Numerical computation of the scattering properties of large arbitrary shaped particle by MLFMA and VCRM

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Abstract

The Surface Integral Equation (SIE) with Multilevel Fast Multipole Algorithm (MLFMA) is an efficient full wave numerical method for computing scattering properties by a large particle of arbitrary shape. It can be well parallelized with Message Passing Interface (MPI) on a memory distributed computer system and obtain accurate results for relatively large particles with size parameter reach up more than 500 efficiently. The recently developed high frequency asymptotic method, called Vectorial Complex Rays Model (VCRM) is proved to be especially suitable for computing scattering by a large particle of arbitrary shape. Accuracy of these two methods on spherical particles has been well studied by comparisons with the rigorous Lorenz-Mie theory (LMT) but less on non spherical particles. In this paper, scattering properties by large elliptical particles with different aspect ratios are computed by using both the SIE with MLFMA and the VCRM. Good agreements between these two methods validate accuracy of them and show great capability of the SIE with MLFMA at the same time. At last, scattering by a large irregular shaped particle is also computed by the SIE with MLFMA.

1 Introduction

In various research fields, we need to solve light scattering problems by arbitrary particles, such as atmospheric radiative transfer, bio-optics and climatology. In fact, particles encountered in nature (ice crystals, dust aerosols, raindrops and cells in biophysical systems) are often irregularly shaped and have a wide range of sizes. In order to achieve accurate and efficient results, various methods are developed which can be classified in three categories: rigorous methods, numerical methods and approximate methods. LMT [1-2] is a rigorous method and has been widely used in light scattering problems by homogenous spheres, layered spherical particles and infinitely long cylinders. However, it is difficult to treat the scattering properties by realistically complex shaped particles. For this reason, numerical methods such as the discrete dipole approximation (DDA) [3], the finite difference time-domain technique (FDTD) [4, 5] and the T-matrix method [6, 7] have been developed and are used in practice. But for all these numerical methods, the computational requirements increase quickly with size, such that they become inapplicable when the particle size is extremely large. So the development of the efficient algorithm is crucial for each method.

SIE is one of the robust and accuracy full-electro-magnetic wave methods for scattering of an arbitrary shaped particle. In this paper, the multilevel fast multipole algorithm (MLFMA) [8, 9, 10] based on the SIE was employed to reduce both the time and the memory complexity. To further improve the efficiency of MLFMA, MPI [8, 9] on a memory distributed computer system is used. This algorithm is of high accuracy and has capability to deal with arbitrary shaped particles of size parameter as large as 500.

Besides the above mentioned methods, various approximate approaches have been developed to obtain scattering properties of large particles, such as geometrical optics (GO) [11] and physical optics [12, 13]. These approaches are applicable when the size of the particle is much larger than the wavelength of the incident beam. VCRM [14, 15] developed by Ren et al. is suitable to deal with the scattering of irregular large particles of smooth surface. In VCRM, the waves are described by vectorial complex rays. By introducing a new property: the curvature of the wavefront and using the vectors in ray tracing, the method is more accurate and flexible than classical GO for arbitrary shaped particles. The accuracy of VCRM has been investigated by comparisons with LMT for spherical particles. It has been successfully applied to the calculation of scattering by ellipsoidal particles [14, 15, 16] and infinite elliptical cylinders [17, 18]. Various new physical phenomena in light scattering by non-spherical particles have been revealed.

Both MLFMA and VCRM have achieved good agreement with LMT on spherical particles. But there is no further discussion between these two methods for scattering by non spherical particle. Comparison between the MLFMA and VCRM for elliptical particles will be presented in this paper, along with computed results of scattering properties of a large complex shaped particle.

The body of the paper is organized as follows: VCRM and MLFMA will be briefly presented in Section 2. The numerical accuracy and capability of the two methods will be discussed in Section 3 with the computed results.

2 Theoretical basis

2.1 Vectorial Complex Ray Model – VCRM

Vectorial Complex Ray Model (VCRM) is based on the geometrical optics but a new property – the wave front curvatures – is introduced. This property permits to account the wavelike behaviour of light, the convergent or divergent of the wave. Thus, a ray is described not only by its amplitude, phase, polarization, propagation direction, but also by the curvatures of the wave front of the wave that the ray presents. All these features evolve at each interaction of ray with the particle surface. Particularly, the curvature matrix of the emergent wave after each interaction of the ray with the particle surface is calculated according to the curvature matrix of the incident wave and the local curvature of the particle surface by using the wave front equation.

The significant benefits of this approach are: a). the wave properties are integrated in the ray model; b). the divergence/convergence of the wave is deduced by the wave front curvature; c). the phase shift due to the focal lines is determined directly by the curvature of the wave front.

2.2 Multilevel Fast Multipole Algorithm – MLFMA

We consider the electromagnetic scattering problem of a homogeneous particle of any shape illuminated by a wave (Figure. 1). Let S be the surface of particle, (ε_1,μ_1) and (ε_2,μ_2) the permittivity and permeability in the outer and inner regions of the particle respectively. The scattered electromagnetic filed at any point can be obtained by the equivalent electric and magnetic currents $\mathbf{J}$ and $\mathbf{M}$ on the surface of the particle which are determined by the electric and magnetic field integral equations according to [19]:

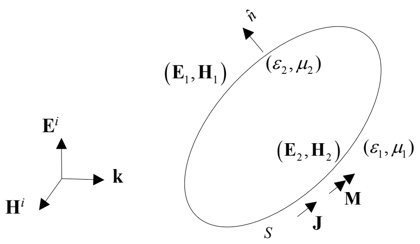

Figure 1 Sketch map of homogeneous particle

$$\mathbf{E}_1 - Z_1\mathbf{L}_1(\mathbf{J}) + \mathbf{K}_1(\mathbf{M}) = \mathbf{E}^i \qquad (1)$$

$$\mathbf{H}_1 - Z_1^{-1}\mathbf{L}_1(\mathbf{M}) - \mathbf{K}_1(\mathbf{J}) = \mathbf{H}^i \qquad (2)$$

$$\mathbf{E}_2 - Z_2\mathbf{L}_2(\mathbf{J}) + \mathbf{K}_2(\mathbf{M}) = 0 \qquad (3)$$

$$\mathbf{H}_2 - Z_2^{-1}\mathbf{L}_2(\mathbf{M}) - \mathbf{K}_2(\mathbf{J}) = 0 \qquad (4)$$

where $Z_1 = \sqrt{\mu_1/\varepsilon_1}$, $(\mathbf{E}^{\mathrm{i}},\mathbf{H}^{\mathrm{i}})$ denote the incident fields, and the operators and are defined as:

$$\mathbf{L}_l\{\mathbf{X}\}(r) = jk_l\int\left[\mathbf{X}(r') + \frac{1}{k_l^2}\nabla\left(\nabla'\cdot\mathbf{X}(r')\right)\right]G_l(r,r')dr' \qquad (5)$$

$$\mathbf{K}_l\{\mathbf{X}\}(r) = \int dr'\mathbf{X}(r')\times\nabla' G_l(r,r') \qquad (6)$$

Following the Combined Tangential Formulation (CTF) [5] we obtain following equations which are free of internal-resonance problem.

$$\hat{t}\cdot[\mathbf{L}_1 + \mathbf{L}_2]\{\mathbf{J}\} - \hat{t}\cdot[Z_1^{-1}\mathbf{K}_1 + Z_2^{-1}\mathbf{K}_2]\{\mathbf{M}\} = -Z_1^{-1}\hat{t}\cdot\mathbf{E}^i(\vec{r}) \qquad (7)$$

$$\hat{t}\cdot[Z_1\mathbf{K}_1 + Z_2\mathbf{K}_2]\{\mathbf{J}\} + \hat{t}\cdot[\mathbf{L}_1 + \mathbf{L}_2]\{\mathbf{M}\} = -Z_1\hat{t}\cdot\mathbf{H}^i(\vec{r}) \qquad (8)$$

where $\hat{t}$ is a tangential vector of the surface.

In the implementation, the dielectric surface is meshed by triangular patches. Within each patch, Rao, Wilton and Glisson (RWG) vector basis functions [19] are applied to expand the unknown equivalent electric and magnetic currents. With using the standard Galerkin's method, a complete matrix equation system can be obtained. The required matrix-vector multiplications are performed efficiently with the multilevel fast multipole algorithm (MLFMA) which can reduce both the time and the memory. MPI parallelization is applied to further improve the efficiency of MLFMA.

3 Numberical results and discussion

In this section, we just show numerical results on a sphere with radius of 50 μm and an ellipsoid having the same volume. Detailed computation information together with other results including scattering by an irregular shaped large particle will be presented during the LIP-2014 conference.

The elongation of the particles is characterized through a couple of aspect ratios, defined as $\kappa_1 = c/a$, $\kappa_2 = c/b$ with *a*, *b* and *c* denoting the semi-axes of the ellipsoid along the *x*, *y* and *z* directions respectively. We have $\kappa_1 = \kappa_2 = 1.0$ for sphere, $\kappa_1 = \kappa_2$ for spheroids and $\kappa_1 \neq \kappa_2$ for ellipsoids.

The first example is a spherical water droplet (*m*=1.33) with radius of 50 μm. The incident plane wave is polarized in *x* direction with wavelength of 0.785 μm. The scattering intensity in *xz* plane computed by MLFMA together with those obtained by LMT and VCRM are plotted in figure 2. It can be seen from this figure that both VCRM and MLFMA agree well with LMT. But there are slit differences between VCRM and LMT when the scattering angle ranged from about $60°\sim120°$ while MLFMA agrees with LMT well. This is because in VCRM the surface wave effect has not yet taken into consideration. But the overall accuracy of VCRM is good.

The next example is an ellipsoid with *a*=35.47, *b*=49.66, *c*=70.95 i.e. $\kappa_1 = 2.0$ and $\kappa_2 = 1.43$. This ellipsoid has the same volume of the sphere with radius of 50 μm. The computed scattering diagrams in *xz* plane computed by VCRM and MLFMA are shown in figure 3. As expected, these two results agree with each other, but a significant difference is observed for the scattering angles range from about $60°\sim120°$. Also, the difference is due to the surface wave effect and the diffraction effect near rainbow angle.

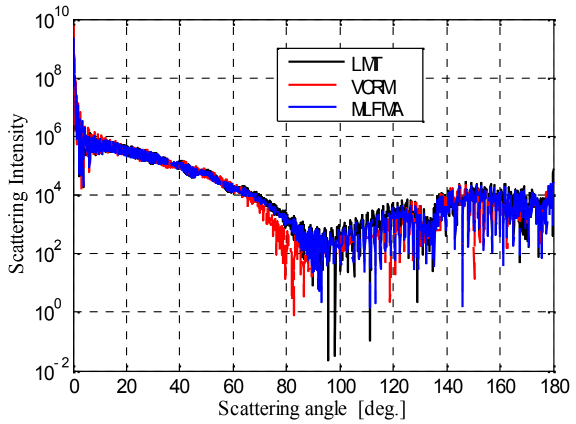

***Figure 2** Comparison of scattering diagrams computed by LMT, VCRM and MLFMA for a water droplet of refractive index m=1.33 and radius 50 μm illuminate by a plane wave of wavelength 0.785 μm for horizontal polarization.*

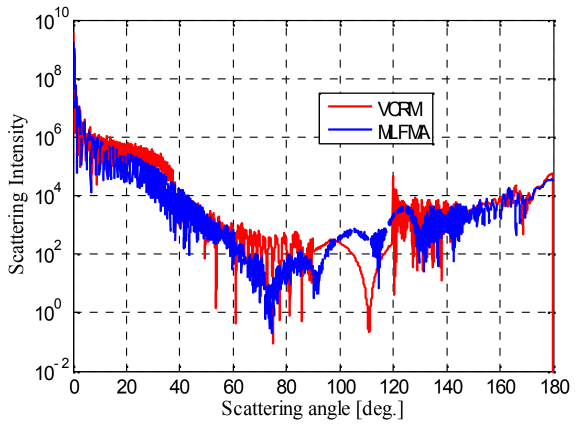

***Figure 3** Comparison of scattering diagrams computed by VCRM and MLFMA for an ellipsoidal water droplet with* $\kappa_1 = 2.0$ *and* $\kappa_2 = 1.43$ *having the same volume of a sphere with radius 50 μm. Other parameters are the same as in Figure 2.*

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