Simulations of scattering by extremely oblate particles with the discrete dipole approximation

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The discrete dipole approximation (DDA) is a widely used method to simulate scattering and absorption of electromagnetic waves by particles of arbitrary shape and internal structure [1]. In most cases the DDA is used with a cubic lattice of dipoles, although theoretically dipoles (voxels) of any shape can be used, for example cuboid (rectangular parallelepiped). Still, the issues associated with the latter has been resolved only in 2015 [2]. Those "rectangular dipoles" allow significant reduction of computational time for some cases. Consider, for example, a graphene nanoplate with sizes 9 μm × 9 μm × 20 nm [2]. Dipole size has to be small to fit into the nanoplate thickness, which implies redundantly large number of dipoles to cover the width. By contrast, rectangular dipoles can be optimized for particular aspect ratios of the scatterer.

In this work we take the next step, by analyzing the rectangular-dipole formulation of the DDA in the limit of very small thicknesses of both dipole and scatterer. Taking the limit of zero thickness greatly simplifies the theoretical formulation, resulting in effectively 2D representation, where all optical quantities scale with various powers of particle thickness. It is equivalent to the Rayleigh–Debye–Gans approximation combined with the boundary conditions at the plane interface. We also proved that the scattering quantities computed with the standard (3D) code are independent of number of dipoles along the particle thickness, when the latter is sufficiently small.

Although the simulations based on the 2D theory are much faster than the standard DDA even for multi-layered structures (no linear system need to be solved), it can still be conveniently done within the framework of the DDA. Thus, we have implemented this capability as the development branch of ADDA: https://github.com/adda-team/adda/tree/2d_dda, as a natural extension of the existing command line options. After the simulation, ADDA generates standard output files, values in which are scaled to the corresponding powers of thickness. This can be used for various applications, including simulations of finite-width metasurfaces.

References

[1] Yurkin, M. A., and A. G. Hoekstra, 2007: The discrete dipole approximation: an overview and recent developments. *J. Quant. Spectrosc. Radiat. Transfer* **106**, 558–89.
[2] Smunev, D. A., P. C. Chaumet, and M. A. Yurkin, 2015: Rectangular dipoles in the discrete dipole approximation *J. Quant. Spectrosc. Radiat. Transfer* **156**, 67–79.

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