# Performance of Iterative Solvers in the Discrete Dipole Approximation

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***Abstract*—The discrete dipole approximation (DDA) is a variant of volume-integral equation method, which speed largely depends on the iterative solution of system of linear equations. I systematically studied the performance of this solution, varying the particle refractive index, DDA formulation (including non-standard ones), and several Krylov-subspace iterative solvers. For that I used publicly available ADDA code, so the conclusions can be directly employed by the practitioners of the DDA. Apart from the expected strong dependence on the refractive index, the number of iterations significantly differs between the DDA formulations, especially for purely real refractive indices. For small particles the number of iterations versus refractive index can be estimated by a simple relation, previously derived from analysis of the spectrum of the interaction matrix.**

## I. Introduction

The discrete dipole approximation (DDA) is a method to simulate scattering and absorption of electromagnetic waves by particles of arbitrary shape and internal structure [1], [2]. Initially the DDA was proposed by Purcell and Pennypacker [3] on the basis of the physical picture of the point dipoles set, which was further advocated by Draine and Flatau [1]. The DDA is commonly associated with a regular cubic discretization of the particle, since it allows the use of the fast Fourier transform (FFT) to greatly accelerate computations [4]. It is this appealingly simple description of the method coupled with availability of optimized open-source codes [1], [5] that led to numerous applications of the DDA varying from interstellar dust to nanoparticles and biological cells. In many cases the DDA is used in a black-box mode by researchers who are only marginally familiar with computational electromagnetics (CEM).

However, the DDA can also be rigorously derived by discretization of the volume integral equation (VIE) for the electric field [6], [2]. In particular, the rare modification of the DDA, named "integration of Green's tensor" (IGT) [7], [8], is equivalent to the VIE for the electric current (J-VIE) with pulse basis functions and point matching [9]. This viewpoint on the DDA is favored by CEM experts, but even they may raise eyebrows at consideration of a standard "point-dipole" DDA, in which the integral of the Green's tensor over the cubical cell is evaluated through a single-point approximation. The latter is completely wrong for nearby cells; still, even such simplest DDA is a "numerically exact" method, converging to the exact solution with refining discretization [2].

The computational bottleneck of the DDA lies with the solution of a large system of linear equations, commonly performed by the iterative solver with FFT-accelerated matrix–vector product. The corresponding interaction matrix **A** 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 methods [10]. Naturally, numerical performance of such iterative solvers in the DDA has attracted a lot of interest over the years. However, most papers focus only on some of the relevant parameters: specific iterative solvers [11], [12], DDA formulation [13], [14], and particle size [15], shape [16], and refractive index $m$ [8], [17], [18]. Some researchers have also related the convergence of the iterative solver to the eigenspectrum of **A** [8], [19].

The goal of this report is to systematically study the performance of the iterative solver (i.e. required number of iterations $N_{\text{iter}}$), varying as much of the relevant parameters as possible. In doing so I try to bridge the worlds of typical DDA users and CEM experts. The tested DDA formulations and iterative solvers are those implemented in the existing publicly available code [5], thus ignoring the more advanced VIE formulations [18]. However, the obtained results are assessed from a CEM viewpoint. In particular, the dependence of $N_{\text{iter}}$ on $m$ is compared to the spectrum-based theoretical prediction for small particles.

## II. Simulations and Discussion

All simulations were performed with ADDA code [5], using the default convergence threshold ($10^{-5}$) for relative residual. The tests, reported in this extended abstract, are all based on a small sphere ($kD = 1$, where $k$ is the wavenumber), discretized using 32 dipoles per diameter $D$. The conference presentation will also include the results for a different particle shape (cube), and larger size ($kD = 10$). The following results are presented as contour plots of $N_{\text{iter}}$ versus complex $m$; the real and imaginary parts of the latter are independently varied from 0 to 10 in step of 0.5 with subsequent interpolation between the nodes.

### A. Different DDA formulations

There are three principally different DDA formulations, implemented in ADDA: point-dipole interaction (standard DDA), IGT, and "filtered coupled dipoles" (FCD) – based on application of antialiasing filter to the Green's tensor [14], [20]. All three have different expression for all elements of **A** and,

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hence, may lead to different behavior of iterative solvers. By contrast, many different expressions for dipole polarizability [2] only slightly modify the diagonal elements of the interaction matrix. Moreover, those modifications are negligible for small dipole sizes. Therefore, only the simplest Clausius-Mossotti (CM) polarizability expression is used as a representative example of the standard DDA. The IGT formulation is used with approximate evaluation of the corresponding integrals, denoted as $\mathrm{IGT_{SO}}$ in the ADDA manual [21], which was tested not to influence $N_{\mathrm{iter}}$. The results for CM, IGT, and FCD, all using the quasi-minimal residual (QMR) iterative solver, are shown in Figs. 1-3, respectively.

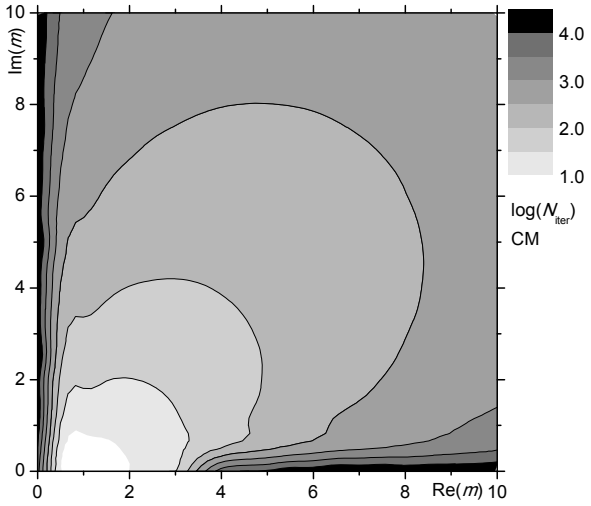


Fig. 1. Contour plot of $N_{\mathrm{iter}}$ for QMR iterative solver (in log scale) versus $m$ for $kD = 1$ sphere, using the CM formulation.

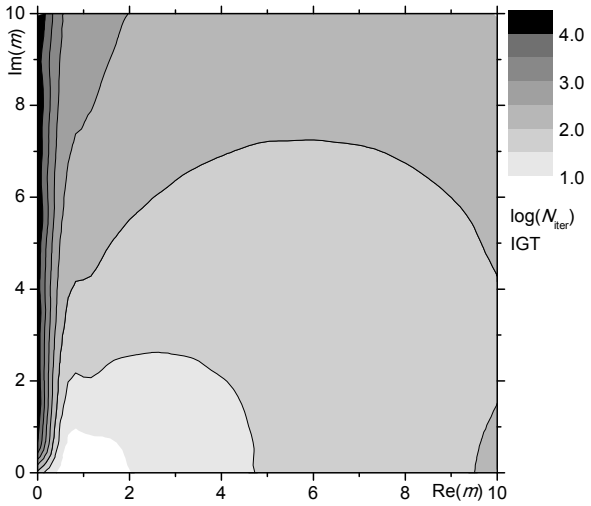


Fig. 2. Same as Fig. 1 but using the IGT formulation.

The performance of the CM formulation in terms of $N_{\mathrm{iter}}$ is always inferior to the other two. Especially troubling is the poor performance for purely real $m$, especially since such $m$ are commonly used for testing purposes [12], [15], [18]. This artefact can be explained by the spectrum of the matrix **A**, which is a discretization of the integral scattering operator. Rahola [19] showed that the spectrum of this operator for any homogenous scatterer is a line in the complex plane going from 1 to $m^2$ (so-called, essential spectrum [22]), except for a small amount of points, corresponding to resonances for the specific size and shape. It is accepted that the spectrum of **A** for particles much smaller than the wavelength approximate that of the integral operator [14], [22], which explains why $N_{\mathrm{iter}}$ only weakly depends on the discretization level. However, the spectrum of **A** do not necessarily falls strictly within the abovementioned essential bounds. In particular, CM formulation is known to spill outside these bounds leading to unphysical resonances along the positive real axis of $m$ [8], [14]. By contrast, both the FCD [14] and the IGT [8] have not shown any spill out, at least in a few test cases. However, the general proof of such favorable behavior is lacking.

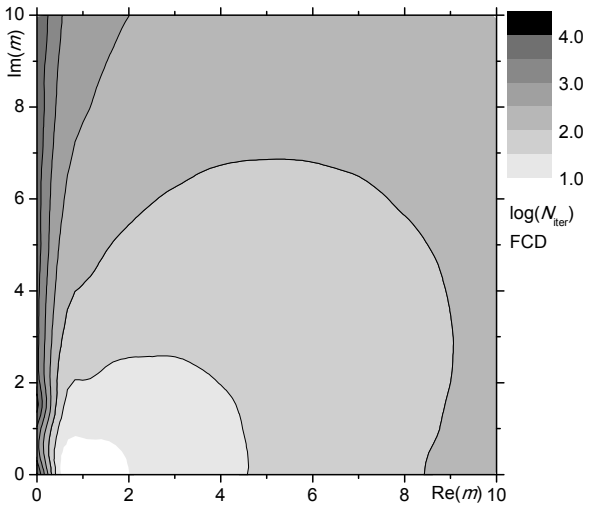


Fig. 3. Same as Fig. 1 but using the FCD formulation.

Also unclear is how one can explain the remaining differences between the FCD and the IGT. The former is faster near the imaginary axis of $m$, while the latter – near the real axis.

### *B. Different iterative solvers*

I tested all iterative solvers implemented in ADDA [21]: Bi-conjugate gradient (Bi-CG), Bi-CG stabilized (Bi-CGStab), enhanced Bi-CGStab(2), conjugate gradient applied to normalized equations with minimization of the residual norm (CGNR), CSYM, QMR and its modification based on 2-term recurrence ($\mathrm{QMR_2}$). All of them were used with the FCD formulation, as discussed above. The QMR results were shown above in Fig. 3 and they are very similar to that for $\mathrm{QMR_2}$ and Bi-CG (data not shown), which is expected due to close relation between those methods.

The results for CSYM, CGNR, and Bi-CGStab are shown in Figs. 4-6, respectively. For CGNR and Bi-CGStab the quantity shown is $2N_{\mathrm{iter}}$ since these methods do not employ the symmetry of **A** and require two matrix–vector products per iteration. The corresponding results for Bi-CGStab(2) (data not shown) are very similar to that of Bi-CGStab, as expected.

The performance of CSYM is always better than that of CGNR, in accordance with its design, but both these methods are significantly inferior to other options. The latter is because

they operate on a Hermitian matrix $\mathbf{A}^H\mathbf{A}$, which has less favorable spectral properties than $\mathbf{A}$. However, their convergence is guaranteed (at least, in infinite precision arithmetic) and is not susceptible to breakdowns [23].

Bi-CGStab shows intermediate results, but is almost always inferior to the QMR. However, Bi-CGStab may become more competitive for larger sizes, when the performance of all iterative solvers is less predictable [15].

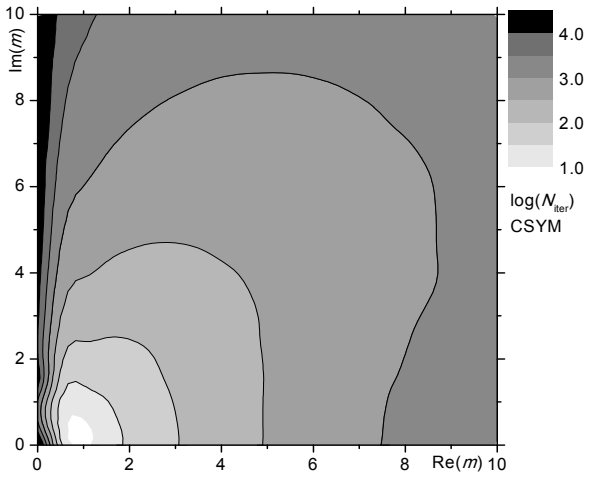


Fig. 4. Contour plot of $N_{\text{iter}}$ for CSYM iterative solver (in log scale) versus $m$ for $kD = 1$ sphere, using the FCD formulation.

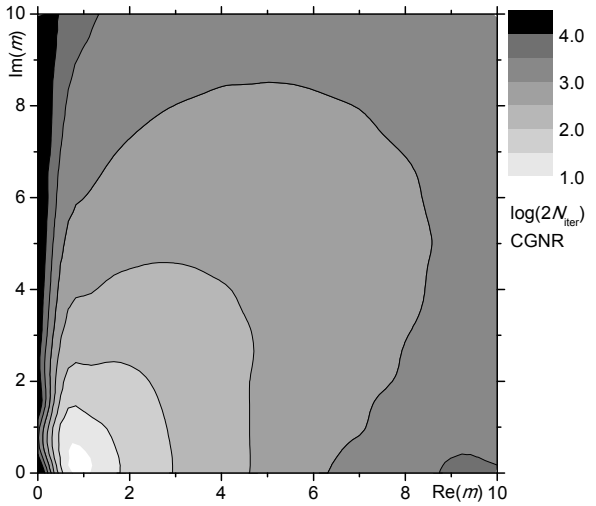


Fig. 5. Same as Fig. 4 but for CGNR iterative solver.

### C. Theoretical estimate for number of iterations

Rahola [19] showed that the spectrum of the integral scattering operator for any homogenous scatterer is a line in the complex plane going from 1 to $m^2$, except for a small amount of points, corresponding to resonances for the specific size and shape. For particles much smaller than the wavelength the resonances are not present, allowing estimation for the optimal reduction factor for any Krylov-space iterative method. This, in turn, was used to derive a simple estimate for number of iterations [24]

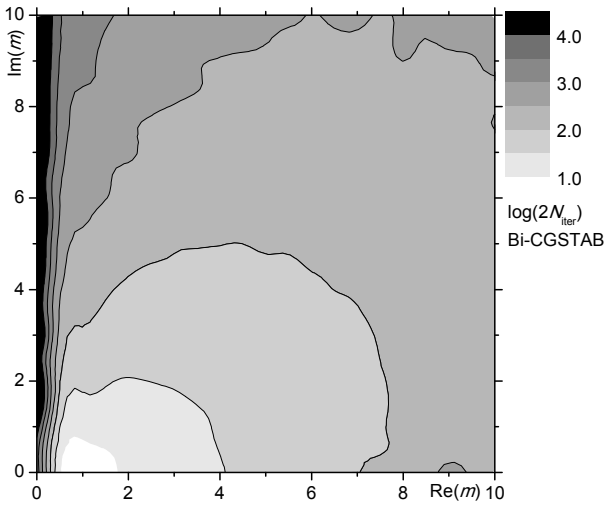


Fig. 6. Same as Fig. 4 but for Bi-CGStab iterative solver.

$$N_{\text{iter}} \approx \frac{5\ln 10}{\ln\left|(m+1)/(m-1)\right|}. \qquad (1)$$

It was tested against DDA simulations for refractive indices of gold in the visible, showing agreement within a factor of two [24]. Equation (1) is plotted in Fig. 7 and shows good qualitative agreement with Fig. 2 and Fig. 3, except for the neighborhood of the imaginary axis. There the integral operator becomes singular, implying infinitely large $N_{\text{iter}}$. However, the actual $N_{\text{iter}}$ obtained from a finite discretization of this operator is always finite.

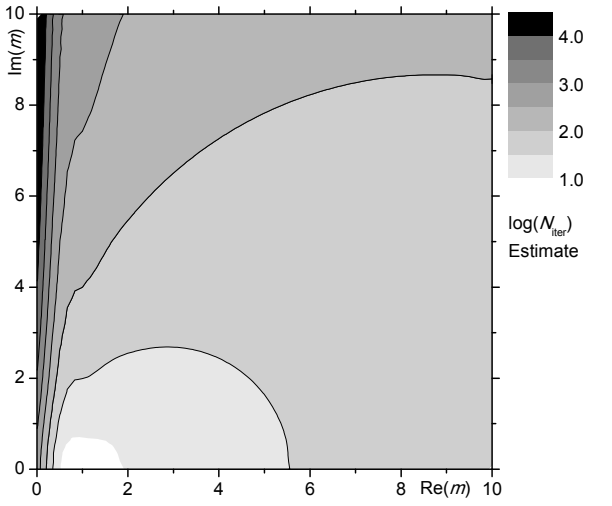


Fig. 7. Contour plot of $N_{\text{iter}}$ (in log scale) versus $m$ according to Eq. (1).

Using similar assumptions the spectrum of matrix $\mathbf{A}^H\mathbf{A}$ can also be described by a line, which allows one to derive an estimate for $N_{\text{iter}}$ of CGNR and CSYM solvers. Those results will be reported at the conference.

Unfortunately, the simple estimates fail for larger particles, where the particle size becomes an important parameter. While dependence of $N_{\text{iter}}$ on size is very complicated in the resonance region (size is comparable to the wavelength), it may allow for

an asymptotic formula for much larger sizes. For instance, linear scaling has been reported, when $m$ has a large imaginary part [25].

## CONCLUSION

The performance of iterative solvers largely depends on the refractive index and on the DDA formulation. While the effect of refractive index is widely acknowledged, the effect of DDA formulation is mostly ignored by the DDA users (who often ignore the existence of non-standard formulations altogether). By contrast, this should not surprise the CEM community, where the close relation between the VIE formulation, the spectrum of the interaction matrix, and the number of iterations is well-known [9], [18].

Among the tested iterative solvers QMR and related ones, which operate on a matrix itself and employ its complex-symmetric property, showed the best performance, at least for small particles. The estimate of $N_{\text{iter}}$ versus $m$, previously derived from the spectrum of the interaction matrix, agrees qualitatively well with results for IGT (or FCD) formulations of the DDA for a $kD = 1$ sphere. This may help one to accurately estimate the required computational resources for DDA simulations of nanoparticles.

## ACKNOWLEDGMENT

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