608E 00	− 0.51953604E 01	− 0.19666417E 01	0.90706996E 01
− 0.46474057E 01	0.27969636E 01	− 0.16303335E 01	0.79812006E 00
− 0.22383800E–00			
$i = 4$			
− 0.41927865E–00	0.17238123E 01	− 0.52755643E 01	− 0.72470224E 00
0.67044574E 01	− 0.30840075E 01	0.16267280E 01	− 0.76033820E 00
0.20889316E–00			
$i = 5$			
0.25654308E–00	− 0.97080200E 00	0.22877170E 01	− 0.56744949E 01
0.56843419E–11	0.56744949E 01	− 0.22877170E 01	0.97080200E 00
− 0.25654308E–00			
$i = 6$			
− 0.20889316E–00	0.76033820E 00	− 0.16267280E 01	0.30840075E 01
− 0.67044574E 01	0.72470224E 00	0.52755643E 01	− 0.17238123E 01
0.41927865E–00			
$i = 7$			
0.22383800E–00	− 0.79812006E 00	0.16303335E 01	− 0.27969636E 01
0.46474057E 01	− 0.90706996E 01	0.19666417E 01	0.51953605E 01
− 0.99779608E 00			
$i = 8$			
− 0.33923594E–00	0.11961277E 01	− 0.23856884E 01	0.39077266E 01
− 0.58950087E 01	0.88594615E 01	− 0.15529632E 02	0.55540647E 01
0.46321847E 01			
$i = 9$			
0.10328869 E 01	− 0.36223711E 01	0.71444762E 01	− 0.11463908E 02
0.16634325E 02	− 0.23009713E 02	0.31847722E 02	− 0.49462602E 02
0.30899183E 02			

6. The Approximating System of Differential Equations

Using quadrature on the integral terms and the foregoing approximations for the partial derivatives, Eq. (1.1) is replaced by

$$\frac{dS_{ij}(z)}{dz} + \frac{1-v_i^2}{v_i z} \sum_{k=1}^{N} \alpha_k^{(i)} S_{kj} + \frac{1-v_j^2}{v_j z} \sum_{k=1}^{N} \alpha_k^{(j)} S_{ik} + \left(\frac{1}{v_i} + \frac{1}{v_j}\right) S_{ij}$$
$$- \frac{v_i^2 + v_j^2}{v_i^2 v_j^2} \frac{S_{ij}}{z} = \lambda \left[1 + \frac{1}{2} \sum_{k=1}^{N} S_{ik} \frac{w_k}{v_k}\right] \left[1 + \frac{1}{2} \sum_{k=1}^{N} S_{kj} \frac{w_k}{v_k}\right], \tag{6.1}$$

$z \geq a$, with initial conditions $S_{ij}(a) = 0$, $i, j = 1, 2, \ldots, N$.

7. Numerical Results

The above procedures for the calculation of S are carried out on an IBM-7044 with FORTRAN IV source programs. In the first series of numerical experiments, we produce the S function for a shell by integrating the system of differential equations (6.1). We call this Method I. We use formulas of order $N = 7$ and $N = 9$, and integration step sizes of 0.005 and 0.0025. There is agreement among calculations for comparable cases.

With $N = 7$ and a step size of 0.005, we vary the inner radius of the shell, $a = 100$, 500, and 1000. We compare reflected intensities, $r = S/4v$, for the shell against the corresponding intensities for the plane-parallel slab, which should be obtained as a $\to \infty$. The results are shown in Fig. 2. The reflection function r is shown for the case in which the albedo is 1 and the thickness is 3 for three angles of incidence that are approximately 13.0°, 60.0°, and 88.5°. We see immediately that the curves for the shell geometry always lie on or above the curves for the slab. In particular, the curve for 88.5°, with $a = 100$, lies as much as 50% above the curve for the slab. As the inner radius a is increased, the r function for the shell approaches that for the slab. The two cases are graphically indistinguishable for $a = 1000$. For the angle of incidence 60°, we have drawn a dashed curve for $a = 50$. It is the result of a calculation with $N = 5$, since the calculation for $N = 7$ is unstable.

Computations of the reflection function r are also carried out with variations of the perturbation technique. The partial derivatives $(S_0)_v$ and $(S_0)_u$ which appear in (3.3) are in the first instance approximated by formula (5.1) in Method IIa, and secondly are produced as solutions of systems of differential equations in Method IIb. Checks consisting of varying the order of the quadrature formula, varying the step length of integration, and increasing the inner radius are positive.

A comparison of the results of Methods I, IIa, and IIb shows satisfactory agreement. Figure 3 shows three sets of curves for the reflection function r, for

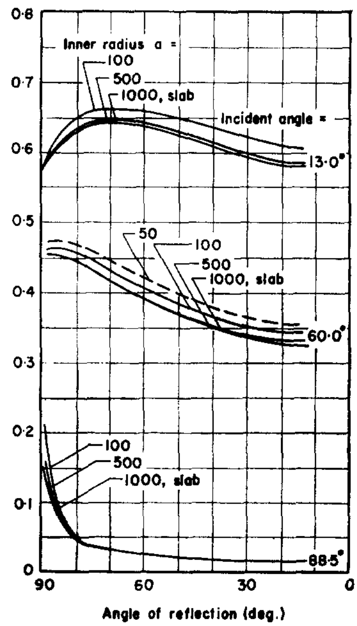

FIG. 2. Some reflected intensity patterns for shells with albedo $\lambda = 1$ and thickness $x = 3$, for various angles of incidence.

the case in which the albedo is 1, the inner radius is 50, and the thickness is 3. Each set corresponds to a different angle of incidence, 17.6°, 60.0°, and 87.3°. The order of the quadrature formula is $N = 5$. Four curves are plotted for each angle, although in some instances they lie on top of one another. These curves are labeled "Slab," "I," "IIa," and "IIb", in an obvious notation. Computing times to produce the data for Fig. 2, as well as tables of reflection functions for all shell thicknesses between 0.0 and 3.0, in increments of 0.1, are 37 seconds for Method I; 1 minute, 6 seconds for Method IIa; and 1 minute, 23 seconds for Method IIb.

Our program is in standard FORTRAN language and requires an extended training for its use. This is an important point.

Computing times for the different methods are short. The perturbation technique, however, has the advantage of producing reflection functions for a variety of shell inner radii in a single calculation [9]. This technique is found to be stable, and gives good results even when the ratio x/a is fairly large. This ratio is 3/50 for the case represented by Fig. 2.

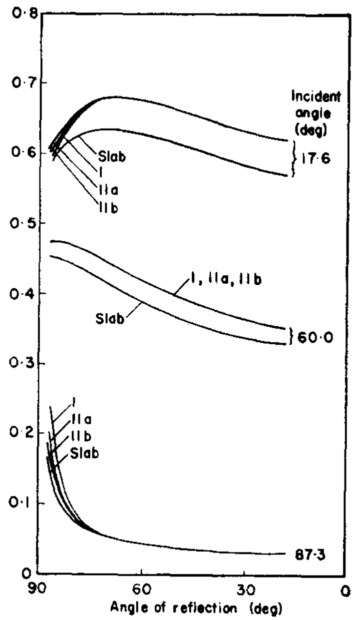

FIG. 3. Some reflected intensity patterns for a shell with albedo $\lambda = 1$, inner radius $a = 50$, and thickness $x = 3$, for various angles of incidence.

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