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A comparison of pseudo-spectral and discrete dipole methods in numerical simulation of single particle light scattering.

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Scattering of light by atmospheric aerosols may be simulated by a number of numerical methods. Here we compare the computational efficiency and numerical accuracy of two popular and robust approaches: the pseudo-spectral time domain method (PSTD) and discrete dipole approximation method (DDA). While each method may be used for scatterers of arbitrary shape, here we consider only spherical particles so that we may use exact Lorenz-Mie solutions as a standard of truth.

We consider a range of size parameters from 10 to 100, and a range of indices of refraction from 1.0 to 2.0 (only real cases are considered here). Our measure of computational efficiency is the cpu time it takes for a method to produce a specified level of accuracy in the extinction efficiency and the phase function.

We find the relative performance of the two methods depends on both size parameter and index of refraction. For indices of refraction less than 1.2 and all size parameters in our range, the DDA appears to superior: prescribed levels of accuracy are attained, and obtained with less computational expense than with PSTD. For indices of refraction above 1.2 the situation changes: for each index value, there is a critical size parameter above which PSTD outperforms DDA: either the DDA failed to converge or the time required for convergence exceeded the time required by PSTD. This critical value of size parameter decreases from 80 to 30 as the refractive index increases from 1.2 to 1.4. For large refractive indices (>1.6), PSTD outperforms DDA for all size parameters in our chosen range.