Features and capabilities of the discrete dipole approximation code ADDA 1.0

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ADDA [1] is an open-source parallel implementation of the discrete dipole approximation (DDA [2]), capable of simulating light scattering by particles of arbitrary shape and composition in a wide range of particle sizes. It is used by more than 50 researchers worldwide. At the ASI we will present a poster, describing features of ADDA version 1.0, which is scheduled to be released in the summer of 2010.

ADDA is applicable to any finite particle in a vacuum (or any non-absorbing homogeneous medium). Scatterer's shape may be chosen from a number of predefined options or specified by an arbitrary set of dipoles. The scatterer can either be homogeneous or consist of several (up to 255) homogeneous domains. The refractive index of each domain may be anisotropic, specified by a diagonal tensor. The orientation of the particle and the direction of the incident beam may be varied, including orientation averaging. The incident light may be either a plane wave or a (tightly-focused) Gaussian beam.

Since the DDA is a numerically exact solution of the macroscopic Maxwell equations, there are no fundamental limits on the size of the scatterer. Practical limits are determined only by the available computer memory and tolerable computation time. Both grow at least cubically with size, when the latter is larger than the wavelength. ADDA can effectively parallelize a single DDA simulation between different cores, processors or computers. Thus, size limitations can be largely alleviated if ADDA is run on a cluster or a supercomputer. For instance, light scattering by spheres with a refractive index of 1.05 and size parameters up to 320 has been accurately simulated.

ADDA can produce a wide variety of scattering quantities: scattering, absorption, and extinction cross sections, asymmetry parameter, angle-resolved amplitude and Mueller matrices, and radiation forces. Electric fields in and near the particle can also be computed. The code features powerful command line interface and a checkpoint system, allowing one to conveniently perform multiple parallel simulations. High numerical efficiency and accuracy of an earlier version of ADDA was proven in comparison with other codes [3].

Acknowledgement. M.Y. is supported by the program of the Russian Government "Research and educational personnel of innovative Russia" (contract P2497).

References

[1] http://code.google.com/p/a-dda

[2] 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).

[3] A. Penttila, E. Zubko, K. Lumme, K. Muinonen, M. A. Yurkin, B. T. Draine, J. Rahola, A. G. Hoekstra, and Y. Shkuratov, "Comparison between discrete dipole implementations and exact techniques," J. Quant. Spectrosc. Radiat. Transfer **106**, 417–436 (2007).