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NUMERICAL ESTIMATION OF DERIVATIVES WITH AN APPLICATION TO RADIATIVE TRANSFER IN SPHERICAL SHELLS

H. H. Kagiwada, R. E. Kalaba and R. E. Bellman

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The RAND Corporation
SANTA MONICA • CALIFORNIA

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PREFACE

This Memorandum is a result of RAND's continuing study of Satellite Meteorology for the National Aeronautics and Space Administration under contract NASr-21(07). To achieve more realism, the authors are extending their previous study of isotropic and anisotropic scattering in slab geometry to shell geometry. They wish to be able to assess quantitatively the effects of sphericity on radiation fields. The ultimate aim of this study is to more fully exploit the mathematical and computational capabilities of the modern digital computer in the study of radiative transfer in planetary atmospheres.

SUMMARY

The invariant imbedding equation for the scattering function for shell geometry is a nonlinear partial differential-integral equation, and its numerical solution presents difficulties.

A simple method for integration of the above equation is presented. Integrals are approximated by finite sums using Gaussian quadrature, and partial derivatives are approximated by linear combinations of functional values. The original problem is approximated by a large system of ordinary differential equations with known initial conditions.

Requisite auxiliary constants for numerical differentiation are given, as are the results of some trial calculations for the case of conservative isotropic scattering. Noteworthy differences between slab and shell geometry are observed, especially with grazing angles.

Author

CONTENTS

I. INTRODUCTION

Of current interest in radiative transfer is the problem of diffuse reflection by a medium having a spherical geometry.[1-3] When conical flux of net flux π per unit normal area is incident on a spherical, hollow shell of inner radius a, and outer radius z, the equation for the scattering function is

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

where λ is the albedo for single scattering, and u and v are the cosines of the incident and reflected angles, respectively. This is an integro-differential equation, in which partial derivatives with respect to z, v, and u occur, and integrals over v and u are present. The initial conditions are

$$S(a,v,u) = 0, \qquad (2)$$

for a perfectly absorbing core. The S function is symmetric in the arguments u and v.

To solve this problem with the use of a digital computer, we wish to replace Eq. (1) by an approximate system of ordinary differential equations. We choose to have z be the independent variable. Our first task is to obtain formulas for the estimation of the derivatives of S with respect to v and u.

II. ESTIMATION OF DERIVATIVES

Consider the function $f(x)$ which is evaluated at the N roots, x_i, of the shifted Legendre polynomial of degree N.[4] We wish to approximate the first derivative of f evaluated at one of the roots by means of a linear estimator

$$f'(x_i) \cong \sum_{j=1}^{N} \alpha_j^{(i)} f(x_j), \qquad i=1,2,\dots,N. \tag{3}$$

We require that formula (3) be exact for all polynomials of degree N-1 or less,

$$f(x) = \sum_{k=0}^{N-1} a_k x^k. \tag{4}$$

We then have to solve the N linear algebraic equations in the N unknowns, $\alpha_1^{(i)}, \alpha_2^{(i)}, \dots, \alpha_N^{(i)}$,

$$\sum_{j=1}^{N} x_j^k \alpha_j^{(i)} = k\, x_i^{k-1}, \qquad k=0,1,\dots,N-1, \tag{5}$$

or

$$\sum_{j=1}^{N} x_j^{k-1} \alpha_j^{(i)} = (k-1) x_i^{k-2}, \qquad k=1,2,\dots,N. \tag{5'}$$

Here, i is a parameter which may take on the values $i=1,2,\dots,N$.

Note that the matrix of coefficients $\left\{x_j^{k-1}\right\}$ is the Vandermonde matrix, the inverse of which is given in Appendix 6 of Ref. 4.

Let $\left\{ y_{jk} \right\}$ be the inverse matrix. Then the solution of Eq. (5′) is given by

$$\alpha_j^{(i)} = \sum_{k=1}^{N} y_{jk} \, b_k \, , \tag{6}$$

where

$$b_k = (k-1)x_i^{k-2}, \qquad k=1,2,\ldots,N. \tag{7}$$

We refer the reader to Ref. 4 for the method of calculation of the elements of the inverse matrix and for the numerical tables of these elements.

The values of the coefficients $\alpha_j^{(i)}$ have been calculated, and they are given in Tables 1, 2, and 3, for N=5, 7 and 9, respectively.

i = 1	-0.10134081E 02	0.15403904E 02	-0.80870874E 01	0.39207982E 01	-0.11035337E 01
i = 2	-0.19205120E 01	-0.15167064E 01	0.48055013E 01	-0.18571160E 01	0.48883323E-00
i = 3	0.60233632E 00	-0.28707765E 01	-0.35527137E-14	0.28707765E 01	-0.60233632E 00
i = 4	-0.48883323E-00	0.18571160E 01	-0.48055013E 01	0.15167064E 01	0.19205120E 01
i = 5	0.11035337E 01	-0.39207982E 01	0.80870874E 01	-0.15403904E 02	0.10134081E 02

Table 1. The coefficients $\alpha_j^{(i)}$ for N = 5

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 2. The coefficients $\alpha_j^{(i)}$ for N = 7

i = 1			
-0.30899183E 02	0.49462602E 02	-0.31847722E 02	0.23009713E 02
-0.16634325E 02	0.11463908E 02	-0.71444762E 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			
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	0.51953604E 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			
0.10328869E 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			

Table 3. The coefficients $\alpha_j^{(i)}$ for N = 9

This method for the estimation of derivatives was tested on the following cases: $f(x) = 1, x, x^2, \ldots, x^6, 1 - e^{-x}, 1 - e^{-4x}$, $\sin 2\pi x/3$. The results were excellent for the polynomials and for the case $1 - e^{-x}$, with accuracy to six decimal places. Accuracy to two decimal places was obtained for the function $1 - e^{-4x}$. For the final test case, four to five correct figures resulted. The most unfavorable trial was that for $f(x) = 1 - e^{-4x}$, a function which rapidly decreases, then levels off, so that its derivative is at first large, then nearly zero.

III. APPLICATION TO THE SPHERICAL SHELL PROBLEM

We return to the computational solution of the S function of Eqs. (1) and (2). We allow the variables v and u to take on only the values $\{v_i\}$, where v_i is the i^{th} root of the Legendre polynomial of degree N, shifted to the interval (0,1).[4] We then express S as a function of one argument, z,

$$S_{ij}(z) = S(z, v_i, v_j), \tag{8}$$

the subscripts i and j indicating the angular parameters. The derivatives of S with respect to v and u are calculated using the formulas

$$\left[\frac{\partial S(z,v,u)}{\partial v}\right]_{v=v_i, u=v_j} \cong \sum_{k=1}^{N} \alpha_k^{(i)} S_{kj}(z), \tag{9}$$

$$\left[\frac{\partial S(z,v,u)}{\partial u}\right]_{v=v_i, u=v_j} \cong \sum_{k=1}^{N} \alpha_k^{(i)} S_{ik}(z). \tag{10}$$

The definite integrals in Eq. (1) are approximated to a high degree of accuracy by the use of Gaussian quadrature.[5] The integrands are evaluated at the roots of the N^{th}-shifted Legendre polynomial,[4] v_i, i = 1,2,...,N. The corresponding weights are w_i, i = 1,2,...,N. We have our desired system of approximating ordinary differential equations,

$$\frac{dS_{ij}(z)}{dz} + \frac{1 - v_i^2}{v_i z} \sum_{k=1}^{N} \alpha_k^{(i)} S_{kj} + \frac{1 - v_j^2}{v_j z} \sum_{k=1}^{N} \alpha_k^{(j)} S_{ik}$$

$$+ \left(\frac{1}{v_i} + \frac{1}{v_j}\right) S_{ij} - \frac{v_i^2 + v_j^2}{v_i^2 v_j^2} \frac{S_{ij}}{z} \tag{11}$$

$$= \lambda \left[1 + \frac{1}{2} \sum_{k=1}^{N} S_{ik} \frac{w_k}{v_k}\right] \left[1 + \frac{1}{2} \sum_{k=1}^{N} S_{kj} \frac{w_k}{v_k}\right],$$

with initial conditions

$$S_{ij}(a) = 0, \tag{12}$$

for $i=1,2,\ldots,N$, $j=1,2,\ldots,N$, and $z \geq a$.

We produced values of reflected intensities,

$$r_{ij}(z) = \frac{S_{ij}(z)}{4 v_i}, \tag{13}$$

for various values of the albedo λ, and for various inner radii a, and shell thicknesses

$$x = z - a. \tag{14}$$

The computations were carried out on an IBM 7044 with a FORTRAN IV source program.

For internal checking purposes, we compared our results for $N = 7$ against the results for $N = 9$. We also compared results using an integration step size of 0.005 against those using one-half this size, or 0.0025. We found complete agreement among the calculations.

We varied the inner radius of the shell, a = 100, 500, 1000, and we compared the intensities, r, against the corresponding intensities for the plane-parallel slab,[6] which should be obtained as $a \to \infty$. The results are shown in Fig. 1. The function r is shown for the case $\lambda = 1$, $x = 3$, for three angles of incidence, 13.0, 6.00, and 88.5 degrees. 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 degrees, with a = 100, lies as much as 50 per cent above the curve for the slab. As the inner radius a is increased, the function r 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 in a dashed curve for a = 50. It was produced from a calculation with N = 5, since the calculations for N = 7 "blew up." This point requires further investigation.

We feel that this method for the numerical estimation of derivatives is a useful one for many applications, due to its simplicity and accuracy. In the near future, we shall produce S and r functions for the shell problem by means of a perturbation technique. A comparison of the results will result in a better evaluation of the present method.

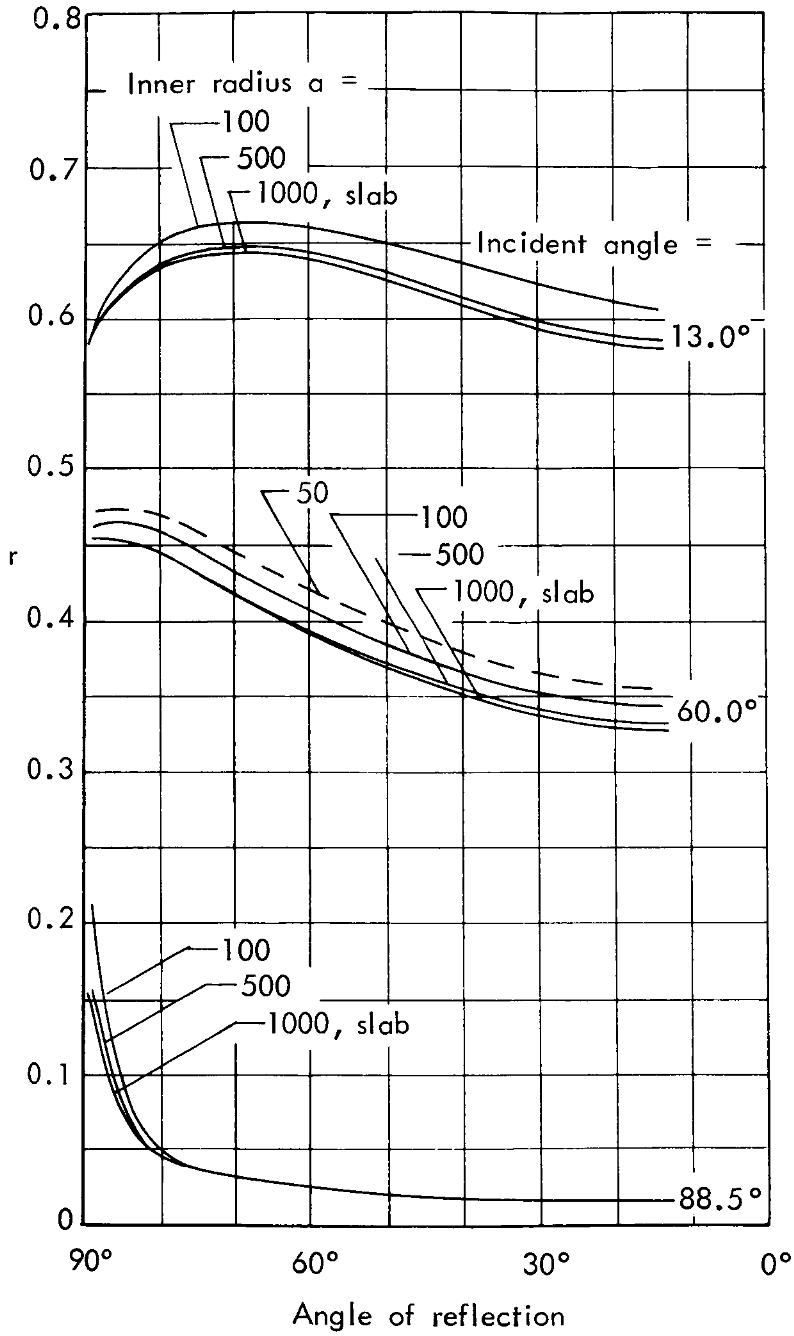

Fig.1 — Some reflected intensity patterns for shells with albedo $\lambda = 1$ and thickness $x = 3$, for various angles of incidence

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