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Comparison of the pseudo-spectral time domain method and the discrete dipole approximation for light scattering by ice spheres

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ABSTRACT

The pseudo-spectral time domain method (PSTD) and the discrete dipole approximation (DDA) are two popular numerically rigorous methods used to model the single-scattering properties of arbitrarily shaped dielectric particles. Stemming from a previous comparison made between the PSTD and DDA for non-absorptive particles, this study expands the comparison to include absorptive cases, and shows the relative strengths of the two methods for application to ice crystal light scattering. The scattering properties of spheres with realistic ice refractive indice, whose analytic solutions can be obtained by using the Lorenz–Mie theory, are considered. Refractive indices of ice at 30 wavelengths ranging from 0.2 μm to 100 μm are separated into three groups based on the imaginary parts of the refractive indices (i.e., $m_i < 10^{-3}$, $10^{-3} \le m_i \le 10^{-1}$, and $m_i > 10^{-1}$). The two methods are compared in terms of the computational time needed to reach the same accuracy. This study indicates that the performance of either the PSTD or DDA depends on both the real part and the imaginary part of the particle refractive index. For ice spheres with the imaginary part of the refractive index less than 10^{-3} and at size parameters exceeding 40, the PSTD is more efficient than the DDA. The PSTD also has a wider capability range for particles at larger sizes. At wavelengths where ice is moderately absorptive ($10^{-3} < m_i < 10^{-1}$ in this study), the critical size parameter decreases as the real part of the refractive index increases. At size parameters below the critical size parameter, the DDA outperforms the PSTD. Furthermore, when the ice becomes strongly absorptive, the DDA is approximately twice as fast as the PSTD for particles with size parameters reaching up to 100.

1. Introduction

Light scattering by dielectric particles is fundamental to the study of bio-optics, astrophysics, atmospheric radiative transfer simulations, and remote sensing applications [1]. Accurate and efficient computations of the single-scattering properties of various particles, e.g., red blood cells or atmospheric aerosol particles, are required in these fields of study. In single-scattering calculations, the 'size parameter', which is proportional to the particle size in comparison with the incident light wavelength, is crucially important and defined as $x = \pi L/\lambda$ (L is the maximum length of the particle, and λ is the incident wavelength). For particles much smaller than the incident wavelength, i.e., $x \ll 1$, the Rayleigh theory is generally

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applied, and in the large particle regime, $x \gg 1$, the geometric optics approximations are both useful and computationally feasible. In the intermediate region with x being in the few tens or hundreds, Maxwell's equations are normally solved numerically for light scattering by non-spherical particles, but the available analytic solution, i.e., the Lorenz–Mie theory [2,3], is only applicable for spheres and infinite cylinders.

Various numerical algorithms have been developed and applied to model the single-scattering properties of dielectric particles in the resonant region, i.e., the T-matrix [4–7], the discrete dipole approximation (DDA) [8–10], the finite-difference time domain method (FDTD) [11–13], and the pseudo-spectral time domain method (PSTD) [14–16]. This study focuses on two popular approaches: the PSTD and the DDA. The PSTD, which solves Maxwell's curl equations in the time domain, uses a spectral method to calculate spatial derivatives; whereas, the DDA solves an electromagnetic integral equation in the frequency domain. Note that the DDA has been extended to consider magnetic dipoles for applications to material science [17]. The two methods discretize the particles using either grid cells or dipoles in the spatial domain, and can be applied to particles with arbitrary shapes and compositions. Both the PSTD and DDA have been widely applied to simulate the scattering properties of atmospheric particles, e.g., ice crystals [15,18,19] and dust particles [20–23], and have been compared with other methods such as the FDTD [23,24] and T-matrix [16,25]. The implementations of the two methods have been parallelized and applied to particles much larger than the incident wavelength. Liu et al. [16] used the PSTD to simulate the light scattering by spheres with refractive indices of ice and size parameters up to 200 and by randomly oriented non-spherical particles with size parameters over 100. The efficiency of the DDA depends strongly on the particle refractive index, and maximum size parameters of 130 and 320 for spheres with respective refractive indices of 1.2 and 1.05 have been achieved [26,27].

Although sharing a similar range of applicability for light scattering simulations, the efficiency and accuracy of the PSTD and DDA show substantial variations at different refractive indices and particle sizes. Liu et al. [28] have studied the capabilities and relative strengths of the PSTD and DDA for light scattering by spheres and spheroids. With the exact scattering properties of spheres given by the Lorenz–Mie theory, the same accuracy criteria were prescribed for the two methods, and the computational time was compared in a fair manner. For a small refractive index, a critical size parameter was found below which the DDA outperformed the PSTD. The value of the critical size parameter decreased from 80 to 30 as the refractive index increased from 1.2 to 1.4. For particles with refractive indices larger than 1.4, the PSTD became more efficient than the DDA for spheres with size parameters larger than 10 and had a broader range of applicability for large sized particles. However, Liu et al. [28] focused on the real part of refractive index (with the imaginary part of the refractive index assumed to be 0). Meanwhile, the PSTD showed much higher accuracy for absorptive particles than those of non-absorptive cases [16], and Yurkin et al. [24] found that the performance of the DDA was also significantly affected by the imaginary part of the refractive index. As realistic particles are always absorptive to some degree, a comparison between the PSTD and DDA for absorbing refractive indices, which was mentioned as future work by both Yurkin et al. [24] and Liu et al. [28], is more meaningful from a practical application perspective.

This study presents an expanded comparison between the PSTD and DDA by using realistic refractive indices of ice at wavelengths ranging from 0.2 μm to 100 μm. The present results are intended to show the relative performances of the two methods for both non-absorptive and absorptive cases, and, thus, to provide a reference for further applications of ice crystal single-scattering simulations. Section 2 details the methods for the comparison, and Section 3 discusses the results. Section 4 summarizes the study.

2. Comparison between the PSTD and DDA

Both the PSTD and DDA show a wide range of applications to light scattering by ice crystals within cirrus clouds. The accuracy and efficiency of the PSTD and DDA simulations become extremely important, because various particle geometries, sizes, and refractive indices (at different wavelengths) need to be considered for atmospheric applications. The appropriate model will not only save significant computational resources, but will also provide more robust and accurate results. This study is intended to provide a detailed comparison of the two methods for light scattering simulations over a wide range of particle sizes and refractive indices. The ADDA code (v.1.1), developed by Yurkin and Hoekstra [27], and the PSTD code, improved and parallelized by Liu et al. [16,28], are used for the comparison. A more detailed discussion of the two implementations can be found in Liu et al. [28], and the basic simulation variables and parameters are kept the same as in their study. In particular, the ADDA was run with default settings, including the lattice dispersion relation (LDR) formulation and the quasi-minimal residual (QMR) iterative solver. The only difference is the threshold of the latter, which was set to 10^{-3}. We note that the ADDA code has several options to choose the DDA formulations and the iterative solver, the optimizing of which may have a profound influence on the code performance [28,29]; however, such optimization is out of scope of this paper.

By discretizing the scattering particles using grid cells (PSTD) or dipoles (DDA), the PSTD and DDA have almost no limitations on the particle geometries. However, to quantify the accuracies of the PSTD and DDA for a fair comparison, the single-scattering properties of spheres are simulated, because exact solutions can be given by the Lorenz–Mie theory. The same accuracy criteria for the extinction efficiency (Q_{ext}) and the phase function (P_{11}) are prescribed, and computational times used by the two methods with the same resources are directly compared. The computational times depend on the size of the computational domain, i.e., the number of grid cells or dipoles, and the number of time steps in the time domain simulations for the PSTD or iterations by the iterative solver for the DDA (N_{iter}). The number of time steps in the PSTD simulations will be specified as N_{trip} in this study,