Electromagnetic Scattering by Spheroidal Particles

H. A. Eide, K. Stamnes, and F. M. Schulz
University of Alaska, Fairbanks
Fairbanks, Alaska

J. J. Stamnes
University of Bergen
Norway

Abstract

Clouds are of paramount importance for the global energy balance and, thereby, our climate. Changes in cloud cover and phase (liquid water versus ice), for example, through increased greenhouse forcing, may have significant and as of yet unknown impacts on our climate. The global climate models (GCMs) designed to predict future climate, usually model the effects of clouds using the scattering and absorption properties of spherical particles at high latitudes as well as at high enough altitudes anywhere on our planet. This leads to errors of undetermined magnitude because the clouds there consist of ice crystals that are far from spherical in shape. Ice particles usually take on needle-like or flat, disk-like shapes. The GCMs therefore cannot correctly predict the evolution of our climate.

We have developed a new method for calculating the single scattering solution for spheroidal particles. The single scattering solution is needed for every particle shape that we want to include in a GCM. The spheroidal particles can easily be made to closely resemble actual ice particles, and we can hence, more accurately model the scattering and absorption of radiation by polar and high altitude clouds. An important part of the single scattering solution for spheroidal particles is the calculation of the expansion coefficients that we need in the angular and radial spheroidal functions. Problems that hampered previous implementations for finding these coefficients have been overcome, and we can now handle realistic sizes and shapes, as well as particle absorption in an effective manner.

In this paper, we present our new method for computation of expansion coefficients.

Introduction

In the separation of variables method (SVM) for scattering by spheroidal particles, a critical point is the calculation of the eigenvectors (or coefficients) for the corresponding eigenfunctions. Traditionally, the method attributed to Bouwkamp (1941) is used for this purpose. Here, we present a new method that yields high precision eigenvalues as well as the eigenvectors (coefficients) needed in the eigenfunction expansions. This is accomplished in an efficient and reliable manner using readily available computer routines. The method is not limited to real or purely imaginary values of the size parameter c, and high precision results have been obtained as well for values of c ($c \leq 40$) for which benchmark results are available. When we use this method together with routines for calculating the spheroidal functions, we get excellent agreement with published results (Hanish et al. 1970; Van Buren et al. 1975), but we need to conduct further tests to establish if this new method constitutes an improvement compared to Bouwkamp's method.

In a companion paper (Schulz et al. 1998a), a method for computing the T-matrix with the SVM is presented. In this paper, we show results obtained by using our method to compute the coefficients and this modified SVM approach, and we give an overview of our current and future work on this subject.

The Spheroidal Differential Equation

As is well known, the Helmholtz scalar wave equation $\left(\nabla^2 + k^2\right)\Psi = 0$ is separable in the spheroidal coordinate system. The solution is given by

$$\Psi = S(\eta)R(\xi)\Phi(\phi) \qquad (1)$$

where S, R, and Φ are the angular, radial, and azimuthal components, respectively. As an example, the radial function of the first kind for the case of a prolate spheroidal particle can be written as

$$R_{mn}^{(1)}(c,\xi) = N_k^{mn}(c,\xi)\times \sum_{k=0,1}^{\infty} i^{k+m-n} d_k^{mn}(c)\frac{(2m+k)!}{k!} j_{m+r}(c\xi) \qquad (2)$$

where $N_k^{mn}(c,\xi)$ is a normalization constant, and the indices m and n determine the kind and order of the functions, respectively. In this case, the function $R_{mn}^{(1)}(c,\xi)$ is an infinite expansion in spherical Bessel functions, $j_{m+r}(c\xi)$, with expansion coefficients $d_k^{mn}(c)$. The angular functions S are given in a similar fashion as expansions involving the same expansion coefficients. The major problem in computing these functions is calculating the expansion coefficients $d_k^{mn}(c)$.

All the differential equations for this problem are of the form

$$\frac{d}{dz}\left[\left(1-z^2\right)\frac{du}{dz}\right]+\left[\lambda - c^2 z^2 - \frac{\mu^2}{1-z^2}\right]u = 0 \qquad (3)$$

where u = R,S, z = η,ξ, and λ and μ are separation constants. It is easily seen that this equation has three singularities. At z = ± 1, we have two regular singularities, and at z = ∞ we have an irregular singularity. If we express this solution by a series of known mathematical functions, we get recursion formulas for the expansion coefficients. It is found that these series solutions only will converge for certain λ, denoted by $\lambda_{\mu\nu}$. Furthermore, we are only concerned with those solutions that satisfy the wave equation inside or outside a prolate or oblate spheroid. That is, we require the series solutions to be single-valued and finite at the poles. In order for this to be true, the constants, μ and ν, have to be integers (Meixner and Schäfke 1954). We denote the eigenvalues by λ_{mn} instead of $\lambda_{\mu\nu}$ for this reason. Furthermore, we can restrict m to be zero or positive.

Recurrence Relations

We want to determine the eigenvalues λ_{mn} for those solutions of Eq. (3) that are finite at η = ±1. The corresponding eigenfunctions $S_{mn}(c\eta)$ are the prolate spheroidal angular functions of the first kind, of order m and degree n, and $R_{mn}(c,\xi)$ are the prolate spheroidal radial functions of the same kind, order, and degree. By replacing c with -ic in Eq. (3), we get the oblate spheroidal eigenvalues, $\lambda_{mn}(-ic)$, and the corresponding angular and radial eigenfunctions.

We have the following recurrence relations between the coefficients λ_{mn} in the eigenvalue problem (Flammer 1957):

$$\alpha_k d_{k+2} + \left(\beta_k - \lambda_{mn}\right)d_k + \gamma_k d_{k-2} = 0. \qquad (4)$$

The coefficients α, β, γ are given by

$$\alpha_k = \frac{(2m+k+2)(2m+k+1)c^2}{(2m+k+3)(2m+k+5)} \qquad (5a)$$

$$\beta_k = (m+k)(m+k+1) + \frac{2(m+k)(m+k+1)-2m^2-1}{(2m+2k-1)(2m+2k+3)}c^2 \qquad (5b)$$

$$\gamma_k = \frac{k(k-1)\,c^2}{(2m+2k-3)(2m+2k-1)}. \qquad (5c)$$

Based on these recurrence relations, one can define infinite continued fractions from which both the eigenvalues, λ_{mn}, and the corresponding coefficients $d_k^{mn}(c)$, can be computed by an iterative scheme. Although the classical iterative procedure works well in many cases when one has access to accurate initial estimates for the eigenvalues, it is difficult to turn it into a reliable algorithm for automatic machine computation. Therefore, we use an alternative procedure that is well adapted to automatic machine computation, because it requires no initial estimates of the eigenvalues λ or coefficients d. Also, it is reliable and accurate and based on readily available computer algorithms. The new procedure is simply based on realizing that the recurrence relations, mentioned above, can be used to reformulate the computational task as an algebraic eigenvalue problem. The procedure leads to a tridiagonal matrix from which the eigenvalues (characteristic values) and the corresponding eigenvectors (coefficients) can be determined by applying a standard computer library routine for solving eigenvalue problems. These routines are readily available and they can also handle complex valued problems. We use LAPACK library routines for solving the complex eigenvalue problem. A simplified version of this method is often used to find starting values for λ that can be used in the Bouwkamp iterative method. In the Bouwkamp method, one typically solves a small eigenvalue problem for approximate values of the λs only. Next, one refines these λs, and then use them in the iterative scheme to determine the coefficients d. Recently, a method in which the λs are completely determined by solving the complex eigenvalue problem was presented (Qinan et al. 1997), but here also the iterative scheme was used to determine the coefficients d. Our new approach fully solves the algebraic eigenvalue problem so that we obtain not only the eigenvalues λ, but also the coefficients d. The eigenvalue problem involves the diagonalization of a matrix of infinite dimension. However, the size of the eigenvalue matrix required in order to yield accurate results is moderate; hence, allowing for an efficient and reliable computation of the coefficients for realistic values of the size parameter c. We seldom need matrices larger than $(2c+n) \times (2c+n)$.

Preliminary Results

We have implemented the new method and compared it with published results (Hanish et al. 1970; Van Buren et al. 1975). However, benchmark values are only available for purely real or purely imaginary values of c. Large values of c are also missing in the literature ($c > 40$). The first tests therefore were limited to purely real and imaginary values of c for which Hanish et. al. (1970) and Van Buren (1975) have published extensive tables ($0.1 \le c \le 40.0$, $m = 0,1,2,3$). The computer program employed for generating the benchmark tables of radial and angular spheroidal functions (Van Buren et al. 1970; King et al. 1970) contain routines that make use of the Bouwkamp method for finding the eigenvalues and coefficients. We replaced these parts of the original routines that compute the eigenvalues, λ, and the coefficients, d, with our routines using the method described above. We found excellent agreement (up to the 22nd decimal point) in most cases. The original program and the one modified to use our method takes about the same amount of computing time, but as mentioned above, the original program can only handle purely real or imaginary c's.

A simple scalar solution to the axisymmetric single scattering problem in the oblate spheroidal coordinate system is given by

$$\Phi(\xi,\eta) = \sum_{n=0}^{\infty} B_n S_{0,n}^{(1)}(ic,\eta)\, R_{0,n}^{(1)}(ic,-i\xi)$$

where the B_n's are determined by the boundary conditions, and the spheroidal functions $S_{0,n}^{(1)}(ic,\eta)$ and $R_{0,n}^{(1)}(ic,-i\xi)$ are calculated using the expansion coefficients, d, calculated with the new method. As the incident field we can take a simple plane-wave as expressed in the following plane-wave expansion

$$e^{ikr} = 2\sum_{n=0}^{\infty} \frac{i^n}{N_{0,n}} S_{0,n}(ic,1)\, S_{0,n}(ic,\eta) R_{0,n}^{(1)}(ic,-i\xi)$$

for a wave traveling along the axis of symmetry. A simple boundary condition is the so-called "hard" boundary condition, which implies that the total field is zero on the surface of the spheroid. By equating these expressions for $\xi = \xi_0$, the surface of the spheroid, we obtain the solutions shown in Figures 1, 2, 3, and 4.

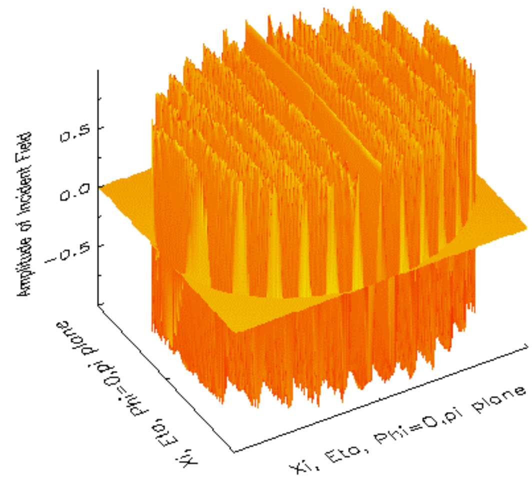

Figure 1. This figure shows an example of the amplitude of a plane wave field, or a plane wave expansion in oblate spheroidal coordinates. The field is traveling in the direction of the minor axis. This is the field used as the incident field in the following figures. (For a color version of this figure, please see *http://www.arm.gov/docs/documents/technical/conf_9803/eide-98.pdf*.)

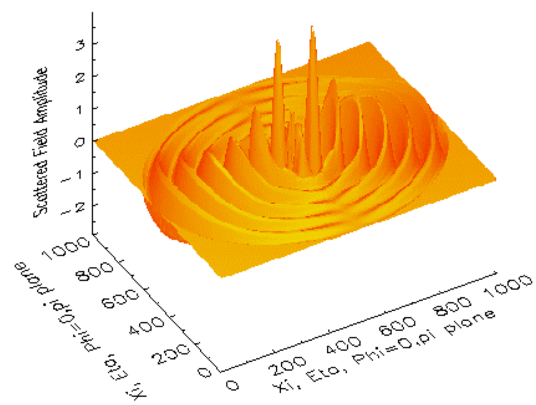

Figure 2. Amplitude of the scattered field in the vicinity of a oblate spheroidal particle with a real c of 3.0. The incident field is a plane wave traveling in the direction of the minor axis (see Figure 1). We have used "hard" boundary conditions. (For a color version of this figure, please see *http://www.arm.gov/docs/documents/technical/conf_9803/eide-98.pdf*.)

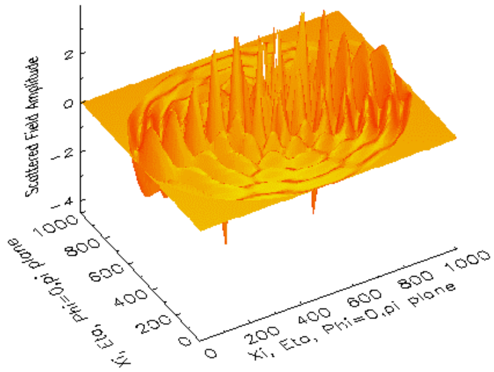

Figure 3. Amplitude of the scattered field in the vicinity of a oblate spheroidal particle like in Figure 2. Now with a real c of 5.0. (For a color version of this figure, please see *http://www.arm.gov/docs/documents/technical/conf_9803/eide-98.pdf*.)

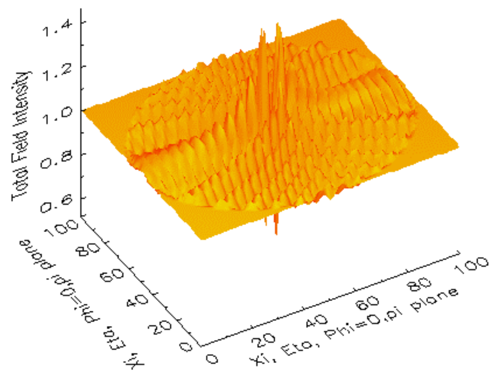

Figure 4. Intensity of the total scalar field (incident + scattered field) in the vicinity of a oblate spheroidal particle with a real c of 1.0. The incident field is a plane wave traveling in the direction of the minor axis (see Figure 1). We have used "hard" boundary conditions like those in the other figures. (For a color version of this figure, please see *http://www.arm.gov/docs/documents/technical/conf_9803/eide-98.pdf*.)

Future Work

In future work we will compare the results obtained and the computational resources required to run the VDISORT code (Schulz et al. 1998b) using Bouwkamp's method and our new method. We will then get results for extreme size parameters and aspect ratios, and we will examine the consequences of using a "spherical" particle model in radiative transfer applications by executing the VDISORT code with a "spherical" as well as a "non-spherical" particle model as input.

We also plan to quantify the impact of particle shape on radiative energy disposition by comparing results obtained with a "spherical" particle model with those obtained with a "non-spherical" particle model as input to a scalar radiative transfer code (e.g., DISORT). Eventually our goal is to parameterize the impact of particle shape on atmospheric warming/cooling rates in such a way that the shape effect can be incorporated into GCMs.

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