The discrete dipole approximation: from Maxwell's equations to practical applications

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Light scattering is widely used in remote sensing of various objects ranging from metal nanoparticles and macromolecules to atmospheric aerosols and interstellar dust. Moreover, the structure of electromagnetic fields near a particle is of major importance for other phenomena, such as the surface-enhanced Raman scattering (SERS) or the electron energy-loss spectroscopy (EELS). All these applications require accurate simulations of interaction of electromagnetic fields with particles of arbitrary shape and internal structure. The discrete dipole approximation (DDA) is one of the general methods to handle such problems [1].

The DDA is a numerically exact method derived from the volume-integral form of the frequency-domain Maxwell's equation for the electric field [2], and is a special case of method of moments. It commonly employs a regular rectangular grid of dipoles, leading to the computational complexity (and required memory) linear in the number of dipoles. This allows one to solve the problems with up to 1 billion dipoles using modern supercomputers [3]. Overall, the DDA is widely used for light-scattering and near-field simulations, thanks to the availability of robust and easy-to-used open-source codes, such as DDSCAT [4] and ADDA [3].

Importantly, the DDA can be applied to a broad range of electromagnetic applications apart from the standard problem of far-field scattering by single isolated particles. This includes complicated environments (e.g., particles on substrate) and unusual incident fields (leading to the SERS and EELS). The DDA can even be applied to simulate fluctuation phenomena, i.e. the near-field radiative transfer and Casimir forces, which are related to the Green's tensor in the presence of a particle. The only drawback is that the latter applications require much larger computational resources.

References

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