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Robust DDA simulations for exciting sources inside a particle

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The discrete dipole approximation (DDA) is a general method to simulate interaction of electromagnetic waves with particles of arbitrary shape and internal structure. Historically, the DDA is applied to scattering of plane waves or shaped beams, but can also be used with point dipole sources. Placing such source near a nanoparticle allows one to simulate emission (or decay rate) enhancement, relevant to fluorescent enhancement and surface-enhanced Raman scattering (SERS) of molecules.

Internal sources are a natural next step, relevant for encapsulated emitters and fluctuational phenomena, such as near-field radiative heat transfer and Casimir forces. However, such extension is confusing in several aspects. Theoretically, it incurs application of strongly singular integral operator to a non-square-integrable incident field, making it unclear whether the source is placed inside a particle or inside a cavity. Practically, the standard DDA based on interaction of point dipoles is known to be highly sensitive to the position of the source with respect to the voxel lattice. While certain empirical corrections are known to produce reasonable results, they are in stark contrast to the numerically-exact aura of the DDA established for other excitation scenarios.

To fill this comprehension gap, we have extended the rigorous derivation of the DDA from the volume-integral equation to the singular incident fields and derived the relation between several terms in the DDA numerical scheme. While this relation is not generally satisfied for point-dipole formulation of the DDA (explaining the abovementioned confusion), it is surprisingly valid for both modern DDA formulations, namely filtered coupled dipoles (FCD) and integration of Green's tensor (IGT). For the FCD, one only need to modify the incident field at the closest voxel, which we implemented in the open-source ADDA code. The IGT formulation works out of the box, benefiting from the semi-analytical evaluation of the integrals that has been recently implemented in ADDA. We used ADDA to simulate the emission enhancement of a point source moved inside a sphere. Both FCD and IGT results are almost constant at the voxel scale and agree with the prediction of the Lorenz-Mie theory, while the point-dipole formulation suffers from superfluous oscillations.