A SCATTERING SIMULATION MODEL FOR NONSPHERICAL AEROSOL PARTICLES BASED ON PARALLEL FDTD SCHEME

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ABSTRACT:

In order to simulate the scattering properties of nonspherical aerosol particles in visible and near infrared band precisely and efficiently, a scattering computation model for aerosol particles based on parallel FDTD (Finite Difference Time Domain) is developed. The basic principle of FDTD is introduced, and a new parallel computation scheme for FDTD is proposed, and is realized by MPI repeated non-blocking communication technique. The FDTD scattering model is validated against Lorenz-Mie theory and T Matrix method. Simulation results show that, the scattering properties obtained parallel FDTD scattering model are qualitatively in good agreement with the T matrix method and Lorenz-Mie theory, validating the accuracy of our model. The relative simulation error of Müeller is slightly larger in forward scattering directions than that in backward directions for particles with small size parameter, while for large particles, the result is opposite.

1. INTRODUCTION

In the visible and near-infrared waveband, the uncertainty remaining the light scattering properties still an important factor limits the simulation accuracy of atmospheric radiative transfer). The IPCC report pointed it out that(IPCC, 2007), though the direct radiative forcing of aerosol was improved, the ambiguity of the estimation are still remarkable due to the lack of adequate knowledge of the optical properties of nonspherical aerosol particles and ice crystals (Liou, 2003; Liou et al., 2013). Owning to this reason, the light scattering computational technique for particles with irregular shape has become a hotpot in the field of radiative transfer (Herman et al., 2005; Yang et al., 2015; Hu et al., 2014).

Many scattering computational models are established to calculate the light scattering properties, such as T Matrix Method (Mishchenko and Travis, 1998), Discrete Dipole Approximation(DDA)(Draine, 1988) and the Finite Difference Time Domain (FDTD) (Mishchenko et al., 2000; Yang and Liou, 1995). For T Matrix method, the light scattering process is solved by the extended boundary condition method (EBCM) (Mishchenko et al., 2000), due to the difficulty in surface integral process for particles with irregular shape, this model is mainly applied to rotational symmetrical particles (like spheroid and cylinder, et al.). In DDA, the nonspherical particle is discretized by a certain number of dipoles, and the simulation of the light scattering process is converted into the solving of the polarization states of these dipoles. Owning to the advantages of its principle, DDA can calculate the light scattering by particles with arbitrary shape and complex compositions. However, in its computational process, large matrix equation is needed to be solved, which will be time-consuming and unstable as the particle size and refractive index become large. For this reason, DDA is mainly suitable for “optical soft” particles or particles with small size. Compared with DDA, FDTD can overcome the computational instability for particles with large refractive index, and become a popular calculation model for light scattering simulation(Yang and Liou, 1995). In the early time, the FDTD is only applied to particles with a size parameter smaller than 40 due to the laggard computer technology. Yet as the development of the supercomputer, the limitation is not existed again, and FDTD can be applied to light scattering simulation of large particle by resorting to parallel computational technique.

In this paper a parallelized FDTD scattering model is established based on MPI (Message Passing interface) technique. Our paper is organized as follows, in section 2, the principle of FDTD is introduced, and then the parallel computational scheme is designed in section 3. At last, a brief conclusion is given.

2. THE BASIC PRINCIPLE OF FDTD

Light propagation in the medium can be totally described by the Maxwell curl equations, which can be written as:

$$\nabla \times \mathbf{H} = \varepsilon \frac{\partial \mathbf{E}}{\partial t} + \sigma \mathbf{E}; \tag{1}$$

$$\nabla \times \mathbf{E} = -\mu \frac{\partial \mathbf{H}}{\partial t} - \sigma_m \mathbf{H}. \tag{2}$$

Where, $\mathbf{E}$ and $\mathbf{H}$ are the intensity vectors of the electric and magnetic field, ε and μ are the permittivity and permeability of the medium; σ and σ_m represent the electric conductivity and magnetic conductivity, respectively. ε and σ can be calculated from the complex refractive index $m = m_r - jm_i$ by

$$\varepsilon = \varepsilon_0 (m_r^2 - m_i^2), \quad \sigma = 2\omega m_r m_i \varepsilon_0; \tag{3}$$

where, ω is the angular frequency, ε_0 is the permittivity of vacuum.

In the implementation of FDTD, the space and time derivatives of the electric and magnetic fields are approximated using central difference method so that they bound computational errors and ensure numerical stability of the algorithm. Hence, time is approximated by discrete time steps, and a marching-in-time procedure is used to track the evolution of the fields from their initial values at the initial time t=0. The basic principle of FDTD is introduced as follows:

The establishing of the iterative formulation. In Cartesian coordinate system, the Maxwell curl equation is firstly converted to the scale one, then the equations of each field component is discretized in time and space by using central difference approximation, after some simplifications, the step-by-step iteration equation for the electromagnetic field can be obtained. Without loss of generality, we take E_x and H_x as the example to show the iteration equations, written as

$$E_x^{n+1}\left(i+\frac{1}{2},j,k\right) = CA(m)\cdot E_x^{n}\left(i+\frac{1}{2},j,k\right) + CB(m)\left[\frac{H_z^{n+1/2}\left(i+\frac{1}{2},j+\frac{1}{2},k\right) - H_z^{n+1/2}\left(i+\frac{1}{2},j-\frac{1}{2},k\right)}{\Delta y} - \frac{H_y^{n+1/2}\left(i+\frac{1}{2},j,k+\frac{1}{2}\right) - H_y^{n+1/2}\left(i+\frac{1}{2},j,k-\frac{1}{2}\right)}{\Delta z}\right] \tag{4}$$

$$H_x^{n+1/2}\left(i,j+\frac{1}{2},k+\frac{1}{2}\right) = CP(m)\cdot H_x^{n-1/2}\left(i,j+\frac{1}{2},k+\frac{1}{2}\right) + CQ(m)\left[\frac{E_z^{n}\left(i,j+1,k+\frac{1}{2}\right) - E_z^{n}\left(i,j,k+\frac{1}{2}\right)}{\Delta y} - \frac{E_y^{n}\left(i,j+\frac{1}{2},k+1\right) - E_y^{n}\left(i,j+\frac{1}{2},k\right)}{\Delta z}\right] \tag{5}$$

Where, m=(i+1/2, j, k) is the discrete coordinates of the field components; Δx, Δy and Δz are the discrete lengths along x, y and Z axes, respectively, Δt is the discrete time interval. In Eq.(4), *CA* and *CB* are the iterative coefficients for the electric field, which can be calculated by

$$CA(m) = \frac{2\varepsilon - \sigma\Delta t}{2\varepsilon + \sigma\Delta t}, \; CB(m) = \frac{2\Delta t}{2\varepsilon + \sigma\Delta t}. \tag{6}$$

In the iterative equations of the magnetic field, the coefficients *CP* and *CQ* can be calculate by the following equations, given as

$$CP(m) = \frac{2\mu - \sigma_m\Delta t}{2\mu + \sigma_m\Delta t}, \quad CQ(m) = \frac{2\Delta t}{2\mu + \sigma_m\Delta t}; \tag{7}$$

In the discrete scheme of FDTD, the spatial distribution of electromagnetic field components at each discrete grid satisfies the Yee cell. The electric and magnetic fields are sampled alternately in time sequence, and the sampling interval is $\Delta t/2$ different from each other[27].

Stability condition of FDTD. FDTD model is an explicit difference scheme for Maxwell curl equations. In order to ensure the convergence of the iteration process, the time difference interval and the spatial gird size must satisfy Courant stability conditions, i.e. the following relations must be satisfied:

$$\Delta t \le \frac{1}{c\sqrt{\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} + \frac{1}{(\Delta z)^2}}}; \tag{8}$$

If the Yee is a cubic, namely, $\Delta x = \Delta y = \Delta z = \delta$, then the equation above can be simplified as

$$\Delta t \le \frac{1}{c\sqrt{3}\delta}. \tag{9}$$

Parallel Computing Framework of FDTD. The flow chart of parallel FDTD scattering model is shown in Figure 1. The process can be divided into three steps: task assignment and initialization, FDTD iteration of the electromagnetic field and particle scattering properties calculation. Task assignment is carried out by the main process, after the task is determined, the computational task is sent to each slaver process; particle scattering properties calculation is carried out by each process sub-region, and the data collection, processing and output are

3. THE PARALLIZATION OF FDTD

The basic principle of the parallel design scheme of FDTD is to divide the computational region into several sub-regions equally and distribute them to each process. The unification of the light scattering simulation is realized by data exchange and communication between processes on the partition plane. In this paper, the one-dimensional zoning model along the z-axis is applied to divide the computational domain.

carried out by the main process, besides, amplitude extraction and phase correction, near-far field transformation and scattering parameter calculation are also accomplished by the main process. The FDTD iteration of the electromagnetic field is the main part of the parallel design, its main task is to realize the iterative calculation of electromagnetic field components. In this part, MPI repetitive non-blocking parallel communication technique is used to the parallel computational design.

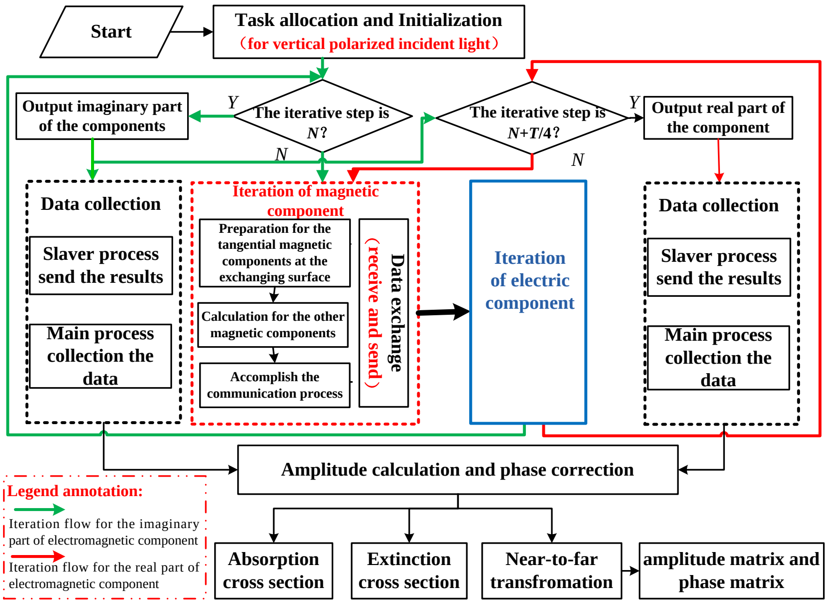


Figure 1. The basic flowchart of parallel FDTD computational model.

Design of data exchange scheme for connection surface. In the FDTD scattering model, the calculation of any field component requires four another adjacent field components, so in the iteration process, it is necessary to exchange the electromagnetic data on the sub-region junction surface. Considering the particularity of FDTD model, a parallel design scheme that only exchanges the magnetic field components is given.

Without loss of generality, the data exchange scheme of the K sub-region is illustrated as an example. As shown in Figure 2, the data exchange process can be divided into two steps: Firstly, the tangential magnetic field components H_x and H_y at K=K$_0$ on the left connecting surface are calculated and sent to process k-1. These data is mainly used for the calculation of the tangent of the right connecting surface in the k-1 sub-region. Furthermore, the tangential magnetic field components H_x and H_y at K=K$_1$ on the right surface are calculated and sent to the k+1 process, which is mainly used for the calculation of E_x and E_y components on the left connection surface of the k+1 process. At the same time, this process receives the tangential magnetic field component data of its left and right sides. In this scheme, the tangential electric field components E_x and E_y on both sides of the connection surface are need not to be exchanged. The reason is that the corresponding tangential electric field components E_x and E_y can be obtained on the basis of the magnetic field components after obtaining the tangential magnetic field components on the connection surface.

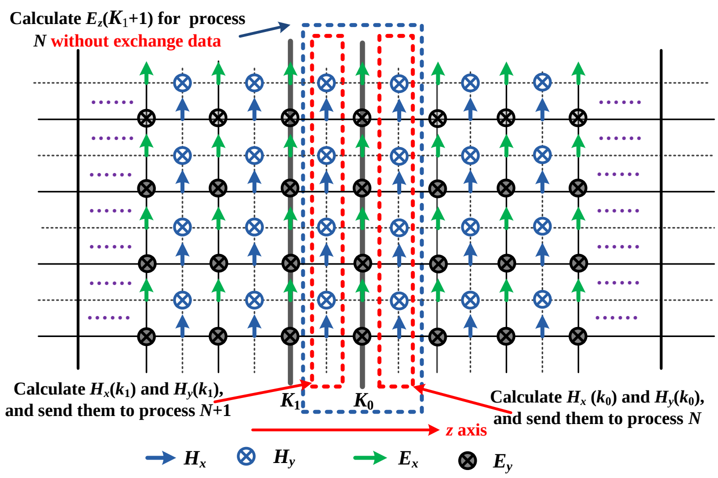


Figure 2. The data exchange scheme of the exterior surface for parallel FDTD scattering model

4. MODEL RESULT ANALYSIS AND VALIDATION

The parallelized FDTD scattering model is implemented based on FORTRAN and MPI software packages. In order to realize parallel computing of the programs, a parallel computing platform is built independently. This platform consists of four computers of the same type, which are connected by a Gigabit switch. The CPU of the computer is Intel i5 (3.1GHz). Next, the calculation accuracy and performance of the model are verified and analyzed.

The Müeller matrix validation for spheroid particle. Let incident light propagates parallel to Z axis, the light wavelength is set as λ=0.86μm, and discrete grid size in calculation domain is taken to be λ/40, the complex refractive index is taken as 1.414-0.00i, and the lengths of the rotational and horizontal axis are set as *a*=0.7μm and *b*=1.4μm, respectively. The Müeller matrix is calculated by FDTD and T matrix method, respectively, and the results are shown in Figure 3.

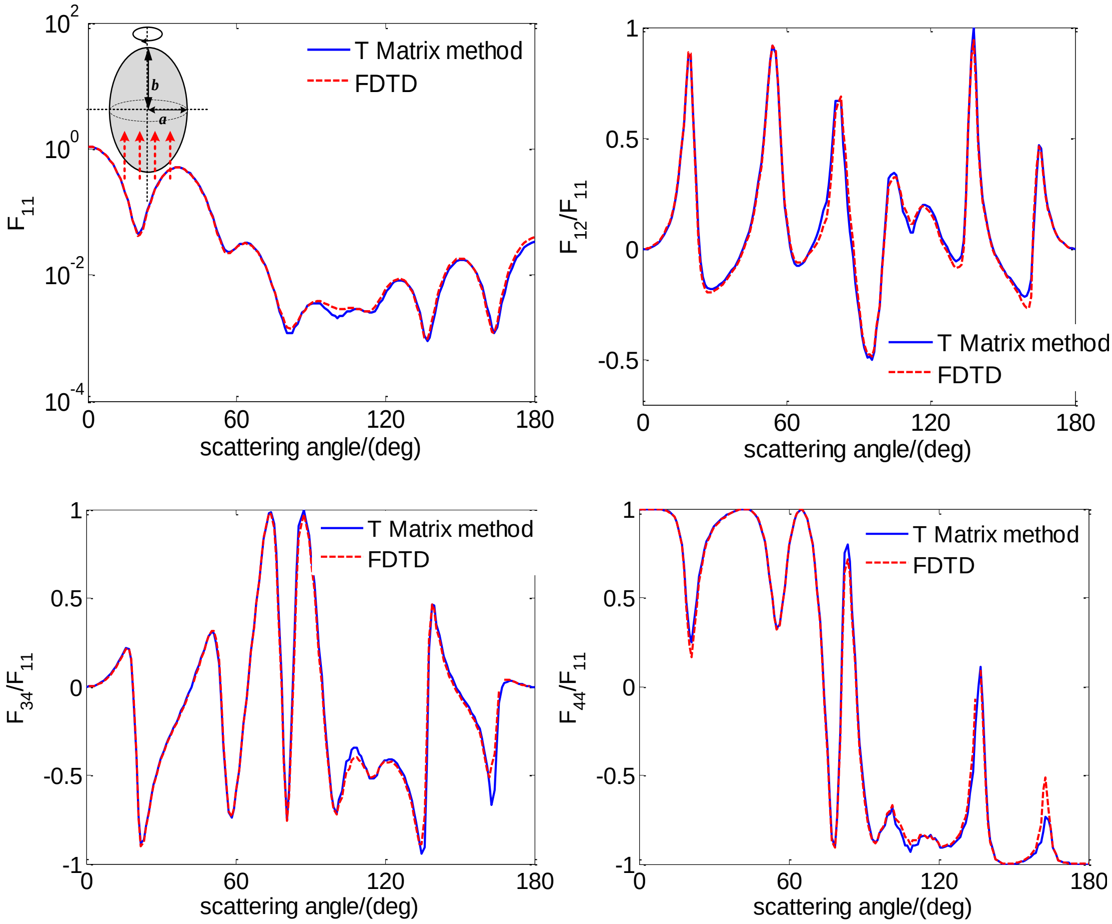


Figure 3. Comparison of the Müeller Matrix simulated by T Matrix method and parallel FDTD model for spheroid particle.

Overall, the Müeller matrix curve obtained by the FDTD model coincides with that simulated by T matrix method in the scattering angle range from 0° to 180°. In the forward scattering direction (0 ~90°), The average relative errors of F_{11}、F_{12}、F_{34} and F_{44} are only 3.1%, 4.2%, 3.3% and 3.5% respectively. In the backward scattering direction, the simulation accuracy of Müeller matrix is slightly lower, especially in the region where the matrix elements vary sharply with the scattering angle, the simulation curve of FDTD might deviate from the result of T matrix method.

The Müeller matrix validation for cylindrical particle. In this simulation, the incident light wavelength is taken as λ=0.86μm, the propagation direction of incident light, the discrete grid size and the complex refractive index of particles are set the same as those of spheroid particle. Setting the diameter and length of cylindrical particle as D=1.0 um and L=2.0 um, and taking the bottom surface of the particle perpendicular to the z-axis, the Müeller matrix is calculated by FDTD model and T-matrix method respectively. The results are shown in Figure 4.

From the figure, it can be seen that the simulation results of the two models are in good agreement, which verifies the accuracy of the model. Similar to the results of spheroid particle, the relative simulation error of FDTD in the backward scattering direction is larger than that in the forward scattering direction, especially in the scattering angle interval where the curve changes drastically. The consistency between the two models is slightly worse.

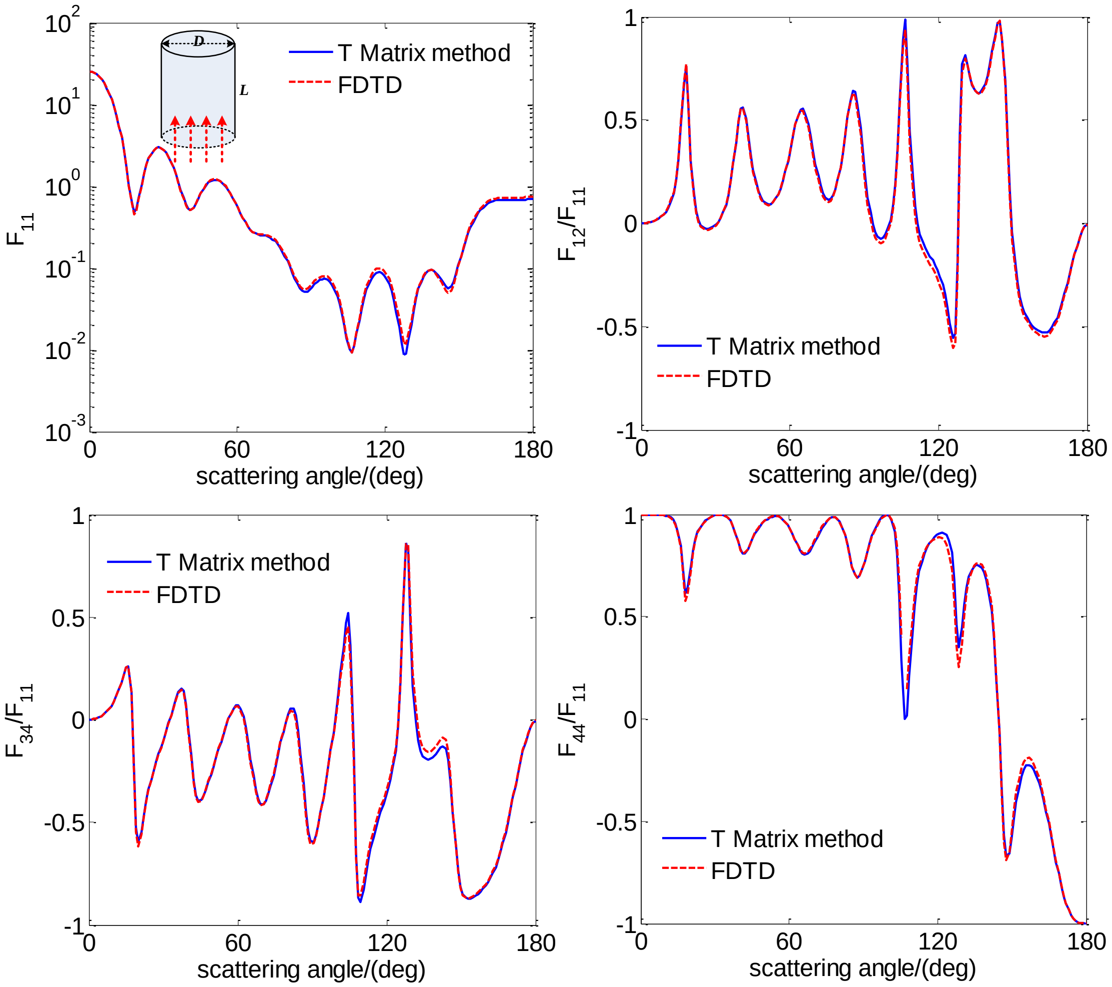
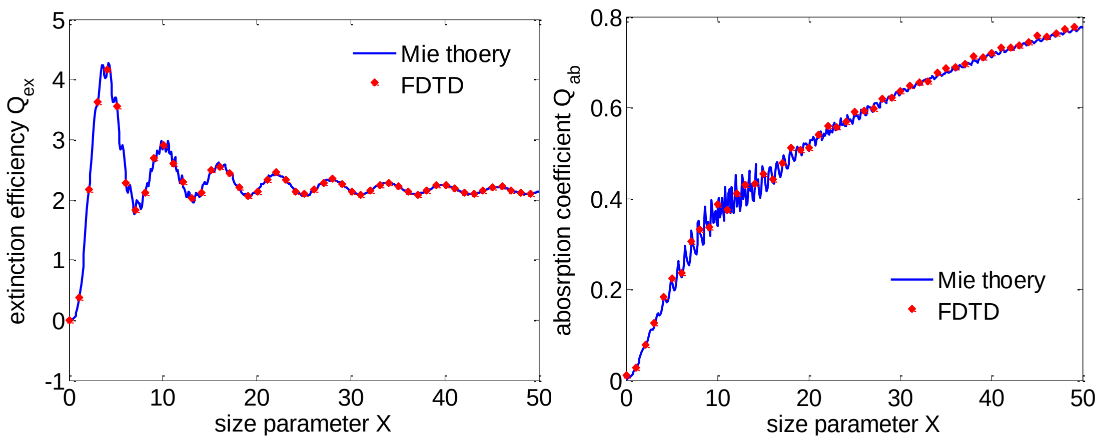


Figure 4. Comparison of the Müeller Matrix simulated by T Matrix method and parallel FDTD model for cylindrical particle.

The validation of integral scattering properties. In this comparison, the incident light wavelength is taken as 0.8um, the particle is set as a sphere with its size parameter X changes from 1 to 50, and the complex refractive index is set to be 1.33-0.005i. The integrated scattering parameters (extinction efficiency Q_{ex}, absorption efficiency Q_{ab} and single scattering albedo SSA) are simulated by FDTD and Mie scattering theory, the results are shown in Figure 5.

The results show that the integral scattering parameters obtained by the two models are in good agreement in the variation range of size parameter X, where the maximum simulation errors of extinction efficiency Q_{ex}, absorption efficiency Q_{ab} and single scattering albedo SSA are 3.63%, 4.67% and 0.5% respectively. In terms of error magnitude, the simulation accuracy of particle integral scattering parameters is higher than that of Müeller matrix.



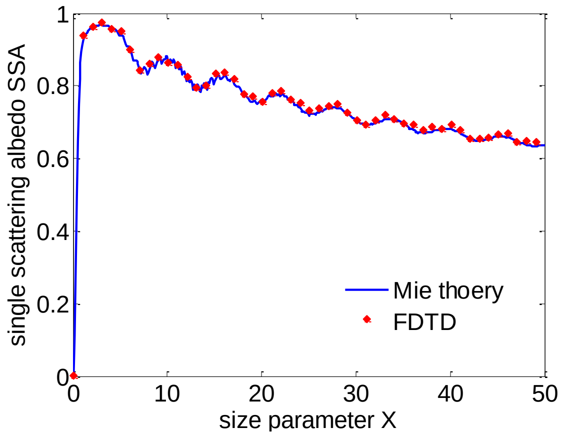


Figure 5. Comparison of the extinction coefficient, absorption coefficient and single scattering albedo simulated by Mie scattering theory and parallel FDTD method.

5. CONCLUSION

In order to simulate light scattering by nonspherical aerosols efficiently, a parallelized FDTD scattering model is proposed. The basic principle of FDTD is briefly introduced, and the FDTD is parallelized by MPI repetitive non-blocking communication technique. Finally, the calculation accuracy of the model is verified and analyzed. The results show that the results of parallel FDTD scattering model and T-matrix method are in good agreement, which verifies the accuracy of the model. The simulation accuracy of forward scattering direction of Müeller scattering matrix is higher than that of backward scattering direction. In the scattering angle range where the Müeller matrix curves changes sharply, the modeling accuracy of FDTD is relatively lower. The reasons is that FDTD is an approximate calculation, there is a step error in particle shape construction process.

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