A parallelized Pseudo Spectral Time Domain Model for the light scattering simulation for aerosol particles with irregular shapes and inhomogeneous compositions

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To improve the precision of climate modeling and atmospheric remote sensing, radiative transfer models (RTM) that can accurately calculate the radiation transferred through the atmosphere with aerosols and cloud are required [1–3]. As the fundamental input parameters for the radiative transfer simulation, the light scattering properties of aerosols (especially these in solar spectrum) should be accurately modeled [4–7]. However, due to the irregular shapes and inhomogeneous compositions of aerosol particles (like mineral dust, soot, etc.), their light scattering processes have not been adequately understood, and substantial uncertainties still remain in their optical properties [8,9]. To simplify the scattering process of aerosol particles, in the RTMs widely used now, nonspherical aerosol particles are usually taken as the spherical ones with equivalent volume or surface area, which will definitely decrease the computational accuracy of radiative transfer [6,10–12]. Many researchers have also found that the nonspherical shapes of aerosol particles exert a significant influence on the polarized components of radiation [6,9,13].

To improve the modeling accuracy of radiative transfer, the scattering properties of aerosol particles with irregular shapes and inhomogeneous compositions should be accurately simulated. To this end, a light scattering model for nonspherical particles is established based on the Pseudo Spectral Time Domain Model (PSTD) technique. This model is comprised of three modules, i.e., the preprocessing module, electromagnetic field computational module and scattering parameter calculation module. In this model, the Perfectly Matched Layer with Auxiliary Differential Equation (ADE–PML), an excellent absorption boundary condition (ABC) in FDTD, is generalized for PSTD scheme, and the weighted Total Field/Scattered Field (TF/SF) technique is employed to introduce the incident light into 3D computational domain. To improve the computational efficiency, the model is further parallelized by the OpenMP technique. The modeling accuracy of PSTD is validated against Lorenz–Mie, Aden–Kerker and *T*-matrix theory for spheres, inhomogeneous particles and nonspherical particles, and the influence of the spatial resolution and the thickness of ADE–PML on the modeling accuracy is discussed as well. At last, the parallel computational efficiency of the model is also analyzed. The results show that an excellent agreement is achieved between the results of PSTD and those well-tested scattering models, where the simulation errors of extinction efficiencies are generally smaller than 1%, indicating the high accuracy of our model. Though with a low spatial resolution, reliable modeling precision still can be achieved by PSTD model, especially for large particles. To suppress the electromagnetic wave reflected by the absorption layers, a 6-layer ADE–PML should be set in the computational domain at least.

References

[1] Liou, K. N., 2003: *An Introduction to Atmospheric Radiation.* Academic Press, San Diego.

[2] Zhang, F., Y.-N. Shi, J. Li, *et al.*, 2017: Variational iteration method for infrared radiative transfer in a scattering medium. *J. Atmos. Sci.* **74**, 419–430.

[3] Rao, R., 2012: *Modern Optics.* Scientific express, Beijing.

[4] Sun, W., G. Videen, Q. Fu, and Y. Hu. 2013: Scattered-field FDTD and PSTD algorithms with CPML absorbing boundary conditions for light scattering by aerosols. *J. Quant. Spectrosc. Radiat. Transfer.* **131**,166–74.

[5] Mishchenko, M. I., and L. D. Travis. 1997: Satellite retrieval of aerosol properties over the ocean using polarization as well as intensity of reflected sunlight. *J. Geophys. Res.***102**,16989–17014.

[6] Dubovik, O., A. Sinyuk, T. Lapyonok, *et al.*, 2006: Application of spheroid models to account for aerosol particle nonsphericity in remote sensing of desert dust. *J. Geophys. Res.***111**, D11208.

[7] Hu, S., T. Gao, H. Li, *et al.*, 2016: Effect of atmospheric refraction on radiative transfer in visible and near-infrared band: model development, validation, and applications. *J. Geophys. Res.* **121**, 2349–2368.

[8] Mishchenko, M. I., J. W. Hovenier, and L. D. Travis. 2000: *Light Scattering by Nonspherical Particles: Theory, Measurements, and Applications.* Academic Press, San Diego.

[9] Cheng, T. H., X. F. Gu, *et al.*, 2010: The reflection and polarization properties of non-spherical aerosol particles. *J. Quant. Spectrosc. Radiat. Transfer.* **111**, 895–906.

[10] Curtis, D. B., B. Meland, and M. Aycibin. 2008: A laboratory investigation of light scattering from representative components of mineral dust aerosol at a wavelength of 550 nm. *J. Geophys. Res.* **113**, D08210.

[11] Han, Y., T. Wang, R. Rao, *et al.*, 2008: Progress in the study of physic-optics characteristics of atmospheric aerosols, *Acta Phys. Sin.* **57**, 7396.

[12] Han, Y., R. Rao, Y. Wang, *et al.*, 2012:Inversive method on atmospheric aerosol scattering phase function. *Infrared Laser Eng.* **41**, 3051.

[13] Herman, M., J. L. Deuzé, A. Marchand, *et al.*, 2005: Aerosol remote sensing from POLDER/ADEOS over the ocean: improved retrieval using a nonspherical particle model. *J. Geophys. Res.* **110**, D10S02.

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