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The boundary element method for light scattering by ice crystals and its implementation in BEM++

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ABSTRACT

A number of methods exist for solving the problem of electromagnetic scattering by atmospheric ice crystals. Amongst these methods, only a few are used to generate "benchmark" results in the atmospheric science community. Most notably, the T-matrix method, Discrete Dipole Approximation, and the Finite-Difference Time-Domain method. The Boundary Element Method (BEM), however, has received considerably less attention in this community despite its extensive use and development in other areas of applied mathematics and engineering. Recently the group of Betcke et al. (2015 [1]) at University College London has released a high performance open source boundary element library called BEM++. In this paper, we employ BEM++ to calculate the scattering properties of hexagonal ice columns of fixed orientation, as well as more complicated particles such as hollow columns and bullet-rosettes. The results for hexagonal columns are compared to those obtained using a highly accurate and well-established T-matrix method (Baran et al., 2001 [2]) for a range of different wavelengths and size parameters. It is shown that the results are in excellent agreement and that BEM++ is a fast alternative to the T-matrix method and others for generating benchmark results. However, the large memory requirements of BEM++ cause it to be limited to size parameters ~15 on a standard desktop PC if an accuracy of roughly 1% is required. The main advantages of BEM++ over many other methods are its flexibility to be applied to homogeneous dielectric particles of arbitrarily complex shape, and its open availability. This flexibility is illustrated by the application of BEM++ to scattering by hollow columns with different cavity types, as well as bullet-rosettes with 2–6 branches.

1. Introduction

It has been well established that understanding the scattering properties of atmospheric ice crystals is important in modelling the radiation balance of cirrus clouds [3–5]. Due to the wide coverage of cirrus over the Earth (~30% at any one time in the mid-latitudes, and ~60–80% in the tropics [3,5,6]), these clouds in turn play an important role in the earth–atmosphere radiation balance.

The ice crystals within cirrus exhibit a large array of sizes and shapes [7–9]. This, combined with the frequency range of radiation incident upon the clouds (from microwave to ultraviolet), leads to a huge variety of scattering problems to be solved. Over the years, many methods have been developed for tackling different problems within the myriad combinations of particle shape, size and incident radiation frequency. These methods fall into two main camps.

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The first contains asymptotic or "approximate" methods which utilise the high-frequency behaviour of light to justify the implementation of geometrical techniques. Examples include Geometric Optics [10], the Kirchhoff approximation [11–13], and Ray Tracing with Diffraction on Facets [14]. These methods are applicable to particles of large size parameter.

The second camp contains the so-called "exact" methods which either discretise the underlying Maxwell's equations and solve the resultant discrete system, or propose a separation of variables ansatz and obtain the coefficients by enforcing the boundary conditions at the ice crystal's surface. Such methods include the T-matrix method [15–17], the invariant imbedding T-matrix method [18], the Discrete Dipole Approximation (DDA) [19], and Finite-Difference Time-Domain (FDTD) method [20]. These methods have a computational cost that scales with size parameter and hence are typically feasible only at small to moderate size parameters. We note briefly that exact methods which bridge these two camps exist. However their development is still in its early stages and, at present, they are limited to scalar problems (see e.g. [21,22]).

One exact method that has received scant attention in the atmospheric physics community, apart from some application to simple shapes with exploitable symmetries [23,24], is the Boundary Element Method (BEM) which, in its most standard form (i.e., not hybrid, see [21]), is applicable to small to moderate size parameter particles of arbitrary shape and at any wavelength. Moreover, a high-performance boundary element library called BEM++ has recently been developed and made open-source at http://www.bempp.org by the group of Betcke et al. [1].

Within the BEM framework, Maxwell's equations are reformulated as a system of boundary integral equations on the particle's surface via the Stratton–Chu formulae. This has the advantage of reducing a problem defined on a three-dimensional infinite domain to a problem defined on a two-dimensional finite domain. The equations are solved to obtain the electric and magnetic surface currents which may then be substituted into the Stratton–Chu formulae (or their far-field asymptotic form) to obtain the field anywhere.

This paper analyses the performance of BEM++ in its application to the scattering problems associated with atmospheric non-spherical ice. In particular, its performance is compared to that of a well-established standard T-matrix method [15] for the problem of scattering by hexagonal ice columns. We go on to demonstrate BEM++'s utility for scattering problems involving complex particle shapes, such as hexagonal columns with cavities and bullet-rosettes. The single-scattering properties we consider in this paper are not at present direct outputs from BEM++. However, example Python scripts which generate these from BEM++'s output can be downloaded from the corresponding author's webpage http://sites.google.com/site/samuelpgroth.

The paper is organised as follows. In Section 2, we state the electromagnetic scattering problem to be solved. Section 3 gives a brief outline of the reformulation of the problem as a system of boundary integral equations, which is performed utilising the Stratton–Chu formulae. Section 4 recalls the definitions of the amplitude scattering matrix and other important scattering properties, and also how they are computed from the outputs of BEM++. In Section 5, the settings of various error tolerances within BEM++ are discussed. Sections 6–8 comprise the results portion of the paper. Section 6 compares the solution of scattering by a sphere with BEM++ to the exact solution, obtained via Mie–Lorenz theory, in order to ascertain the accuracy of BEM++ and decide upon the appropriate mesh resolution to be used. Section 7 looks at scattering by hexagonal columns, comparing the solution with BEM++ to that obtained using a T-matrix method. In Section 8 BEM++ is applied to scattering by hexagonal columns with different types of cavity, and bullet-rosettes, problems which are beyond the applicability of current standard T-matrix methods. Here we also test that the reciprocity condition holds. Performing this test is an important verification tool for numerical methods [25]. The final section contains some discussion and concluding remarks.

2. Problem statement

Consider the scattering of a monochromatic plane wave with time-dependence $e^{-i\omega t}$ by a homogeneous, isotropic dielectric scatterer Ω_1 (see Fig. 1) with a complex refractive index $n=\sqrt{\epsilon\mu}$, where ϵ and μ are the permittivity and permeability, respectively, of the material composing Ω_1. It is assumed that Ω_1 is surrounded by a homogeneous medium $\Omega_2 := \mathbb{R}^3 \backslash \overline{\Omega_1}$ with unit refractive index.

The transmission problem is to find the fields $\{\mathbf{E}_1, \mathbf{H}_1\}$ and $\{\mathbf{E}_2, \mathbf{H}_2\}$ in Ω_1 and Ω_2, respectively, satisfying Maxwell's equations

$$\nabla \times \mathbf{E_1} = i\omega\mu_1\mathbf{H}_1, \quad \nabla \times \mathbf{H}_1 = -i\omega\epsilon_1\mathbf{E}_1 \text{ in } \Omega_1, \tag{1}$$

$$\nabla \times \mathbf{E_2} = i\omega\mu_2\mathbf{H}_2, \quad \nabla \times \mathbf{H}_2 = -i\omega\epsilon_2\mathbf{E}_2 \text{ in } \Omega_2, \tag{2}$$

along with the *transmission conditions* on the interface $\Gamma := \partial\Omega_1$:

$$\mathbf{n} \times \mathbf{E}_1 = \mathbf{n} \times \mathbf{E}_2 \quad \text{and} \quad \mathbf{n} \times \mathbf{H}_1 = \mathbf{n} \times \mathbf{H}_1. \tag{3}$$

In addition, the scattered fields, defined as $\mathbf{E}^s := \mathbf{E}_2 - \mathbf{E}^i$, $\mathbf{H}^s := \mathbf{H}_2 - \mathbf{H}^i$ where $\{\mathbf{E}^i, \mathbf{H}^i\}$ is the incident electromagnetic field, are required to satisfy the Silver–Müller radiation condition

$$\sqrt{\mu}\hat{\mathbf{x}} \times \mathbf{H}^s + \sqrt{\varepsilon}\mathbf{E}^s = o\left(\frac{1}{r}\right) \quad \text{as } r := |\mathbf{x}| \to \infty \tag{4}$$

uniformly in all directions $\hat{\mathbf{x}} := \mathbf{x}/r$.

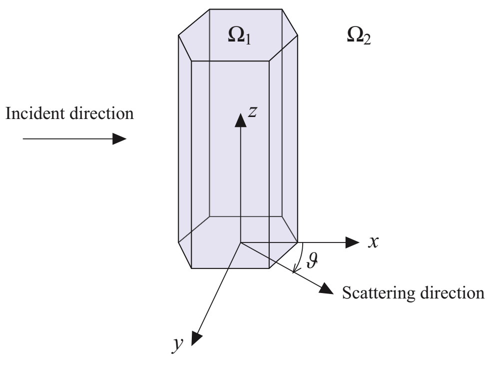

Fig. 1. Scattering setup.