COMPARATIVE STRENGTHS OF A PSEUDO-SPECTRAL TIME DOMAIN METHOD IN NUMERICAL SIMULATION OF SINGLE PARTICLE OPTICAL SCATTERING

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Abstract. We present some results on the relative performance of the pseudo-spectral time domain, finite difference time domain, and DDA methods in calculating single-particle optical scattering properties. Our interest is in particles with size parameters in excess of 10. Using as test case a homogeneous spherical particle we have found that the pseudo-spectral time domain method is generally more efficient (uses less cpu time for a given accuracy) than the finite-difference time domain method. The DDA method appears to be superior to the pseudo-spectral method for indices of refraction less than 1.5, but as the index of refraction increases, the pseudo-spectral method becomes superior. We present here some results for particles with size parameters 10 and 30, and indices of refraction 1.3117 and 1.7.

1. Introduction.

We give here an indication of the potential of a pseudo-spectral time-domain (PSTD) method currently under development for the numerical simulation particle optical scattering properties of atmospheric aerosols. We are interested in such aerosols as ice, soot and mineral dust that have particle size parameter (x) above 10. As x increases beyond 10, calculations quickly become quite demanding of cpu time. This makes it important to understand how cpu requirements of the PSTD method compare with those of other methods, given a level of accuracy, as size parameters and indices of refraction (m) increase.

Although our main interest is in simulation of scattering properties of aggregates of non-symmetric and non-homogenous particles, a useful preliminary step is to test the method in the case that the aerosol is a single, homogeneous, spherically symmetric particle, for which we can use Mie solution values for phase matrix elements in our error assessment.

We present here early results on the relative performance of pseudo-spectral, finite difference time domain, and DDA methods. In this report we focus on the numerical approximation to the phase function P_{11}. We show some results with the PSTD at size parameters ($x = 10, 30$), but otherwise confine our performance comparison report to the single particle size parameter 10. We consider two indices of refraction: $m = 1.3117$, characteristic of ice crystals, and $m = 1.7$, which is in the range of the real parts of m for commonly occurring soot aerosols.

2. Methods.

The finite-difference time-domain (FDTD) [4, 3] and the discrete-dipole-approximation (DDA) [2, 5] are two widely used methods for the solution of light scattering by arbitrarily shaped particles. The pseudo-spectral time-domain (PSTD) method is quite widely used in fluid dynamics studies, but only rather recently has been introduced in optical scattering studies [1]. This method uses Fast Fourier Transform methods to give spectral accuracy at low cpu cost in calculation of spatial derivatives. The same centered time step (leapfrog) method is used in the PSTD and FDTD methods, and each of these methods includes a perfectly matched boundary layer, as well as the same near-to-far-field transform method.

3. Results.

Figures 1 and 2 show calculations of the normalized phase function P_{11} using the pseudo-spectral method, for a particle size parameter $x = 10$ (Fig. 1) and $x = 30$ (Fig. 2). Each figure shows the Mie solution and two pseudo-spectral calculations: one with volume averaged permittivity near particle edges, and the other with center-determined permittivity. For the smaller size parameter, the errors are evidently quite small, except in the back-scattering direction. There, the volume-centered method produces better results. Fig. 2 shows the same improvement of back-scattering with center-determined permittivity, but indicates that errors are beginning to appear at side angles.
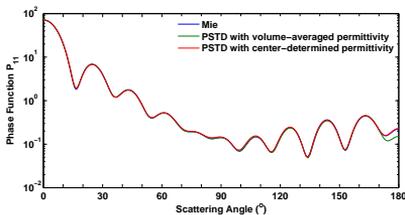
Figure 1. PSTD: x=10, m = 1.3117
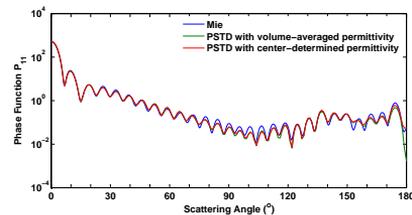
Figure 2. PSTD: x=30, m= 1.3117

Figures 3 and 4 show comparisons of the relative errors, expressed as percentages

$$E_{rel} = \frac{|\,numerical\, -\, exact\,|}{|exact|} \times 100$$

for calculations using the FDTD, PSTD, and ADDA methods. In the figures, the color indicates the relative error. The abscissa in each display is the scattering angle, while the ordinate is labeled on the left with the spatial resolution (in either gridpoints per wavelength or dipoles per wavelength, as appropriate). *It is important to note that the resolution ranges considered differ in the figures.* The horizontal lines indicate cpu time, indicated on the right. In the interpretation of these figures it is also important to recognize that the ordinate scale is logarithmic, and that relative error maxima occur at angles with relative minima of P_{11}: large relative error in calculating the deepest minima is to be expected.
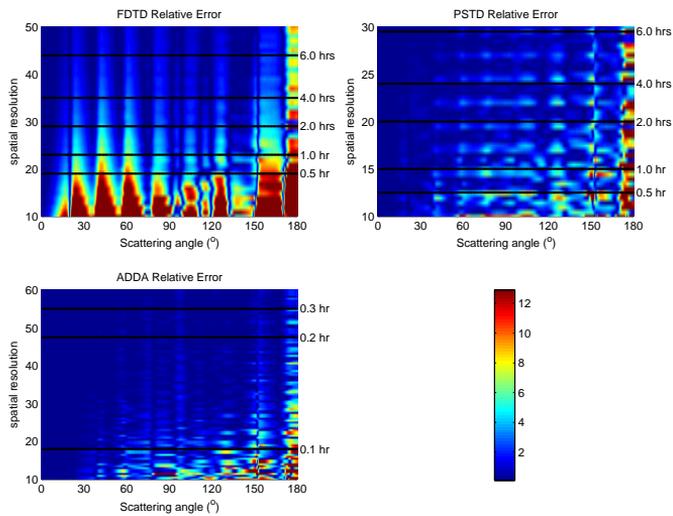
Figure 3. Relative errors (%) and cpu times for FDTD, PSTD, and ADDA methods: $x = 10$ and $m = 1.3117$ in all cases.
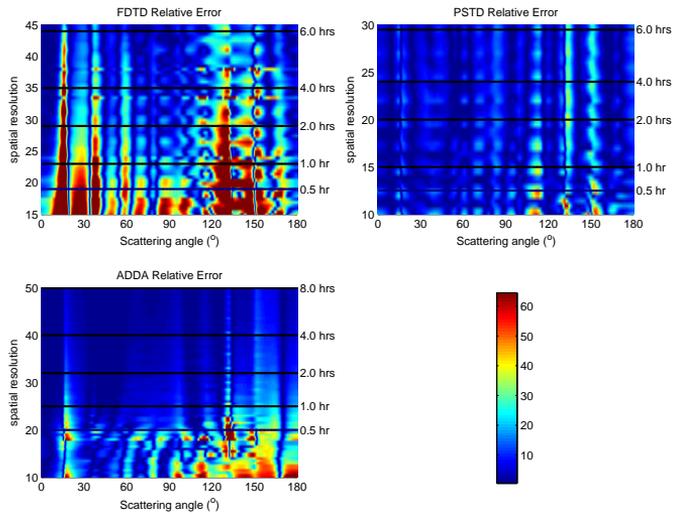
Figure 4. Relative errors (%) and cpu times for FDTD, PSTD, and ADDA methods: $x = 10$ and $m = 1.7$ in all cases.

At $m = 1.3117$ the ADDA method is clearly superior to the FDTD method on the basis of both error level and cpu time, and to the PSTD method on the basis of cpu time

(though only marginally better on the basis of error level). Figure 4 shows the comparison to change substantially when the index of refraction is increased to 1.7. All errors have risen in the range of resolutions shown. The ADDA has greatly increased its cpu time and resolution requirements in order to hold down the level of relative error. The PSTD appears now to show the best performance.

4. Discussion and Conclusions.

We presented some comparisons of relative errors and cpu times in numerical simulations of single-scattering properties spherical homogeneous particles using the PSTD, FDTD, and DDA methods. For a fixed particle size parameter $x = 10$, we found that the DDA method performs better, in terms of having more desirable error/cpu usage characteristics, than the other two methods when the index of refraction was 1.3117. However, we found that for index of refraction 1.7, the PSTD appeared to perform better. We have no reason to believe that the PSTD will not continue to show relative strength at larger size parameters and refractive indices, and are currently conducting experiments in this regime.

All results reported here were calculated on the same hardware, the 2592-core IBM Idataplex Cluster with 2.8GHz Nehelem processors and a 4xQDR Infiniband interconnect, at the Texas A&M Supercomputing Facility. Total cpu times would be different on other machines, so the relative times are the more significant data.

Acknowledgments

References

[1] W. H. Liu, "The PSTD algorithm: a time-domain method requiring only two cells per wavelength,"Microwave Opt. Technol. Lett. **15**, 158-165 (1997).
[2] E. M. Purcell and C. R. Pennypacker, "Scattering and absorption of light by nonspherical dielectric grains," Astrophys. J. **186**, 705-714 (1973).
[3] P. Yang and K. N. Liou, "Finite-difference time domain method for light scattering by small ice crystals in three-dimensional space,"J. Opt. Soc. Am. A **13**, 2072-2085 (1996).
[4] S. K. Yee, "Numerical solution of initial boundary value problems involving Maxwell's equations in isotropic media", IEEE Trans. Antennas Propag. **14**, 302-307 (1966).
[5] M. A. Yurkin and A. G. Hoekstra, "The discrete dipole approximation: An overview and recent developments," J. Quant. Spectrosc. Radiat. Transfer. **106**, 558-589 (2007).

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