**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.

Keywords: Fast multi-pole, plane wave expansion, finite-difference time-domain, ray-by-ray, near-to-far field mapping

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 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]:

$$\begin{pmatrix} I_s \\ Q_s \\ U_s \\ V_s \end{pmatrix} \bigg|_{r \gg \lambda} = \frac{\sigma_s}{4\pi r^2} \begin{pmatrix} P_{11} & P_{12} & 0 & 0 \\ P_{12} & P_{22} & 0 & 0 \\ 0 & 0 & P_{33} & P_{34} \\ 0 & 0 & -P_{34} & P_{44} \end{pmatrix} \begin{pmatrix} I_i \\ Q_i \\ U_i \\ V_i \end{pmatrix} \quad (1)$$

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.

2.1. Volume integration algorithm for FDTD

In FDTD, the far field can be conventionally calculated using a volume integration algorithm [50]:

$$\begin{aligned} \mathbf{E}^s(\mathbf{r})|_{kr \rightarrow \infty} = & \frac{k^2 \exp(ikr)}{4\pi r} \iiint_V [\epsilon(\mathbf{r}') - 1] \{ \mathbf{E}(\mathbf{r}') \\ & - \hat{\mathbf{r}}[\hat{\mathbf{r}} \cdot \mathbf{E}(\mathbf{r}')] \} \exp(-ik\hat{\mathbf{r}} \cdot \mathbf{r}') d^3\mathbf{r}' \end{aligned} \quad (2)$$

where

- $\mathbf{E}^s$ = the scattered far electric field;
- $\mathbf{E}$ = the near electric field;
- $\mathbf{r}$ = the observation point;
- $\hat{\mathbf{r}}$ = the unit vector of $\mathbf{r}$, indicating the scattering direction of interest;
- r = the amplitude of $\mathbf{r}$;
- $\mathbf{r}'$ = the near-field position vector;
- ϵ = the permittivity;
- k = the wave number of the incident wave in vacuum ($k = 2\pi/\lambda$ where λ is the wavelength in vacuum);
- V = the volume domain that the particle occupies.

The term $\exp(-ik\hat{\mathbf{r}} \cdot \mathbf{r}')$ in Eq. (2) involves the near-field position vector and the scattering direction, indicating the number of operations to be $O(N \cdot N_s)$, where N is the number of near-field cells, and N_s is the number of scattering directions. This number of operations can be quite large when the particle is large (e.g., for a particle 20 times the incident wavelength, N can be millions) and the far field is of interest in many directions (e.g., N_s is often tens of thousands).

To reduce the number of operations, we use a method that “uncouples” $\hat{\mathbf{r}}$ and $\mathbf{r}'$. We consider using the plane wave expansion [51] to separate the near-field position vector and the scattering direction in the term $\exp(-ik\hat{\mathbf{r}} \cdot \mathbf{r}')$:

$$\exp(-ik\hat{\mathbf{r}} \cdot \mathbf{r}')|_{kr \rightarrow \infty} = \sum_{l=0}^{\infty} i^l (2l+1) j_l(kr') P_l(-\hat{\mathbf{r}}' \cdot \hat{\mathbf{r}}) \quad (3)$$

where

$\hat{\mathbf{r}}' =$ the unit vector of $\mathbf{r}'$;
 $r' =$ the amplitude of $\mathbf{r}'$;
 $j_l(x)$ = the spherical Bessel function of the first kind;
 $P_l(x)$ = the Legendre polynomial.

Eq. (3) is the reduced version of the addition theorem (Eq. 3.12 in [43] page 80, with $\mathbf{D}$ and $\mathbf{d}$ replaced by $\mathbf{r}$ and $\mathbf{r}'$ respectively) when r goes to infinity. Therefore, the present implementation is a reduced version of the FMM. The term $i^l j_l(kr') P_l(\hat{\mathbf{r}}' \cdot \hat{\mathbf{r}})$ is then expressed in terms of the elementary identity in the form [52] (page 410):

$$i^l j_l(kr') P_l(-\hat{\mathbf{r}}' \cdot \hat{\mathbf{r}}) = \frac{1}{4\pi} \iint_{\Omega} \exp(-ik\hat{\mathbf{k}} \cdot \mathbf{r}') P_l(\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}) d\Omega \quad (4)$$

where the integration is over the unit sphere Ω in $\hat{\mathbf{k}}$ space. Substituting Eq. (4) into Eq. (3) yields:

$$\exp(-ik\hat{\mathbf{r}} \cdot \mathbf{r}')|_{kr \rightarrow \infty} = \frac{1}{4\pi} \iint_{\Omega} \left[\exp(-ik\hat{\mathbf{k}} \cdot \mathbf{r}') \sum_{l=0}^{\infty} i^l (2l+1) P_l(\hat{\mathbf{k}} \cdot \hat{\mathbf{r}}) \right] d\Omega \quad (5)$$

Truncating the summation and approximating the integration using the Lebedev quadrature [53] in Eq. (5) yields:

$$\exp(-ik\hat{\mathbf{r}} \cdot \mathbf{r}')|_{kr \rightarrow \infty} = \frac{1}{4\pi} \sum_{m=1}^{M(L)} \left[w_m \cdot \exp(-ik\hat{\mathbf{k}}_m \cdot \mathbf{r}') \sum_{l=0}^L i^l (2l+1) P_l(\hat{\mathbf{k}}_m \cdot \hat{\mathbf{r}}) \right] \quad (6)$$

where M , as a function of L , is the number of Lebedev quadrature points on the unit sphere when the order is L . $M(L) \approx 4L^2/3$ when $L \geq 5$ [53]. w_m is the weight of the m^{th} quadrature point. $\hat{\mathbf{k}}_m$ is the m^{th} unit vector. On the right of Eq. (6), $\hat{\mathbf{r}}$ and $\mathbf{r}'$ are no longer coupled, but are coupled with vector $\hat{\mathbf{k}}_m$ respectively.

For notational clarity, considering $\mathbf{E}(\mathbf{r}') - \hat{\mathbf{r}}[\hat{\mathbf{r}} \cdot \mathbf{E}(\mathbf{r}')] = (\bar{\mathbf{I}} - \hat{\mathbf{r}}\hat{\mathbf{r}}) \cdot \mathbf{E}(\mathbf{r}')$, Eq. (2) can be written in a matrix form as:

$$\mathbf{E}^s(\mathbf{r})|_{kr \rightarrow \infty} = \frac{k^2 \exp(ikr)}{4\pi r} (\bar{\mathbf{I}} - \hat{\mathbf{r}}\hat{\mathbf{r}})^{3 \times 3} \cdot \bar{\bar{\mathbf{E}}}^{3 \times N} \cdot \bar{\mathbf{P}}^N(\hat{\mathbf{r}}) \quad (7)$$

where

$$\bar{\bar{\mathbf{E}}}^{3 \times N}_{p,n} = [\epsilon(\mathbf{r}'_n) - 1] \mathbf{E}^p(\mathbf{r}'_n) \Delta V_n \quad (8)$$

$$\bar{\mathbf{P}}^N_n(\hat{\mathbf{r}}) = \exp(-ik\hat{\mathbf{r}} \cdot \mathbf{r}'_n) \quad (9)$$

The superscripts in Eq. (7) denote the matrix sizes, except the k^2 term. The superscript of $\mathbf{E}$ denotes the spatial dimension, namely 1 for x, 2 for y, and 3 for z. The subscript of $\mathbf{r}'$ denotes the index of the near-field cell. $\bar{\mathbf{I}}$ is a 3x3 identity matrix. ΔV_n is the volume of the n^{th} cell.

Substituting Eq. (6) into Eq. (2) yields a matrix form:

$$\mathbf{E}^s(\mathbf{r})|_{kr \rightarrow \infty} = \frac{k^2 \exp(ikr)}{4\pi r} (\bar{\mathbf{I}} - \hat{\mathbf{r}}\hat{\mathbf{r}})^{3 \times 3} \cdot \bar{\bar{\mathbf{E}}}^{3 \times N} \cdot \bar{\bar{\mathbf{F}}}^{N \times M} \cdot \bar{\mathbf{A}}^M(\hat{\mathbf{r}}) \quad (10)$$

where

$$\bar{\bar{\mathbf{F}}}^{N \times M}_{n,m} = \exp(-ik\hat{\mathbf{k}}_m \cdot \mathbf{r}'_n) \quad (11)$$

$$\bar{\mathbf{A}}^M_m(\hat{\mathbf{r}}) = \frac{w_m}{4\pi} \sum_{l=0}^L i^l (2l+1) P_l(\hat{\mathbf{k}}_m \cdot \hat{\mathbf{r}}) \quad (12)$$

To obtain an approximation with desirable accuracy [43], in Eq. (12), we choose

$$L \approx kd/2 \quad (13)$$

$$M \approx \frac{4}{3}L^2 \approx (kd)^2/3 \quad (14)$$

where d is the largest distance between two points within the particle.

Then the number of operations in Eq. (10) becomes $O([kd]^2N + [kd]^3N_S)$. This is called a “single pole” algorithm, in which the near field is “mapped” to a single pole, the coordinate origin, by calculating the term $\bar{\bar{F}}^{N \times M}$ before the single pole is “mapped” to the far field by calculating the term $\bar{A}^M(\hat{\mathbf{r}})$.

This number of operations increases significantly when kd becomes larger. In order to further decrease the number of operations, we consider using a “multi-pole” algorithm. We divide the particle into several cubical volume boxes, where $\mathbf{c}_b$ is the center of the b^{th} volume box. Writing $\mathbf{r}' = \mathbf{c}_b + (\mathbf{r}' - \mathbf{c}_b)$, Eq. (6) becomes

$$\begin{aligned} \exp(-ik\hat{\mathbf{r}} \cdot \mathbf{r}')|_{kr \rightarrow \infty} \\ = \exp(-ik\hat{\mathbf{r}} \cdot \mathbf{c}_b) \frac{ik}{4\pi} \sum_{m=1}^{M(L)} \left[w_m \right. \\ \left. \cdot \exp(-ik\hat{\mathbf{k}}_m \cdot (\mathbf{r}' - \mathbf{c}_b)) \sum_{l=0}^L i^l (2l+1) P_l(\hat{\mathbf{k}}_m \cdot \hat{\mathbf{r}}) \right] \end{aligned} \quad (15)$$

Substituting Eq. (15) into Eq. (2) yields a matrix equation:

$$\mathbf{E}^s(\mathbf{r})|_{kr \rightarrow \infty} = \frac{k^2 \exp(ikr)}{4\pi r} (\bar{\bar{I}} - \hat{\mathbf{r}}\hat{\mathbf{r}})^{3 \times 3} \cdot \sum_{b=1}^B [\bar{\bar{E}}^{3 \times N_b} \cdot \bar{\bar{P}}^{N_b \times M} \cdot \bar{A}^M(\hat{\mathbf{r}}) Q_b(\hat{\mathbf{r}})] \quad (16)$$

where

$$\bar{\bar{E}}^{3 \times N_b}_{p,n} = \mathbf{E}^p(\mathbf{r}'_q) dV_n |_{\mathbf{r}'_n \in V_b} \quad (17)$$

$$\bar{\bar{P}}^{N_b \times M}_{n,m} = \exp(-ik\hat{\mathbf{k}}_m \cdot \mathbf{r}'_n) |_{\mathbf{r}'_n \in V_b} \quad (18)$$

$$Q_b(\hat{\mathbf{r}}) = \exp(-ik\hat{\mathbf{r}} \cdot \mathbf{c}_b) \quad (19)$$

and

B = the number of volume boxes;

V_b = the domain of the b^{th} box;

N_b = the number of near-field units in the b^{th} box, satisfying $\sum_{b=1}^B N_b = N$.

Eq. (16) constitutes a multiple-pole algorithm with a number of operations on the order of $O(NM + N_S BM + N_S LM)$. From Eq. (15), L and M can be approximately chosen as:

$$L \approx kd_b \approx kd \cdot B^{-1/3} \quad (20)$$

$$M \approx \frac{4}{3}(kd)^2 \cdot B^{-2/3} \quad (21)$$

where d_b = the edge length of each box.

Then the number of operations becomes $O\left([kd]^2 \left[NB^{-\frac{2}{3}} + N_S B^{\frac{1}{3}}\right] + [kd]^3 N_S B^{-1}\right)$. For large particles, when $N \gg N_S$, we choose $B \approx N/N_S$, and the number of operations becomes $O\left([kd]^2 N^{\frac{1}{3}} N_S^{\frac{2}{3}} + [kd]^3 N_S^2 / N\right)$. When $B = 1$, the multi-pole algorithm reduces to the single-pole algorithm. Apparently, for large particles, the number of operations in the multi-pole algorithm is much smaller than in the single-pole algorithm. For small particles (i.e., $N < N_S$ or $kd < 1$), the single-pole algorithm is sufficient, and is still much faster than the conventional method. In summary, we employ the single-pole method if $N < N_S$ or $kd < 1$; otherwise the multi-pole method is used. Note that the total number of operations above in each case is an approximate estimation.

2.2. Surface integration algorithm for RBR

The RBR has been used to calculate the optical properties of large faceted particles [33] with characteristic dimensions larger than several tens of the incident wavelength. Both a volume integration algorithm and a surface integration algorithm to

calculate the far field from the near field are present in the literature. Here we apply the FMM to accelerate the surface integration algorithm. The conventional surface integration algorithm is expressed as:

$$\mathbf{E}^s(\mathbf{r})|_{kr \rightarrow \infty} = \frac{ik \exp(ikr)}{4\pi r} \hat{\mathbf{r}} \times \iint_S \{ \hat{\mathbf{n}}_S \times \mathbf{E}(\mathbf{r}') - \hat{\mathbf{r}} \times [\hat{\mathbf{n}}_S \times \mathbf{H}(\mathbf{r}')] \} \exp(-ik\hat{\mathbf{r}} \cdot \mathbf{r}') d^2\mathbf{r}' \quad (22)$$

where

$\mathbf{E}$ and $\mathbf{H}$ are the electric and magnetic fields at the outside surface of the particle; $\hat{\mathbf{n}}_S$ is the outward-pointing normal vector at the surface.

In RBR this integration is performed for each outgoing ray along the ray tracing process [33], which can then be represented in a matrix form:

$$\mathbf{E}^s(\mathbf{r})|_{kr \rightarrow \infty} = \frac{ik \exp(ikr)}{4\pi r} \left[\hat{\mathbf{r}} \times \bar{\bar{E}}^{3 \times N} + (\bar{\mathbf{I}} - \hat{\mathbf{r}}\hat{\mathbf{r}})^{3 \times 3} \cdot \bar{\bar{H}}^{3 \times N} \right] \cdot \bar{P}^N(\hat{\mathbf{r}}) \quad (23)$$

where

$$\bar{\bar{E}}^{3 \times N}_{p,n} = (\hat{\mathbf{n}}_S \times \mathbf{E})^p|_{\mathbf{r}'_n} \Delta S_n \quad (24)$$

$$\bar{\bar{H}}^{3 \times N}_{p,n} = (\hat{\mathbf{n}}_S \times \mathbf{H})^p|_{\mathbf{r}'_n} \Delta S_n \quad (25)$$

$$\bar{P}^N_n(\hat{\mathbf{r}}) = \exp(-ik\hat{\mathbf{r}} \cdot \mathbf{r}'_n) \quad (26)$$

and N is the number of outgoing rays. ΔS_n is the cross section of the n^{th} outgoing ray on the particle surface. The superscripts of $\hat{\mathbf{n}}_S \times \mathbf{E}$ and $\hat{\mathbf{n}}_S \times \mathbf{H}$ denote the index of dimension, 1 for x, 2 for y, and 3 for z, and the subscripts of $\mathbf{r}'$ denotes the index of outgoing rays. The number of operations is $O(N \cdot N_S)$.

Following the same FMM procedure applied to the volume integration in FDTD (Eq. (6)) to separate the near-field position vector and the scattering direction in the term

$\exp(-ik\hat{\mathbf{r}} \cdot \mathbf{r}')$, and substituting Eq. (6) into Eq. (23), we obtain the single-pole algorithm for the surface integration in a matrix form:

$$\mathbf{E}^s(\mathbf{r})|_{kr \rightarrow \infty} = \frac{ik \exp(ikr)}{4\pi r} [\hat{\mathbf{r}} \times E^{3 \times N} + (I - \hat{\mathbf{r}}\hat{\mathbf{r}})^{3 \times 3} \cdot H^{3 \times N}] \cdot F^{N \times M} \cdot A^M(\hat{\mathbf{r}}) \quad (27)$$

where $F^{N \times M}$ and $A^M(\hat{\mathbf{r}})$ are the same as those in Eq. (10). In order to obtain acceptable accuracy, we still choose L and M as in Eq. (13) and (14) respectively. Then the number of operations becomes $O([kd]^2[N + N_s])$. For large particles, we apply a multi-pole algorithm. We divide the domain of the particle into several boxes,

$$\mathbf{E}^s(\mathbf{r})|_{kr \rightarrow \infty} = \frac{k^2 \exp(ikr)}{4\pi r} \sum_{b=1}^B \left\{ \left[\hat{\mathbf{r}} \times \bar{E}^{3 \times N_b} + (\bar{I} - \hat{\mathbf{r}}\hat{\mathbf{r}})^{3 \times 3} \cdot \bar{H}^{3 \times N_b} \right] \cdot \bar{P}^{N_b \times M} \cdot \bar{A}^M(\hat{\mathbf{r}}) Q_b(\hat{\mathbf{r}}) \right\} \quad (28)$$

where

$$E^{3 \times N_b}_{p,n} = (\hat{\mathbf{n}}_S \times \mathbf{E})^p|_{\mathbf{r}'_n \in V_b} \Delta S_n \quad (29)$$

$$H^{3 \times N_b}_{p,n} = (\hat{\mathbf{n}}_S \times \mathbf{H})^p|_{\mathbf{r}'_n \in V_b} \Delta S_n \quad (30)$$

and N_b is the number of outgoing rays that leaves the particle from the b^{th} non-empty box. B is the number of non-empty boxes (an empty box is one from which no ray leaves the particle). $A^M(\hat{\mathbf{r}})$ and $Q_b(\hat{\mathbf{r}})$ are the same as in Eq. (16). The number of operations of the multi-pole algorithm becomes $O(NM + N_s BM)$. For surface integration, the edge length of each box d_b is proportional to $B^{-1/2}$. Therefore, we approximate L and M as:

$$L \approx kd_b \approx kd \cdot B^{-1/2} \quad (31)$$

$$M \approx 4L^2/3 \approx \frac{4}{3}(kd)^2 \cdot B^{-1} \quad (32)$$

Then the number of operations becomes $O([kd]^2[NB^{-1} + N_s])$. Note that the multi-pole algorithm is always faster than the single-pole algorithm when $kd > 1$, and faster than the conventional algorithm when $N > [kd]^2$.

3. Results

In this section, we compare the optical properties calculated using FMM and other conventional algorithms to analyze the efficiency improvement and accuracy of FMM. The optical properties of a single particle considered here are the extinction efficiency and the 4×4 phase matrix that is dependent on the scattering angle [37]. The present algorithms are designed to accelerate the calculation of the phase matrix.

3.1 Volume integration algorithm for FDTD

We calculate the phase matrix of a single hexagonal column ice crystal to validate FMM in FDTD. The incident wavelength λ is chosen as $0.66\mu\text{m}$ in the visible spectrum. The refractive index of ice at this wavelength is $1.3078 + i1.66 \times 10^{-8}$, the aspect ratio of the column is $2a/H = 1$, and the particle size is $H = 2a = 1\mu\text{m}$, where a and H are the side length of the hexagonal cross section and height of the column, respectively. The grid resolution is chosen as 40 grid points per wavelength. $N_s = 194 \times 360$, where 194 is the number of polar angles (or scattering angles) ranging from 0° for forward scattering to 180° for backward scattering, and 360 is the number of azimuthal angles. The resultant phase matrix is then averaged over the azimuthal angles to represent the random rotation of the particle about the incident direction (the phase function, P_{11} , or radar cross section (RCS), is normalized based on integration over all solid angles, hereafter in this paper). In FMM we arbitrarily choose the box size to be $kd_b = 2$ and the truncation of the plane wave expansion to be $L = 5$. The phase matrix elements as functions of scattering angle

computed using the conventional FDTD and FMM are shown in Fig. 1. The visible similarity of the two results indicates a good reproduction of FDTD results using FMM.

Fig. 1. Comparison of the phase matrix elements computed using the conventional FDTD and the FMM.

To assess the feasibility of using FMM to reproduce FDTD results, we define the relative difference between the two results as:

$$R = \frac{[\int_0^\pi \delta P_{11}^2 \sin(\theta) d\theta]^{1/2}}{[\int_0^\pi P_{11}^2 \sin(\theta) d\theta]^{1/2}} \quad (33)$$

where

δP_{11} = the difference of the phase function between FMM and FDTD;
 P_{11} = the phase function of the conventional FDTD;
 θ = the scattering angle.

R is about 1×10^{-5} for the results shown in Fig. 1. The CPU time for these near-field to far-field calculations are about 1700 seconds for FDTD and 40 seconds for FMM, which suggests a speed-up factor of ≈ 40 . The near-field calculation takes about 380 seconds. Thus the efficiency improvement of the whole simulation is about 5 times. To further validate the FMM method, we carry out additional calculations for different sizes ($H = 2a = 2\mu\text{m}$ and $3\mu\text{m}$), while other conditions (i.e., particle geometry, orientation, box size kd_b , truncation number L) are kept the same. The comparison of CPU time of the two far-field calculations and their relative difference are thus shown in Fig. 2. The speed-up factor is ≈ 40 for the tested particle sizes, while the difference is less than or close to 1×10^{-5} .

Fig. 2. CPU time (left panel) of far-field calculations for FDTD and FMM and their relative difference (right panel) as functions of particle size. The particle geometry and incident wavelength is the same as in Fig. 1. kd_b is fixed as 2. L is fixed as 5.

We next vary kd_b and L to determine the best choice of sub-domain discretization and truncation. A semi-empirical relation between kd_b and L has been given [54-59] as:

$$L \approx \frac{\sqrt{3}}{2}kd_b + \alpha \ln \left(\pi + \frac{\sqrt{3}}{2}kd_b \right) \quad (34)$$

where $\frac{\sqrt{3}}{2}d_b$ is the largest point-to-center distance within a cubic box with edge length of d_b . α is a parameter that controls the accuracy of the plane wave expansion, Eq. (15). Using $\alpha = 1$ results in an accuracy of 10^{-1} , while $\alpha = 5$ results in accuracy of 10^{-6} [43]. The sets of $kd_b = 2, L = 5$ used in the previous calculations correspond to $\alpha = 2.5$. To test the performance of this approximation in our implementation, we repeat the above FMM calculation for size $H = 2a = 3\mu m$ with α varying from 1 to 6. kd_b is set to be 2, 5, and 8 respectively. The CPU times with FMM and differences from the conventional FDTD calculation are shown in Fig. 3. Comparing with the previously chosen sets, $kd_b = 2, \alpha = 2.5$, increasing kd_b and α to $kd_b = 5, \alpha = 3$ further increases efficiency and accuracy of FMM. So the speed-up compared to the conventional FDTD reaches 100 times. Further increasing α from 3 does not increase accuracy as expected. There must be other error sources other than from the approximation of Eq. (15). For example, the floating-point error (real 4 type float number is used in the original FDTD code) may accumulate during the summation in Eq. (16) resulting in a small error in the final result. Fig. 4 shows the variation of CPU time and R as functions of kd_b when we fix $\alpha = 3$. The $kd_b = 34$ case corresponds to a single-pole algorithm calculation. We notice that when $kd_b = 5$, both CPU time and the relative difference reach a minimum. R increases

with kd_b , which can be compensated for by slightly increasing α with kd_b . In all of the above calculations, the number of far-field directions is $N_S = 194 \times 360 \approx 7 \times 10^4$, and the grid cell resolution is $\gamma = 40$ (wavelength/size of cell). According to our analysis in the method section and the results above, we obtain an empirical expression for the best choice of kd_b :

$$kd_b \propto kd \left(\frac{N_S}{N} \right)^{\frac{1}{3}} \propto \gamma^{-1} N_S \approx 5.0 \gamma^{-1} N_S^{1/3} \quad (35)$$

Fig. 3. The same as Fig. 2 but showing the CPU time of FMM calculations and their relative differences from the FDTD results with respect to α .

Fig. 4. The same as Fig. 2 but showing the CPU time of FMM calculations and their relative differences from the FDTD results with respect to kd_b . α is fixed at 3. $kd_b = 34$ corresponds to a single-pole algorithm calculation.

3.2 Surface integration algorithm in ray-by-ray

In this subsection, we test the performance of the FMM in accelerating the surface integration mapping in the RBR method. We calculate the optical properties of a hexagonal column ice crystal with size parameter $kH = 2ka = 100$. The refractive index is still $1.3078 + i1.66 \times 10^{-8}$. The number of incident rays is 3×10^5 . We set $kd_b = 5$ and $\alpha = 3$ to be consistent with the FDTD experiments. The phase matrix elements are shown in Fig. 5. The relative difference, R , between RBR and FMM is about 3×10^{-7} . In particular, the relative difference of backscattering cross sections is about 5×10^{-7} . The CPU time is about 200 seconds for the RBR calculation and 50 seconds for the FMM

calculation, which indicates a speed-up of a factor of 4. Advantage of FMM is that increasing the number of rays will not lead to a significant increase of CPU time, unlike the conventional RBR. When we use 10 times as many rays, or 3×10^6 , and redo the FMM calculation, the relative difference between the new calculation and the old is about 2×10^{-3} . However, the CPU time almost stays the same. When we use 2/3 as many rays, or 2×10^5 , the relative difference is about 10%, which is not acceptable. Therefore, 3×10^5 rays are sufficient for this calculation, but should not be less. However, increasing the number of rays to increase accuracy is feasible using FMM, while costly in the conventional RBR.

Fig. 5. Comparison of the phase matrix elements computed using the conventional RBR and the FMM. The direction of the incident light is shown in the figure.

We further calculate the phase matrices of randomly oriented hexagonal column ice crystals with size parameters $kH = 2ka = 100, 150, 200$ and compare with the results of II-TM and IGOM. The comparison is shown in Fig. 6. We assume the II-TM [30,31] results to be benchmark references. The broad agreement between II-TM and IGOM has been reported in [30]. Here we show that the RBR result also agrees with the other two. Furthermore, RBR agrees much better with II-TM than IGOM does for the backscattering cross section ($P_{11}(180^\circ)$) and polarization terms (i.e., P_{22} , P_{33} , P_{44}).

Fig. 6. Phase matrices of hexagonal column ice crystals with size parameters $kH = 2ka = 100, 150$, and 200 at $0.66\mu\text{m}$ incident light. For display, P_{11} is multiplied by a factor of 10 for $kH = 150$ and 100 for $kH = 200$. Other polarization terms have 0.5 and 1.0 added respectively.

RBR is feasible for particles with not only convex geometries (e.g., hexagonal columns), but also concave geometries (e.g., aggregate of hexagonal columns), in which

re-entrance of rays into the particle is taken into account. For the MODIS (Moderate Resolution Imaging Spectroradiometer) [60,61] Collection 6 (C6) operational cloud property retrievals, ice crystals are assumed to be aggregates consisting of eight hexagonal columns. The detail of this C6 aggregate geometry is described in [38] and [61]. We compute the phase matrices of three C6 ice crystal aggregates with size parameters $kD = 60, 80, 100$, where D is the largest distance between two points within the aggregate. The results of the three methods, II-TM, RBR with FMM, and IGOM are shown in Fig. 7. Notice that there is a better overall agreement between RBR and II-TM than that between IGOM and II-TM.

Fig. 7. The same as Fig. 6 but for three C6 ice crystal aggregates with size parameters $kD = 60, 80, \text{and } 100$.

Fig. 8 shows the extinction efficiency and asymmetry factor of hexagonal ice crystals with various sizes with $0.66\mu\text{m}$ incident light calculated using II-TM, RBR with FMM, and IGOM. As particle size increases, all three methods agree better in both the extinction efficiency and asymmetry factor. This is consistent with the geometric optics approximation used in RBR and IGOM. Notice that the extinction efficiencies obtained with RBR and IGOM are basically the same, which result from the fact that the two methods use the same physical principles to calculate the extinction efficiency. However, the asymmetry factor of RBR agrees much better with II-TM than IGOM does. When the particle size parameter exceeds about 100, the extinction efficiency difference between II-TM and RBR becomes less than 2%, and the asymmetry factor difference is less than 1%.

Fig. 8. Extinction efficiency and asymmetry factor of randomly oriented hexagonal ice crystals as functions of size parameter.

4. Summary and Discussions

The computational efficiency of FDTD and RBR is significantly improved by implementing FMM to accelerate the far-field calculation. In implementations of FDTD, the near-field to far-field calculation takes several times longer than the near-field calculation. Application of FMM reduces the near-field to far-field calculation time consumption by several tens to a hundred times making it negligible compared to the near-field calculation. In addition, FDTD with FMM reproduces the conventional FDTD results with a relative phase function difference, R , of about $10^{-6} \sim 10^{-5}$. For the same particle size, the time consumption of FMM is nearly proportional to the grid resolution, γ , while the conventional far-field calculation is proportional to the grid resolution cubed. This indicates even stronger efficiency improvement when higher grid resolutions (“compact” grids) are used. To determine the best choice of sub-domain sizes in our code, we derive an empirical relationship between the chosen sub-domain box size d_b and the grid resolution, shown in Eq. (35).

Our application of FMM to the far-field calculation significantly reduces the time consumption of RBR. One of the advantages of RBR with FMM is that the CPU time consumption remains almost the same when the number of rays is increased, while the CPU time consumption of the conventional RBR is proportional to the number of rays. Flexibly increasing the number of rays to ensure convergence is thus feasible in our RBR with FMM procedure. A new so-called physical-geometric optics hybrid (PGOH) method has been developed recently [34,35], which is based on the same physics as RBR, but

deals with all parallel rays together in numerical implementation, so it is more efficient than RBR. In fact, RBR is expected to converge to the PGOH result when using an infinite number of rays. However, it is challenging to implement PGOH in the case of particles with complex geometries (e.g., concave geometries such as snow particles [63], ice crystal aggregates [7,64-66], dust [67], and surface roughened particles [68-70]). The RBR method is easy to implement for these complex geometries. IGOM [32] is similar to RBR but considers less interference between rays and is more efficient, especially for randomly oriented particles.

Although applying FMM to FDTD and RBR improves the computational efficiency significantly, the memory demand also increases considerably. For example, computing the optical properties of a particle with a size parameter of about 1000 using RBR with FMM requires approximately 3 gigabytes, whereas only several megabytes are needed if the conventional RBR is used. However, this shortcoming is becoming less severe with current supercomputing resources. .

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