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Extension of the discrete dipole approximation to rectangular cuboid dipoles

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We performed a comprehensive analysis of the extension of the discrete dipole approximation (DDA) to a rectangular cuboid lattice of dipoles. The theoretical analysis of two different approaches, based either on the point-dipole interaction or on the integration of Green's tensor (IGT), was performed starting with the rigorous integral equation for the electric field. We showed that the expressions for polarizability and interaction terms must strictly conform to each other, which resolves the existing controversy in the literature. Moreover, there are large differences between the spectra of the interaction matrix in the static limit for those DDA formulations. In particular, the point-dipole formulation leads to unphysical edges of the spectrum that deteriorate the convergence of the iterative solver with increasing refractive index. This severely limits the applicability of point-dipole DDA formulations with rectangular dipoles in contrast to the case of cubic dipoles. We implemented both above formulations in the open-source code ADDA. It is freely available from the development branch of ADDA (http://code.google.com/p/a-dda/source/browse/branches/rectangular_dipole) and is suitable for general scattering problems.

We performed a number of test simulations to verify the correctness of the implementation and illustrated their performance on a number of test cases. In particular, we considered a graphene sheet, which thickness is much smaller than the wavelength. First, we found that use of IGT is critical even for cubic dipoles, since point-dipole (CLDR) formulation applied to two-dipoles-per-thickness discretization resulted in more than 10 times larger errors. Second, use of IGT with rectangular dipoles leads to more than 100 times faster simulations keeping the satisfactory accuracy. The required memory can be reduced by the same factor allowing one to handle larger scattering problems with a desktop computer. We have also tested the new formulation on a red blood cell – also an oblate particle, but with thickness larger than λ – and noticed only marginal improvement in comparison with the standard DDA. Therefore, we conclude that use of rectangular dipoles is expected to be especially beneficial for strongly oblate and prolate particles, which smallest dimension is much smaller than λ. This class includes many potential applications related to plate- or needle-like particles, e.g., in nanotechnology. More details on these results are available in [Smunev et al., J. Quant. Spectrosc. Radiat. Transfer 156:67–79 (2015), doi: 10.1016/j.jqsrt.2015.01.019].