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Comparison between discrete dipole implementations and exact techniques

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Abstract

The use of the discrete dipole approximation (DDA) method in wave optical scattering simulations is growing quite fast. This is due to the fact that the current computing resources allow to apply DDA to sufficiently large scattering systems. The advantage of DDA is that it is applicable to arbitrary particle shape and configuration of particles. There are several computer implementations of the DDA method, and in this article we will compare four of such implementations in terms of their accuracy, speed and usability. The accuracy is studied by comparing the DDA results against results from either Mie, T-matrix or cluster T-Matrix codes with suitable geometries. It is found that the relative accuracy for intensity is between 2% and 6% for ice and silicate type refractive indices and the absolute accuracy for linear polarization ratio is roughly from 1% to 3%.

Keywords: Scattering; Discrete-dipole approximation

1. Introduction

The importance of light scattering methods in studying the structure of various remotely sensed objects, e.g. in astronomy and in some technological applications has greatly increased in the last years. One obvious reason for this is undoubtedly the enormous and steady increase in the computer power and speed. The information content from the light scattering studies is very large because at its best all the 16 Mueller matrix

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elements as a function of the scattering angle can be derived and related to some unknown physical parameters.

Before light scattering results for any object can be computed the relevant morphology for it must either be known or modeled. Most of the geometries can be divided into two basic classes: solid and particulate. For the solids it is fairly straightforward to model the outer boundary while in the case of particulate material much more free parameters must be considered. First, the sizes and shapes of the constituents must be decided. Second, the packing density (1-porosity) is often a crucial parameter and must either be known or varied which complicates the computations further. For any of existing light scattering codes we must know (or model) the refractive index and in most cases both the real and imaginary parts. The scattering material can also be anisotropic which requires that two or three different indices should be obtained.

Most of the existing light scattering programs can roughly be divided into two categories: those which use the ray optics (RO) or geometric optics (GO) approaches and those which use the exact wave optics (WO) approach. Following Mishchenko et al. [1], we can say that the RO and GO use only the ladder diagrams e.g. the radiative transfer theory (RTT) [2–4], while e.g. the coherent backscattering (CB) uses also the cyclical diagrams.

In the case of the problems which deal with particulate media one of the crucial parameters is the packing density (pD). The classical assumption is that the light scattering by these can be explained by the much simpler RO/GO models if the pD is less that about 5–10%. With higher values of pD the exact WO approach should be used. Unfortunately, up to quite recently the existing light scattering routines and the computers have not been able to do that.

Among the WO methods the discrete dipole approximation (DDA), also known as the coupled dipole approximation, has several special advantages over all the other existing approaches. These are that they can be applied to quite arbitrary shaped geometries which can be inhomogeneous and anisotropic. As already explicitly in its name the DDA has a minor drawback in being an approximation although if infinite CPU time would be possible the results should become exact. The other drawback comes from the fact that if orientation averages are needed then the computationally demanding linear equations must be solved repeatedly. Recent developments in DDA computations include, for instance, the optimization of the DDA computations for scatterers that have identical shapes but differing sizes or refractive indices [5].

Because of the increasing popularity in the DDA codes it would be valuable to quantitatively compare several aspects of these both in relation to each other (speed, accuracy, etc.) and in respect to the absolute accuracy of those. For this we naturally need codes which can handle some geometries in a numerically exact manner. This limits the available geometries to only a few. A fairly obvious choice is to use the T-matrix [6] and the cluster T-matrix [7] codes. We were able to collect a total of four different DDA versions to do this comparison.

This article has been arranged such that in Section 2 we briefly describe the theory of the DDA approach, in Section 3 the four DDA codes are presented, and in Section 4 the details of the comparison and its results are discussed. In Section 5 we draw some conclusions about the performance and properties of different DDA codes.

2. Theory of DDA

Assume that the scattering particles are isotropic and homogeneous, i.e., that their optical properties are fully described by the complex refractive index m. In DDA, the particle is divided into a discrete set of dipoles (or computational cells) on a cubic lattice with dimensionless interdipole distances kd (k is the wave number in free space). The electric field values $\mathbf{E}_j$ ($j = 1, 2, 3, \ldots, N$) are to be derived from a group of linear equations (see e.g. Lumme and Rahola [8]):

$$\mathbf{E}_j = \gamma \mathbf{E}_{0,j} + \beta \sum_{l=1, l\neq j}^{N} \mathbf{T}_{jl} \cdot \mathbf{E}_l, \quad j = 1, 2, 3, \ldots, N, \tag{1}$$

where $\mathbf{E}_{0,j}$ is the incident field value at dipole j, γ and β are complex coefficients (see below), and $\mathbf{T}_{jl}$ is the transformation dyadic ($\mathbf{1}$ being the unit dyadic)

$$\mathbf{T}_{jl} = u_{jl}\mathbf{1} + v_{jl}\mathbf{e}_{jl}\mathbf{e}_{jl}, \tag{2}$$