

Benchmark calculations with the discrete dipole approximation and the T-matrix method for cubes

Maxim A. Yurkin^{a,b} and Michael Kahnert^{c,d}

^a*Institute of Chemical Kinetics and Combustion SB RAS, Institutskaya Str. 3, 630090, Novosibirsk, Russia*
yurkin@gmail.com

^b*Novosibirsk State University, Pirogova Str. 2, 630090, Novosibirsk, Russia*

^c*Swedish Meteorological and Hydrological Institute, Folkborgsvägen 1, SE-601 76, Norrköping, Sweden*
michael.kahnert@smhi.se

^d*Chalmers University of Technology, Department of Earth and Space Science, SE-412 96, Gothenburg, Sweden*

Keywords: discrete dipole approximation, T-matrix, cube, benchmark results

Light scattering by a cube is relevant for many practical applications, including powdered crystal samples, ice crystals in atmosphere, and metallic nanoparticles. But even more often cubes are used in benchmark studies of light-scattering codes to contrast with spheres and spheroids. Although a cube is a geometrically simple object, it is unexpectedly complicated in terms of light-scattering simulation. The Mie theory was proposed more than a century ago, and currently optical properties of spheres can be evaluated with machine precision. By contrast, methods to rigorously evaluate light-scattering by cubes appeared only during the last two decades, and their accuracy is rarely discussed.

In this talk we will present the simulation results of light-scattering by cubes with sizes $kD = 0.1$ and 8 (where k is free-space wavenumber and D is the side length of the cube) and with three values of the refractive index ($1.6 + 0.01i$, $0.1 + i$, and $10 + 10i$) using the discrete dipole approximation (DDA) and the T-matrix method. Our main goal was to push the accuracy of both methods to the limit. For the DDA we used an earlier developed extrapolation technique based on simulation results for different levels of discretization. It allowed us to present unprecedentedly accurate benchmark results with estimated relative uncertainty from 10^{-7} to 10^{-3} depending on cube size and refractive index, as well as on the particular scattering quantity of interest.

For the T-matrix method we analyzed convergence curves (versus the number of multipoles n_{cut}) and showed that some cases feature almost monotonous convergence. Based on this we proposed a simple procedure to fit this curve by a power function, which allowed us to compress the whole convergence curve into a confidence range (i.e. a certain value and its uncertainty estimate). Comparison of the DDA and T-matrix results showed that the obtained estimate is, overall, reliable, although an underestimation of the real error up to a factor of four was obtained in rare cases.

Both the proposed error estimate of the T-matrix method and its difference against the DDA results showed relative errors from 10^{-4} to 0.2. Moreover, T-matrix error estimate was always from 100 to 10^4 times larger than the DDA error estimate. Although we could not directly verify the accuracy claimed by the DDA, even the less remarkable agreement between the two methods is unprecedentedly good in some cases. Thus we believe that the presented benchmark results would be useful for developers of light scattering codes, as well as for those who apply these codes to cubes in practical applications. A detailed account of these results can be found in the paper [1].

- [1] Yurkin MA, Kahnert M. Light scattering by a cube: Accuracy limits of the discrete dipole approximation and the T-matrix method. *J. Quant. Spectrosc. Radiat. Transfer* (2012), doi: 10.1016/j.jqsrt.2012.10.001