Convergence of Iterative Solution of a Linear System in the Framework of the Discrete Dipole Approximation

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Abstract— The discrete dipole approximation (DDA) is a popular method to simulate scattering and absorption of electromagnetic waves by particles of arbitrary shape and internal structure. Initially the DDA was proposed on the basis of the physical picture of the point dipoles set, but it can also be rigorously derived by discretization of the volume integral equation for the electric field. The DDA is commonly associated with a regular cubic discretization of the particle, since it allows the use of the fast Fourier transform to greatly accelerate computations. In this case the computational bottleneck of the DDA lies with the solution of a large system of linear equations, commonly performed by the iterative solver. The corresponding interaction matrix is complex symmetric, which makes the choice of the best iterative solver a hard task even if one limits himself to the family of Krylov-subspace (conjugate-gradient — CG) methods.

The goal of this report is to systematically study the performance of the iterative solver (i.e., required number of iterations), varying as much of the relevant parameters as possible. The tested DDA formulations and iterative solvers are those implemented in the existing open-source code ADDA. This includes the simplest point-dipole interaction formulation (e.g., so-called, lattice dispersion relation) as well as advanced formulations based on filtering the Green's tensor or integrating it over the volume of elementary cube. Iterative solvers include general ones applied to either the original (e.g., Bi-CGStab) or the normalized system (e.g., CGNR), as well as specialized solvers for complex-symmetric systems (quasi-minimal residual, QMR, or Bi-CG).

We also performed a theoretical analysis, based on the spectrum of the interaction matrix, which resulted in the reliable estimation of the number of iterations within a factor of 2 (in a wide range of refractive index) for particles smaller than the wavelength. Both theoretical analysis and extensive simulations highlighted the superiority of the advanced DDA formulations, especially for purely real refractive indices. For particles larger than the wavelength, the theoretical analysis correctly predicts the trend of number of iterations with increasing particle size, given the reasonable assumption about the spectral radius of the interaction matrix. Among the tested iterative methods, the QMR and its variants are the most efficient methods in all regimes.