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Acceleration of the iterative solver in the discrete dipole approximation: Application to the orientation variation of irregularly shaped particles

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Abstract

We have applied a method of reducing the number of iterations required to solve a system of linear equations in the discrete dipole approximation. This method obtains an initial guess of dipole polarization from those with similar particle characteristics (e.g., the size parameter and refractive index) calculated a priori. If the initial guess is closer to the solution, the number of iterations of the linear equation solution becomes smaller than that calculated with an arbitrary initial value.

This method was applied to various particle orientations using spline interpolation of the initial guess of dipole polarization from orientations calculated a priori.

We studied three types of particle model: an aggregate, a deformed sphere with moderate surface roughness, and a particle with a large number of edges. For the particle with a large number of edges, we propose a new model called the overlapping mixture of multiple tetrahedra (OMMT).

The proposed method is most advantageous for particles with moderate surface roughness (e.g., a deformed sphere), for which the calculation time was reduced to 20–40% of the original calculation time. For OMMT and an aggregate, the computation time was reduced to 30–60% and 40–90%, respectively. The differences in the scattering coefficient, absorption coefficient, intensity and polarization introduced by our method were less than 0.008%, 0.03%, 0.1%, and 0.08%, respectively.

If the light scattering properties vary slowly with the orientation variation, interpolation of the results is more efficient than the proposed method and produces only a small difference in the results. However, the interpolation of the results fails for particles such as BCCA64, for which our proposed method produces more accurate results.

Keywords: Light scattering simulation; Efficient calculation; Discrete dipole approximation

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1. Introduction

Light scattering by particles depends on the particle characteristics, such as their size, shape, and chemical composition. Therefore, the light scattering characteristics of cosmic dust and atmospheric aerosols can be used to interpret the data observed for various objects.

The analysis of observed data requires knowledge about how the particle characteristics affect the light scattering properties. These properties can be obtained from light scattering simulations. Among various methods of light scattering simulations, the discrete dipole approximation (DDA) [1–3] is a powerful tool for studying the light scattering characteristics of irregularly shaped particles.

In the DDA calculations, the shape is first described by a number of dipoles, and then the multiple interactions of the incident light with the dipoles are simulated. Compared with other methods, the DDA has the advantage of treating a shape with dipoles. This makes it possible to simulate light scattering for irregularly shaped particles without any symmetry. One disadvantage of the DDA is that a system of linear equations must be solved for all particular values of particle parameters and for each direction of incident light.

An efficient solution method is desirable for calculating the light scattering properties for various sets of particle characteristics. In this study, we applied the method originally proposed by Muinonen and Zubko [4] to reduce the number of iterations required to solve a system of linear equations in the DDA calculation. We modified the method and applied it to variation in particle orientation.

In Section 2, we introduce the method of Muinonen and Zubko [4] along with our modification; to apply to the variation in orientation. In this section, we also introduce the three types of particle that were studied. In Section 3, we investigate the efficiency of the method and show the difference in the final results using the proposed method. In Section 4, we discuss the advantages and disadvantages of the proposed method. Section 5 contains our conclusions.

2. Method

2.1. Reduction of iterations in the DDA

In this study, we use DDSCAT6.1 [1] for the DDA calculations. In the DDA, the particle is described with a number of dipoles and the multiple interactions of incident electric fields with these dipoles are calculated.

The interaction of electric fields with dipoles is described by a set of linear equations [1]:

$$\sum_{k=1}^{N} A_{jk} P_k = E_{\mathrm{inc},j}, \tag{1}$$

where $A_{jk}P_k$ is the contribution to the electric field by the kth dipole, P_k is the dipole polarization of the kth dipole, and $E_{\mathrm{inc},j}$ are the electric fields incident on the jth dipole.

This equation is solved to obtain the dipole polarization P_k of each dipole [1]. Once the solution P_k is obtained, the scattering properties of the particle can be calculated (see [1, Section 3]). The linear equations can be solved using either a direct or an iterative method. The direct method has limited application because it requires a large amount of memory. Therefore, for an efficient calculation, DDA programs developed by researchers are generally based on iterative methods [1,3,5]. For example, in DDSCAT6.1, a system of linear equations are solved by an iterative biconjugate gradient method [6].

In iterative methods, the values of P_k are initially set to an arbitrary value. For DDSCAT6.1, these are initially set to 0.0 [6]. Starting with the arbitrary value of P_k, subsequent iteratively calculated values of P_k converge on the solution and the process stops when the linear equations are considered to be solved within a defined error tolerance h (e.g., 10^{-5}). See [6, Eq. (18)] for details of h.

Muinonen and Zubko [4] proposed an optimization of the DDA calculations for particles with various refractive indices m or particle size parameters x [4]. An example of their method is as follows. The calculations for $x = x_1$ and x_2 $(= x_1 + \Delta x)$ are conducted with a normal DDA calculation as the first step. Then, in the calculation for $x = x_1 - \Delta x$, the initial value is extrapolated from the values of $x = x_1$ and $x = x_2$,