Optimization of the discrete dipole approximation applied to particles on a plane substrate

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Investigating optical properties of particles on a substrate is relevant to different scientific and technical applications. On one hand, the synthesis and use of various nanoparticles commonly occur on a substrate. On the other hand, the substrate and/or interface itself enables one to develop new optical methods, for example, total internal reflection microscopy. The discrete dipole approximation (DDA) is an efficient method for simulating the interaction of the electromagnetic field with particles of arbitrary shape and internal structure. This method, derived from the frequency-domain volume-integral Maxwell equation, is numerically exact, i.e., achieves any required accuracy with sufficient computational resources.

The computational problem of the DDA consists in solving a large system of linear equations. High efficiency is achieved by applying a conjugate-gradient iterative solver with the matrix-vector product computed using the fast Fourier transform (FFT). The presence of the substrate requires one to replace the dipole–dipole interaction term with a more complicated expression including the so-called Sommerfeld integrals. The latter lacks a translational symmetry along the surface normal, seemingly breaking the FFT acceleration. Fortunately, this acceleration can be retained by cleverly rearranging the interaction terms [1]. This new formulation has been implemented in the open-source code ADDA [2], reaching the same computational complexity as in the free space (almost linear in the number of dipoles). Still, the calculation of four Sommerfeld integrals for every possible distance between two dipoles takes significant time, in some cases longer than the rest of the simulation.

The goal of this work is to optimize these calculations by using series expansions and asymptotic approximations of the integrals for small and large distances, respectively, and an interpolation over two cylindrical variables in the intermediate region. This approach significantly reduces the number of runs of the integration routines and, consequently, the simulation time, while keeping the same accuracy. We will present specific timing results and simulation examples at the conference.

References

[1] Yurkin, M. A., and M. Huntemann, 2015: Rigorous and fast discrete dipole approximation for particles near a plane interface *J. Phys. Chem. C* **119**, 29088–29094.

[2] Yurkin, M. A., and A. G. Hoekstra, 2011: The discrete-dipole-approximation code ADDA: capabilities and known limitations. *J. Quant. Spectrosc. Radiat. Transfer* **112**, 2234–2247.

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