

CAPABILITIES OF THE DISCRETE DIPOLE APPROXIMATION FOR SIMULATION LIGHT SCATTERING BY BIOLOGICAL CELLS

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Light scattering is a long used non-invasive method to study biological cells. It is used extensively in flow cytometers, where light scattering by single cells is analyzed. However, solving the direct light scattering problem for single cells still presents lots of difficulties that are mainly caused by the size and shape of the cells. The size is in the range from a few wavelengths (for visible light) to several tens of wavelengths. This size range prohibits the use of long wavelength (Rayleigh) or short wavelength (Geometrical Optics (GO)) approximations. The shape in general is very complex with multiple inclusions, which can be smaller, comparable or considerably larger than the wavelength). This limits the use of quick, accurate techniques to very few cases. Internal inclusions with size comparable to wavelength also greatly complicate the application of GO even to very large cells. Another property of biological cells, which simplifies computations, is index-matching (when they are studied in liquid solution, as is usually the case). This property gives rise to several approximations, e.g. Rayleigh-Debye-Gans and anomalous diffraction, however they usually give satisfactory accuracy only to some measured quantities. Reference [1] is a recent review of light scattering by biological particles, where these issues are discussed in more detail.

Although different new approximations are being developed, e.g. replacing certain cells by simpler shapes, validation of such approximations anyway require rigorous simulation of light scattering by complex-shaped particles. There are two types of methods, which are in principle capable of handling any geometry and size of the scatterers. They numerically solve the Maxwell equations in the time – Finite Difference Time Domain (FDTD) – or frequency – Discrete Dipole Approximation (DDA) – domain. Both methods divide the scatterer in subvolumes that should be much

smaller than the wavelength. Therefore their memory and time requirement rises steeply with size of the scatterer. That was always the main restriction for simulating light scattering by complex-shaped biological cells.

FDTD simulation of biological cells has a long history [2, 3], but it is mainly focused on small cells (because of computational requirement described above). The largest simulations found in the literature are for size parameter 80 [3]. We have recently applied DDA to large-scale simulation of light scattering by red blood cells [4] (size parameter up to 40). In this study we are testing the limits of DDA, using simple shapes, e.g. spheres, which can be solved using analytical techniques. At the workshop we will present results of DDA performance and accuracy of both integral characteristics (cross-sections and asymmetry parameter) and angular dependence of all Mueller matrix elements for particles with sizes and refractive in the range of biological particles, i.e. $30 < x < 130$ and $1.02 < m < 1.2$. We will show that DDA is capable of accurately computing light scattering by biological particles. However, especially for the largest sizes, computation times will be very large, even on state-of-the-art massively parallel supercomputers.

References

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