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Computation of scattering matrix elements of large and complex shaped absorbing particles with multilevel fast multipole algorithm

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ABSTRACT

Light scattering properties of absorbing particles, such as the mineral dusts, attract a wide attention due to its importance in geophysical and environment researches. Due to the absorbing effect, light scattering properties of particles with absorption differ from those without absorption. Simple shaped absorbing particles such as spheres and spheroids have been well studied with different methods but little work on large complex shaped particles has been reported. In this paper, the surface Integral Equation (SIE) with Multilevel Fast Multipole Algorithm (MLFMA) is applied to study scattering properties of large non-spherical absorbing particles. SIEs are carefully discretized with piecewise linear basis functions on triangle patches to model whole surface of the particle, hence computation resource needs increase much more slowly with the particle size parameter than the volume discretized methods. To improve further its capability, MLFMA is well parallelized with Message Passing Interface (MPI) on distributed memory computer platform. Without loss of generality, we choose the computation of scattering matrix elements of absorbing dust particles as an example. The comparison of the scattering matrix elements computed by our method and the discrete dipole approximation method (DDA) for an ellipsoid dust particle shows that the precision of our method is very good. The scattering matrix elements of large ellipsoid dusts with different aspect ratios and size parameters are computed. To show the capability of the presented algorithm for complex shaped particles, scattering by asymmetry Chebyshev particle with size parameter larger than 600 of complex refractive index $m = 1.555 + 0.004i$ and different orientations are studied.

1. Introduction

In atmospheric aerosols researches, we need to study optical properties of dust particles with absorption derived from large desert and semiarid regions, which play an important role in climate forcing assessments, radiative forcing and energy balance [1,2]. Experimental measurements revealed that the majority of the particles are submicron sized [3–6]. D'Almeida et al. have studied the distributions of mineral dust of Saharan and suggested that the size range of mineral particles from 0.01 μm up to 100 μm should be taken in consideration [7]. So we may admit that the size parameter of the dust varies from less than a wavelength to hundreds of wavelengths in the visible range, which make it a challengeable problem. In the past several decades, the scattering and absorption of solar radiation by absorbing mineral dust have been a

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major focus by means of computation [8–14]. Because the mineral particles have various morphology, composition and size, the limitation of detailed knowledge of absorbing dust particles with complex shapes by computation still exists.

Usually, researchers consider the mineral particles as homogenous spheres to gain exact analytical solution by using the classical Lorenz–Mie theory (LMT) [15]. Dubovik et al. proposed the use of oriented spheroids for modeling dust particles and computed light scattering with the *T*-matrix method and the approximated geometric-optics-integral-equation method [8,9,16]. Bi et al. demonstrated by an improved geometric optics method [17] that the ellipsoid model is better than the spheroid model for simulating dust particle optical properties. With respect to the morphological irregularity of dust particles, the shape of Gaussian random sphere is assumed by Muinonen et al. [18] and the ray optics approximation method is used for mineral dusts with size much larger than the wavelength [10,16]. Liu developed concave fractal polyhedral models to compute the single-scattering properties and combined the pseudospectral time-domain method with the improved geometric optics (GO) to enlarge the size parameter range from the Rayleigh to the geometric-optics regimes [11]. Beside these computation methods, the finite difference time-domain technique (FDTD) [13,19] is also applicable in practice.

In all aforementioned work, some of them may achieve a big progress to cover a large size parameter range but the accuracy is often not sufficient; the others can get accurate solutions but without higher degrees of nonsphericity or the particle size is severely limited. For example, LMT is a rigorous method and has been widely used in light scattering metrology [15,20], but it can only be used for regular shape particles such as spheres, spheroids, and infinite cylinders. For this reason, accurate numerical methods such as DDA (Discrete Dipole Approximation) [21,22], FDTD [13,19], and *T*-matrix method [14] are usually applied in practice [23]. In principle, these methods can be applied to arbitrary shaped particles, but in practice the calculable particle size is often limited and the size parameter hardly reaches 500 even for a refractive index near unity, because the computation requirements increase quickly with size parameter. Approximate approaches, such as geometrical optics and physical optics, can obtain acceptable results when the size of the particle is much larger than the wavelength of the incident wave. Therefore, the light scattering by small dust particles or simple shaped large particles is well documented, but the computation of scattering properties of large absorbing particle with complex asymmetric shape still faces great challenges [23,24]. The development of accurate and efficient algorithms for the scattering by large particles of complex geometry is essential for many applications. There are two possible ways to reply this demand: (1) improvement of approximate methods, such as Vectoriel Complex Ray Model (VCRM) recently developed by Ren et al. [25,26]. By introducing a new property – the wave front curvature in the ray model, VCRM permits us to count the divergence/convergence of waves on the curved surface of an arbitrary shape particle of smooth surface, the phase due to the focal lines and finally the interference of all emergent waves and (2) enhancement of numerical approaches, such as MLFMA will be undertaken in this paper. VCRM, even not an exact solution, will be used to validate the MLFMA code.

Among numerical methods, SIE is proved to be a robust and accurate full wave methods for the scattering of arbitrary shaped particles [27,28] and will be applied in this paper. When SIE is used, the multilevel fast multipole algorithm (MLFMA) should be employed to reduce both the time and the memory complexity [29–31]. To improve the efficiency of MLFMA, various approaches of MPI on a memory distributed computer system are developed [32,33,36], among which a hybrid MPI and OpenMP parallelized MLFMA approach is proved to be capable of improving the load-balance and scalability by combing processes and threads flexibly, hence to depress the load imbalance in the pure MPI parallel MLFMA [36]. This hybrid parallelized approach has been applied to the prediction of the radiation pressure force, torque and stress of laser beam on non-spherical particles [37,38] and to the validation of VCRM [39]. It will be employed here with several improvements to enhance further its performance, especially for the treatment of absorbing particles. We will show that with this approach we can deal with arbitrarily shaped large absorbing particles. As a typical example, the scattering matrix of a complex Chebyshev particle of size parameter equal to 600 and refractive index $m = 1.555 + 0.004i$ is studied to show the great capability of the presented approach.

The body of the paper is organized as follows. Section 2 is a brief introduction to SIE with MLFMA. The numerical accuracy and capability of MLFMA for different absorbing mineral dusts will be shown in Section 3. The last section is devoted to the conclusions.

2. Theoretical basis

The theoretical fundamentals of SIE with MLFMA can be found in the monograph [40] and the references therein. We give in this section a brief description of the method to help the understanding of the sketch of our approach and the improvements we made in this paper.

The scattering problem of an arbitrarily shaped homogeneous body undertaken in this paper is illustrated in Fig. 1. The boundary S of the dielectric body is taken as the equivalent surface. $\hat{\mathbf{n}}$ is the unit vector normal to S and points toward outside. The permeability and permittivity

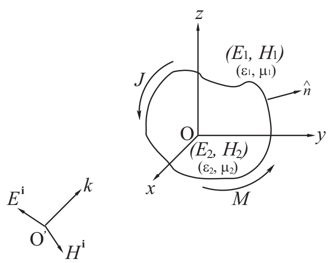

Fig. 1. Sketch of three dimensional homogeneous dielectric body.