The discrete dipole approximation – the jack of all light trades

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The discrete dipole approximation (DDA) is a numerically exact method to simulate interaction of electromagnetic field with particles of arbitrary shape and composition. The method originated in astrophysics to simulate light scattering by cosmic dust. This application along with atmospheric aerosols has been the main driver of the DDA development until the late 1990s. Further on a lot of new nano-related applications emerged, which led not only to new objects but also to new numerical challenges and physical extensions of the DDA.

In this review talk I will start with rigorous derivation of the DDA starting from the integral form of Maxwell’s equation for the electric field. This derivation is paramount to the DDA due to several reasons. First, it rigorously proves the validity of the method and, thus, puts it in line with other numerically exact methods, i.e. its accuracy can be made as good as required given infinite computational resources. It also shows that the DDA is just a special albeit very popular case of wide range of methods described by a term “method of moments”. Second, it allows one to study the origin of the DDA errors (e.g., from shape and discretization) and to develop improvements aimed at specific error types. Moreover, it gives certain a priori predictive power with respect to the DDA accuracy for a given problem. Third, the rigorous derivation gives a solid base for the extension of the DDA to other physical phenomena, discussed below, to prevent one wandering in the dark of trials and errors.

In the last decade the DDA saw an explosion of extensions and improvements. First, they are related to the scattering problem itself, which may include multi-layered substrate and/or periodic boundary conditions. Second, that is numerical improvements such as filtered coupled dipoles, integration of Green’s tensor, and use of rectangular dipoles. Third, extension to the following phenomena: surface-enhanced Raman scattering, metal-enhanced fluorescence, electron-energy-loss spectroscopy, cathodoluminescence, near-field radiative transfer, and nonlinear response to ultrashort laser pulses. Some of those phenomena are deeply related to the Green’s tensor in the presence of a particle. Given such rapid development, the number of remaining challenges is larger than ever, especially with respect to efficient numerical algorithms.

Finally, the method without an efficient computer code is just a beautiful toy for one’s mind. Thus, I will also review existing open-source DDA codes, in particular their adoption of the latest DDA developments.