Short Note

Efficient method of computing a geometric optics integral for light scattering by nonspherical particles

by

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1. Introduction

An effective method for calculating the scattering of light by nonspherical particles which covers all shapes and sizes does not exist because of the complex nature of the solution and the computer time required. The numerical methods thus far developed are applicable mostly to particles in specific size ranges.

Light scattering by nonspherical particles depends on the dimensionless size parameter x , defined as $\pi D/\lambda$, where D is the diameter of the particle and λ is wavelength, as well as on the shape and the refractive index of the particles. For small x (< 50), numerical methods such as the finite-difference time domain (FDTD) method have been applied to calculate light scattering by nonspherical particles (e.g., Yang and Liou, 2000; Ishimoto, 2006). To obtain the scattering properties of nonspherical particles characterized by large x (> 200) a combination of the geometrical ray-tracing technique and Fraunhofer diffraction (GOM1; Yang and Liou, 1996) has been widely used (e.g., Takano and Liou, 1989; Macke *et al.*, 1996; Hess *et al.*, 1998).

For intermediate x , $50 < x < 200$, Muinonen (1989) and Yang and Liou (1996) developed another geometrical optics–integral equation model (GOM2; Yang and Liou, 1996) to compute light scattering by nonspherical particles, but an efficient computational scheme for this model has yet to be developed. This paper examines the factors affecting the computation time of GOM2 and presents a scheme for improving its computational efficiency.

2. Computational scheme

In GOM2, the reflected and refracted near fields are

calculated by the ray-tracing technique in a manner similar to GOM1. The near fields are then transformed to the far fields by applying the electromagnetic equivalence theorem (Yang and Liou, 1996) in the same manner as in the FDTD method (Zhai *et al.*, 2004). Consequently, the accuracy and time consumption of the GOM2 calculations are between those of GOM1 and FDTD.

The scattered far field can be obtained by integrating the electric and magnetic fields over the particle's surface (Yang and Liou, 1996):

$$\mathbf{E}_s(\mathbf{r}) = \frac{e^{ikr}}{-ikr} \cdot \frac{k^2}{4\pi} \mathbf{n}_r \times \int_S [\mathbf{n}_s \times \mathbf{E}(\mathbf{r}') - \mathbf{n}_r \times (\mathbf{n}_s \times \mathbf{H}(\mathbf{r}'))] e^{-ik\mathbf{r}' \cdot \mathbf{n}_r} dS, \quad (1)$$

where $\mathbf{E}(\mathbf{r}')$ and $\mathbf{H}(\mathbf{r}')$ are, respectively, the electric and magnetic fields that include the incident and scattered (reflected and refracted) fields on the particle surface; k is the wave number, defined as $2\pi/\lambda$; $\mathbf{r}$ is the position vector of the observation point; $\mathbf{r}'$ is the position vector of the source point on the particle surface; $\mathbf{n}_r$ is the scattering direction; and $\mathbf{n}_s$ is the outward unit vector normal to the surface. $\mathbf{H}(\mathbf{r}')$ is related to $\mathbf{E}(\mathbf{r}')$ as $\mathbf{H}(\mathbf{r}') = \mathbf{n}_0 \times \mathbf{E}(\mathbf{r}')$, where $\mathbf{n}_0$ is the direction of the outgoing ray (Yang and Liou, 1996).

In the ray-tracing procedure, the incident wave is divided into a number of localized rays, each of which interacts with the particle, resulting in the production of various orders of scattered rays by the Fresnel reflection and refraction on the particle surface. The fundamental equation that incorporates the ray-tracing is given by

$$\mathbf{E}_s(\mathbf{r}) = \frac{e^{ikr}}{-ikr} \cdot \frac{k^2}{4\pi} \sum_{i,p} \left\{ \mathbf{n}_r \times \int_{S_{i,p}} [\mathbf{n}_s \times \mathbf{E}(\mathbf{r}') - \mathbf{n}_r \times (\mathbf{n}_s \times \mathbf{H}(\mathbf{r}'))] e^{-ik\mathbf{r}' \cdot \mathbf{n}_r} dS \right\} \quad (2)$$

where the subscript i denotes an individual localized ray; p is the order of the ray-tracing event ($p = 0$, incident ray; $p = 1$,

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externally reflected ray; $p = 2$, twice refracted ray, and so on) (Yang and Liou, 1996). $S_{i,p}$ is the surface area element from which the near field associated with ray i at event p makes a contribution to the far field. The indices i and p of the variables are omitted in Eq. 2 for simplicity. In this paper, the formulation for only the refracted rays ($p \geq 2$) is presented. The incident and externally reflected rays can be treated in a similar manner.

Let $m (= m_r + i m_i)$ be the refractive index of particles relative to air. $\mathbf{E}(\mathbf{r}')$ and $\mathbf{H}(\mathbf{r}')$ are then expressed as

$$\mathbf{E}(\mathbf{r}') = \mathbf{E}^*(\mathbf{r}') e^{-km_i \sum_{j=1}^{p-1} d_j} e^{ik(\mathbf{n}_i \cdot \mathbf{r}^0 + m_r \sum_{j=1}^{p-1} d_j)}$$

and

$$\mathbf{H}(\mathbf{r}') = \mathbf{H}^*(\mathbf{r}') e^{-km_i \sum_{j=1}^{p-1} d_j} e^{ik(\mathbf{n}_i \cdot \mathbf{r}^0 + m_r \sum_{j=1}^{p-1} d_j)}$$

(Yang and Liou, 1996), where $\mathbf{n}_i$ is the direction of the incident ray, $\mathbf{r}^0$ is the position vector at the point where the incident ray first strikes the particle, and d_j is the distance between two successive reflections inside the particle. $\mathbf{E}^*(\mathbf{r}')$ and $\mathbf{H}^*(\mathbf{r}')$ are determined from the Fresnel equations after rotation of the coordinate axes. The term $e^{-km_i \sum_{j=1}^{p-1} d_j}$ expresses the attenuation of the ray in the particle, and $e^{ik(\mathbf{n}_i \cdot \mathbf{r}^0 + m_r \sum_{j=1}^{p-1} d_j)}$ is the phase shift associated with ray propagation.

We refer to the phase shift term $e^{ik(\mathbf{n}_i \cdot \mathbf{r}^0 + m_r \sum_{j=1}^{p-1} d_j)}$ as $e^{ikf(\mathbf{r}')}$ and to the position vector at the center of the surface area element ($S_{i,p}$) as $\mathbf{r}'_{i,p}$ (Fig. 1). The Fresnel term is invariant over $S_{i,p}$. We assume that the attenuation term over $S_{i,p}$ is represented by the value at its center position ($\mathbf{r}'_{i,p}$). Equation 2 can then be written as

$$\mathbf{E}_s(\mathbf{r}) = \frac{e^{ikr}}{-ikr} \cdot \frac{k^2}{4\pi} \sum_{i,p} \left\{ \mathbf{n}_i \times [\mathbf{n}_i \times \mathbf{E}^*(\mathbf{r}'_{i,p}) - \mathbf{n}_r \times (\mathbf{n}_i \times \mathbf{H}^*(\mathbf{r}'_{i,p}))] \cdot e^{-km_i \sum_{j=1}^{p-1} d_j} e^{ik(f(\mathbf{r}'_{i,p}) - \mathbf{n}_r \cdot \mathbf{r}'_{i,p})} \int_{S_{i,p}} e^{ik[f(\mathbf{r}') - f(\mathbf{r}'_{i,p}) - \mathbf{n}_r \cdot (\mathbf{r} - \mathbf{r}'_{i,p})]} dS \right\}. \quad (3)$$

The Fresnel term, the attenuation term, and the phase shift term at $\mathbf{r}'_{i,p}$ can be calculated by the ray-tracing procedure (Yang and Liou, 1996). The computational difficulty inherent in GOM2 is strongly related to the complexity of the calculation of the integral of the phase of the wave, in which the spacing of the incident rays is an essential parameter. Yang and Liou (1996) noted that the radius of a circular cross section of a ray should be of the order k^{-1} (i.e., ~ 1 size parameter unit) if the phase of the localized waves in $S_{i,p}$ is to be properly represented by using the incident ray at the center of $S_{i,p}$, and this implies that the spacing of incident rays should be ~ 1 size parameter unit. Thus, the required CPU time for GOM2 is proportional to x^2 , whereas for GOM1 the required CPU time is basically independent of the size parameter. This dependence on size is one of the main reasons that the CPU time required for GOM2 is much longer than that required for GOM1.

To sidestep this problem, Yang and Liou (1996) developed an intensity mapping algorithm in which the phase

Fig. 1 Schematic diagram showing the surface area elements on a crystal face used for calculating the integral of the phase shift. $w (= \Delta x/k)$ is the length of the sides of each square in the lattice. Thus, the ray spacing is Δx in size parameter units, $S_{i,p}$ ($p = 0, 1, 2$) are the surface area elements, and $\mathbf{r}'_{i,p}$ is the position vector at the center of $S_{i,p}$.

interference is accounted for approximately by considering the ray spreading of the externally reflected and refracted intensities produced by GOM1. In this paper, we present another approach in which the integral of the phase shift term is computed by using a parallelogram as the fundamental surface area element.

We assume that a particle is bounded by plane faces and that the center of the particle is at the origin of a Cartesian coordinate system. The incident rays are assumed to propagate in the positive z -axis direction. We assume that there is a lattice of uniform squares, each with sides of length $w = \Delta x/k$ (Fig. 1), and that each incident ray is positioned at the center of a square; that is, the ray spacing is Δx in size parameter units.

The first step of ray-tracing is to identify the first particle face that an incident ray intersects. The square that includes the incident ray projects onto the selected face as a parallelogram (Fig. 1) (or onto a plane that includes the selected face if some of the vertices of the parallelogram are beyond the edge of the particle face). After the ray propagates through the particle, the projected area of this parallelogram is another parallelogram on one of the particle's other faces (or on a plane that includes that particle face). The coordinates of the vertices and the center of the parallelogram are calculated by the ray-tracing procedure, along with the function $f(\mathbf{r}')$, which is associated with the phase shift. Once the parallelogram coordinates and the phase of the wave are determined, the integral of the phase over the parallelogram can be calculated analytically (see Appendix). This procedure allows us to relax the restriction that the cross section of the ray must

be ~ 1 size parameter unit.

3. Results

The presented computational scheme involves some uncertainties that may influence the computational accuracy. First, the attenuation term over the area to be integrated is approximated by its value at the center of the parallelogram. Second, the integral of the phase term is calculated over the area of the parallelogram even if some of the vertices are outside the particle face. To assess the computational accuracy, we compared the calculation results for the phase function (P_{11}) and the degree of linear polarization ($-P_{12}/P_{11}$) between the present scheme and the FDTD and GOM1 methods. In addition, we examined the influence of the ray spacing on GOM2 accuracy.

Figure 2 compares the phase function P_{11} as calculated by GOM2, GOM1, and FDTD for hexagonal ice crystals assumed to be randomly oriented in three-dimensional (3D) space and with an aspect ratio ($L/2R$) of 1.7, where R and L are the radius of the hexagon and the length of the crystal, respectively (Fig. 1). The refractive index is $m = 1.29 + i 1.58 \times 10^{-5}$, which is for ice crystals at $\lambda = 1.38 \mu\text{m}$. We used the size parameter $x = 50$ to represent small particles. In the GOM1 result, the haloes at scattering angles of 22° and 46° and peaks at 160° and 180° are clearly seen. The P_{11} results calculated by the GOM2 and FDTD methods agree overall: the 22° and 46° halos disappear, and the back-scattering peak is spread over a wide interval. From these results, we conclude that GOM2 can effectively calculate the phase function P_{11} of hexagonal ice crystals when x is ~ 50 , whereas GOM1 cannot. Note that in the GOM1 computation, the externally reflected and refracted rays contribute to the far field only in the direction determined by Snell's law. As a result, fluctua-

Fig. 2 Comparison of the phase function (P_{11}) calculated by GOM2 ($\Delta x = 1$), GOM1, and FDTD for 3D randomly oriented hexagonal ice crystals where $x = 50$, $L/2R = 1.7$, and $\lambda = 1.38 \mu\text{m}$.

tions often appear in P_{11} with respect to the scattering angle. In this study, the vector normal to the surface $\mathbf{n}_s$ is tilted randomly by $\sim 1^\circ$ around its original direction for each reflection and refraction event in the GOM1 calculation to reduce such fluctuations.

We next examined the sensitivity of the GOM2 calculation accuracy to the ray spacing Δx (Fig. 3). We compared P_{11} and $-P_{12}/P_{11}$ calculation results among $\Delta x = 1, 4$, and 16 , which correspond to $x/50$, $x/12.5$, and $x/3.1$, respectively. The results show that the GOM2 computation can be performed without noticeable degradation of accuracy even with ray spacing Δx as large as $\sim x/10$ (Fig. 3). The calculation with $\Delta x = 1$ for 140 random orientations of a particle took several hours of CPU time on a typical workstation (Dell Precision 690, Xeon/Intel 3.00 GHz in this study). As expected, the CPU times for $\Delta x = 4$ and 16 were approximately $1/16$ and $1/256$, respectively, of the CPU time required for $\Delta x = 1$.

We then compared P_{11} as calculated by GOM2 and

Fig. 3 (a) The phase function P_{11} calculated by GOM2 for 3D randomly oriented hexagonal ice crystals with $x = 50$, $L/2R = 1.7$, and $\lambda = 1.38 \mu\text{m}$. The influence of ray spacing is examined for $\Delta x = 1$, $\Delta x = 4$, and $\Delta x = 16$. (b) Same as (a) but for the degree of linear polarization ($-P_{12}/P_{11}$).

Fig. 4 Comparison of the phase function P_{11} calculated by GOM2 ($\Delta x = 50$) and GOM1 for 3D randomly oriented hexagonal ice crystals with $x = 800$, $L/2R = 1.7$, and $\lambda = 1.38 \mu\text{m}$.

GOM1 for particles with a large size parameter, $x = 800$, with ray spacing $\Delta x = 50$ ($= x/16$) (Fig. 4). At this large size parameter, the P_{11} calculation results are similar between GOM2 and GOM1.

4. Conclusions

The computational efficiency of GOM2 is improved considerably, without noticeable degradation of the accuracy of the phase matrix calculation, by using a parallelogram as the fundamental surface area element for the integral of the phase of the wave. The method presented here is particularly useful in the size parameter range of $50 < x < 200$ where the GOM1 and the FDTD methods are not efficient. It can also be applied to the calculation of the scattering matrix for concave particles such as Voronoi aggregates (Ishimoto *et al.*, 2012); hence, use of this algorithm can improve the processing of remotely sensed light scattering data from nonspherical particles such as mineral dust and ice cloud particles.

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Appendix

Integral of the phase of a wave over the parallelogram

We outline the calculation of the integral of the phase of a wave over a parallelogram $F = \int_{S_{i,p}} e^{ik\{(f(\mathbf{r}') - f(\mathbf{r}'_p)) - \mathbf{n}_r \cdot (\mathbf{r}' - \mathbf{r}'_p)\}} dS$.

First, the coordinate axes are translated so that the center

Fig. A1 The coordinates and phase of the wave at the center and the vertices of the parallelogram after translation and rotation of the coordinate axes. The parallelogram is in the x - y plane and its center is at the origin.

of the parallelogram $S_{i,p}$ coincides with the origin point in the Cartesian coordinate system. By replacing $f(\mathbf{r}') - f(\mathbf{r}'_p)$ and $\mathbf{r}' - \mathbf{r}'_p$ with $f(\mathbf{r}'')$ and $\mathbf{r}''$, F is expressed as $\int_{S_{i,p}} e^{ik\{f(\mathbf{r}'') - \mathbf{n}_r \cdot \mathbf{r}''\}} dS$.

Next, the coordinate axes are rotated so that the parallelogram is in the x - y plane and two edges of the parallelogram are parallel to the y axis (Fig. A1). After the rotation, F is expressed as $\int_{S_{i,p}} e^{ik\{f(\mathbf{r}'') - \mathbf{n}_r \cdot \mathbf{r}''\}} dS$, where $\mathbf{n}_r = [\tilde{n}_x \ \tilde{n}_y \ \tilde{n}_z]^T$ is the direction of light scattering in the new coordinate system.

The phase of the wave inside the parallelogram can be expressed by $f(\mathbf{r}) = f_x x + f_y y$, where the coefficients f_x and f_y are obtained by solving a set of equations, for example, $f^{(4)} = f_x x^{(4)} + f_y y^{(4)}$ and $f^{(1)} = f_x x^{(1)} + f_y y^{(1)}$. If we define $p_x \equiv k(f_x - \tilde{n}_x)$ and $p_y \equiv k(f_y - \tilde{n}_y)$ then $k\{f(\mathbf{r}) - \mathbf{n}_r \cdot \mathbf{r}\}$ is given by $f_x x + f_y y$. The integral of the phase can now be expressed as $F = \int_{-a}^a \int_{cx-b}^{cx+b} e^{i(p_x x + p_y y)} dy dx$ where the parameters a , b , and c are, for example, $a = x^{(4)}$, $b = (y^{(4)} + y^{(1)})/2$, and $c = (y^{(4)} - y^{(1)})/(x^{(4)} - x^{(1)})$. It is now straightforward mathematics

to obtain the final expression $F = 4ab \frac{\sin(p_x b)}{p_x b} \frac{\sin\{(p_y + p_x c)a\}}{(p_y + p_x c)a}$.

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短報

非球形粒子散乱計算における幾何光学積分の効率的手法

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非球形粒子の散乱特性を計算する幾何光学積分法において、積分素面を平行四辺形で表現し光線の位相差を考慮して積分を行うことにより、計算精度を大きく損なうことなく計算効率が向上することを示した。サイズパラメータが 50 以下の粒子の計算が可能な FDTD 法とサイズパラメータが 200 以上の粒子に適用が可能な簡便な幾何光学手法の間が埋まり、氷晶雲や鉱物性エアロゾルの衛星観測データ解析の高度化等への活用が期待できる。