

Can the Discrete Dipole Approximation simulate scattering of particles with size parameter equal to 100?

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Abstract

This study is devoted to exploring the applicability bounds of a modern Discrete Dipole Approximation (DDA) code running on a state-of-the-art massively parallel supercomputer. A number of DDA simulations of light scattering by spheres with different size parameters (x) and refractive indices (m) are performed and compared with the exact solution. Results of DDA performance and simulation errors are presented. We show that DDA is at least applicable in the range of refractive index from 1 to 2, and size parameter up to 130 (for $m < 1.2$). We are currently exploring larger values of m .

1 Introduction

The methods to solve the single light scattering problem can be divided into approximate and exact [1]. Approximate methods include, among others, Rayleigh and Geometrical Optics (GO) approximations, which are applicable, respectively, to particles small and large compared to the wavelength [2]. Exact methods are numerous, but only few of them are applicable to scatterers with complex internal structure. Those are volume integral methods, which solve the Maxwell's equations either in the time domain (Finite Difference Time Domain, FDTD) or frequency domain (Discrete Dipole Approximation, DDA [3]).

In this study we explore the applicability of DDA to simulate light scattering in intermediate size range (to order ten times the wavelength), where no approximation applies. Even when the size of the scatterer is large enough for GO, the internal structure with characteristic sizes comparable to the wavelength may greatly complicate the application of GO [4]. All methods, which are capable to simulate light scattering by complex inhomogeneous objects in this size range, face extreme computational complexity with increasing scatterer's size, because they divide the scatterer in subvolumes that should be much smaller than the wavelength.

We have recently demonstrated that DDA is applicable for biological particles in suspension with size parameters and relative refractive indices in the range $30 < x < 130$ and $1.02 < m < 1.2$, respectively [5]. In this study we extend that work to higher refractive indices (up to 2) to include many more relevant applications.

2 Simulation method

Our code, the Amsterdam DDA (ADDA), is capable of running on a cluster of computers (parallelizing a single DDA computation), which allows us to use practically unlimited numbers of dipoles, since we are not limited by the memory of a single computer [6, 7]. In this study we use the Lattice Dispersion Relation

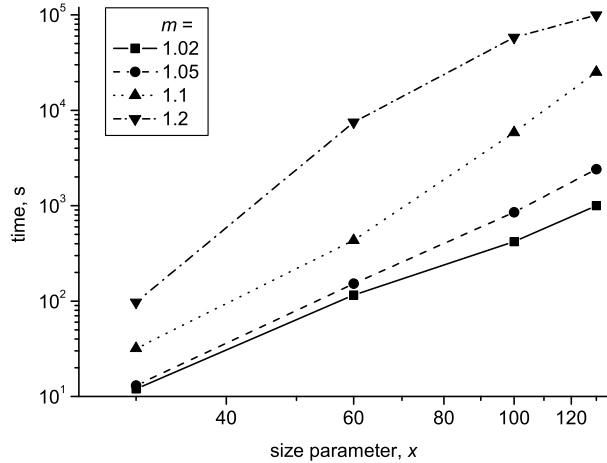


Figure 1: DDA simulation times for spheres with different x and m (on 64 P4-3.4 GHz processors). Two largest computations times for $m = 1.2$ are estimated.

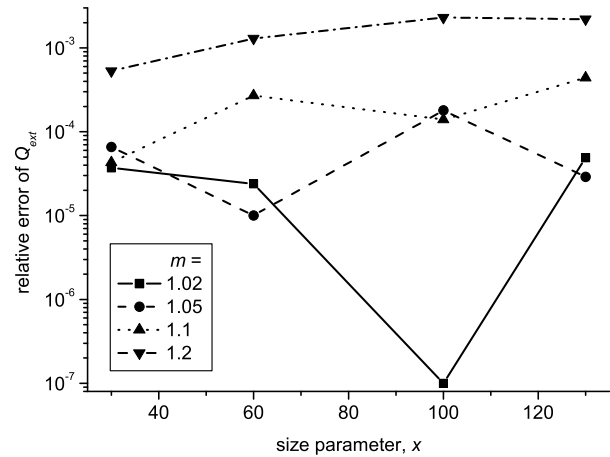


Figure 2: Relative errors of Q_{ext} for spheres with different x and m .

(LDR) [8] for dipole polarizability. We use two iterative methods: Bi-Conjugate Gradient STABILized (Bi-CGSTAB) [9] and Quasi Minimal Residual (QMR) [10]. The former performed better for very large index-matching particles, described in Sect. 3. All the DDA simulations were carried out on the Dutch national computer cluster LISA [11].

Since the DDA method is equally applicable to particles of any shape and internal structure, we test it on simple objects, for which an exact analytical solution is available, and then extend the conclusions to arbitrary shaped scatterers. We use homogenous spheres as test objects and compare DDA simulations with Mie solutions. As a result, we obtain DDA performance statistics (hardware requirements, simulation time) and accuracy of both integral characteristics (cross sections and asymmetry parameter) and angular dependencies of all Mueller matrix elements for different x and m .

3 First results

Here, we present results obtained for the refractive index range of biological particles $1.02 < m < 1.2$. Figure 1 shows DDA simulation times for different spheres (obtained on 64 P4-3.4 GHz processors). The size of a single dipole has been kept constant at $\lambda/12$. The total number of dipoles for the largest simulation was $6 \cdot 10^7$. One can see that simulation time scales approximately cubical with the size parameter and rapidly increases with refractive index. Relative errors of Q_{ext} for these simulations are presented in Fig. 2. They are fairly small. Results for the asymmetry parameter are similar (data not shown).

The angular dependence of S_{11} is presented for two particular cases: $x = 100$, $m = 1.02$ and $x = 130$, $m = 1.2$ in Fig. 3 and Fig. 4, respectively. Those are the cases that give the largest errors in the range of biological particles. One can see that DDA results are in good agreement with the exact solution, however relative errors can be significant at specific angles (near the deep minima). Results for other Mueller matrix elements show the same trends (data not shown).

At the conference we will show results for refractive index up to 2, and for size parameter up to 100. Simulation times are expected to be as large as one week on 128 P4-3.4 GHz processors. This number tells us that such massive DDA computations are only useful to serve as benchmark studies, i.e. providing data to test the quality of other, less expensive approximate methods.

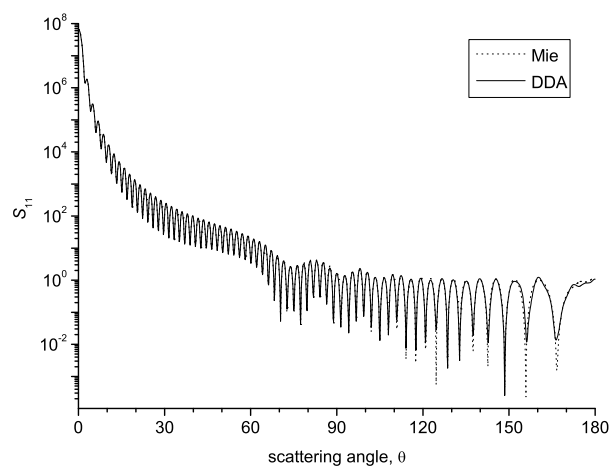


Figure 3: $S_{11}(\theta)$ for a sphere with $x = 100$, $m = 1.02$. Both DDA (solid line) and Mie results (dotted line) are shown.

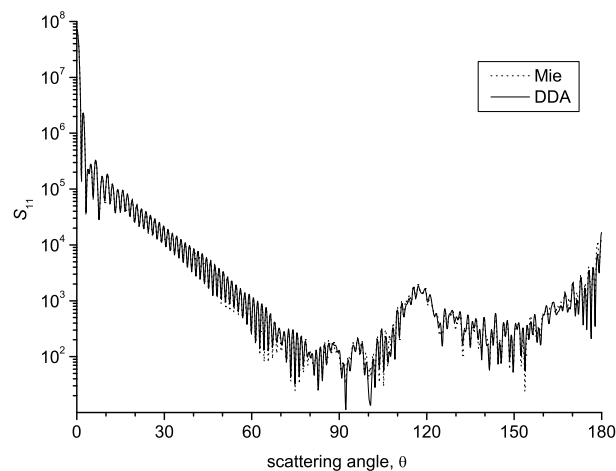


Figure 4: $S_{11}(\theta)$ for a sphere with $x = 130$, $m = 1.2$. Both DDA (solid line) and Mie results (dotted line) are shown.

4 Conclusion

DDA is capable of simulating light scattering by large particles with $m < 2$, however it requires very large, computation times even on state-of-the-art massively parallel supercomputers. For biological particles ($m < 1.2$) DDA is proven to be applicable up to $x = 130$ with overall satisfactory accuracy. Accuracy of integral scattering quantities is very good, while angle-resolved quantities show larger relative errors (especially in minima).

At the conference we will present the bounds of size parameter for practical applicability of DDA (with current code and hardware) for $m < 2$. We will show DDA performance and accuracy of both integral characteristics (cross sections and asymmetry parameter) and angular dependencies of all Mueller matrix elements.

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