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Enhancement of the computational efficiency of the near-to-far field mapping in the finite-difference method and ray-by-ray method with the fast multi-pole plane wave expansion approach

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ABSTRACT

The finite-difference time-domain (FDTD) and ray-by-ray (RBR) methods are techniques used to calculate the optical properties of nonspherical particles for small-to-moderate and large size parameters, respectively. The former is a rigorous method, and the latter is an approximate geometric–physical optics-hybrid method that takes advantage of both high efficiency of the geometric optics approach and high accuracy of the physical optics approach. In these two methods, the far field is calculated by mapping the near field to the far field with consideration of the phase interference. The mapping computation is more time-consuming than the near-field simulation when multiple scattering directions are involved, particularly in the case of the RBR implementation. To overcome the difficulty, in this study the fast multi-pole method is applied to both FDTD and RBR towards accelerating the far-field calculation, without degrading the accuracy of the simulation results.

1. Introduction

Calculating the optical properties of nonspherical objects and particles is important in many research fields. For example, in remote sensing, airborne objects are detected from radar signals scattered back from the objects [1–3]; in atmospheric sciences, the properties of aerosols and ice particles are inferred based on radiometer, radar, and lidar observations and these properties are fundamental to the assessment of the radiative forcings of the aforesaid atmospheric constituents [4–10]; and in medical examination and treatment, the optical analysis of tissue and red blood cells with lasers is used to detect tissue- and blood-related diseases [11–15]. Rigorous methods for these calculations include the finite-difference time-domain (FDTD) method [16–21], pseudo-spectral time-domain method (PSTD) [21–23], discrete dipole approximation (DDA) [24–26], T-matrix method [27–29], invariant imbedding T-matrix method (II-TM) [30,31], to just list a few. Approximate methods include the improved geometric optics method (IGOM) [32], ray-by-ray method (RBR) [33], and physical-geometric optics hybrid method (PGOH) [34,35]. Most rigorous methods are feasible for particles with characteristic dimensions smaller than 20–30 times the incident wavelength, while the

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aforesaid approximate methods generally give reasonable approximations when the particle sizes are larger than 20–30 times the incident wavelengths.

The FDTD solves Maxwell's equations using the second order leap-frog (or central) finite difference scheme to approximate the spatial and temporal derivative terms. Therefore, this method converges to the true solution when using a fine grid mesh along with a long temporal-integration duration. The merits of FDTD are manifested by its easy implementation, easy control of the degree of accuracy via the grid resolution, and feasibility for complex particle shapes. However, CPU time for a single orientation calculation increases by the fourth power of the particle size. For this reason, FDTD is generally impractical to apply to particles larger than 20–30 wavelengths. In fact, the rapid increase in computational time is a common shortcoming of rigorous methods.

The RBR method approximates the near field within the geometric optics framework. Rays are traced following the geometric optics approach. This avoids the tremendous CPU consumption of FDTD. However, the far field is calculated by mapping the electric field associated with each ray to the far-field counterpart. Therefore, a significant amount of CPU time is consumed to calculate the far field when many scattering directions are of interest. The number of rays and required CPU time increase quadratically with the size parameter. Another shortcoming is that this approximation is good only for large faceted particles. For “soft” (i.e., the refractive index close to 1) and weakly absorbing particles, a volume integral algorithm gives a better far-field approximation, whereas for “hard” (i.e., the refractive index much larger than 1) and strongly absorbing particles, a surface integral gives a better far-field approximation [36].

The optical properties of a particle are specified in terms of the extinction cross-section, σ_e, scattering cross-section, σ_s, and a 4×4 phase matrix representing the relationship between the scattered and incident Stokes parameters in the case of randomly oriented particles with an equal number of mirror-imaging positions [37,38]:

$$\left.\begin{pmatrix} I_S \\ Q_S \\ U_S \\ V_S \end{pmatrix}\right|_{r\gg\lambda} = \frac{\sigma_s}{4\pi r^2}\begin{pmatrix} P_{11} & P_{12} & 0 & 0 \\ P_{12} & P_{22} & 0 & 0 \\ 0 & 0 & P_{33} & P_{34} \\ 0 & 0 & -P_{34} & P_{44} \end{pmatrix}\begin{pmatrix} I_i \\ Q_i \\ U_i \\ V_i \end{pmatrix} \tag{1}$$

where r=the distance between the particle and the point of observation; λ=the wavelength of the incident light; $(I_i \ \ Q_i \ \ U_i \ \ V_i)^T$ and $(I_S \ \ Q_S \ \ U_S \ \ V_S)^T$ denote the Stokes parameter vectors associated with the incident and scattered waves, respectively [37].

Note that the phase matrix depends on the scattering direction and particle orientation, and the extinction and scattering cross sections are affected only by particle orientation. Averaging the cross sections and phase matrix over all orientations results in the optical properties of an ensemble of randomly oriented particles (e.g., most ice cloud particles and aerosols). A derivative variable called the extinction efficiency is commonly used to describe the optical properties, which is defined as σ_e/σ_p, where σ_p is the projected area of the particle to the incident light. σ_p is also orientation-dependent and must be averaged over all orientations for randomly oriented particles.

Using FDTD or RBR to calculate the optical properties of nonspherical particles includes two steps [16,33]: (i) simulating the near-field scattered electromagnetic waves inside and around the particle by solving Maxwell's equations within a finite domain including a particle (in FDTD) or by tracing rays following the geometric optics approach (in RBR), and (ii) calculating the extinction and scattering cross-sections and far field (at infinite distance) by mapping the near field to the far field. The phase matrix is then obtained from the far field.

The second step, the far-field calculation, usually consumes more than half of the total computational time in FDTD, or the majority of the total CPU time in RBR. Therefore, accelerating the far-field calculation can significantly improve the efficiency of the two methods. The conventional far-field calculation further consists of: (i) calculating the far field of each near-field unit (a small volume for volume integration mapping, or a small surface area for surface integration mapping) independently and (ii) computing the total far field as the superposition of all of the unit far fields. This becomes quite time consuming when the far-field information is required in many scattering directions. To accelerate the far field calculations, we implement the fast multi-pole method (FMM) [39–43], which consists of: (i) separating the near-field domain into several sub-domains and “gathering” the near field within each sub-domain; (ii) calculating the far field of each sub-domain independently; and (iii) calculating the total far field as the superposition of the far-field contributions by individual rays.

Using this algorithm, the far-field calculation of a tremendously large number of the near-field units is no longer required. Therefore, the CPU time consumption can be significantly reduced. Since originally developed in 1987 [39], the FMM has been widely applied to various problems in numerous research fields [44–47] including solving Maxwell's equations, leading to a reduction of the computational complexity of matrix-vector multiplications from $O(N^2)$ to $O(N)$. In particular, an alternative algorithm using 2D or 3D Fourier Transforms was also used to accelerate the far-field calculation in DDA [48], and another scheme using the plane wave expansion is employed in the near-to-far field transformation from the near field obtained from a method of moments (MoM) [49].

This study is directed towards accelerating the far-field calculation using FMM in FDTD and RBR. Section 2 describes the methods. Section 3 shows results and analyses, and Section 4 presents the summary and discussions.

2. Methods

The far field can be computed with FMM in conjunction with FDTD and RBR. As a comparison, the conventional far-field formalism is also presented here.