Current capabilities of the discrete dipole approximation for very large particles: speed, accuracy, and computational tricks

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The current capabilities of the discrete dipole approximation (DDA) for very large particles are shown together with computation times and errors. I discuss several relevant practical issues, such as an iterative solver and dependence of the performance on the refractive index. Moreover, I discuss the convergence of DDA with refining discretization and show how an extrapolation technique can be used to increase DDA accuracy and provide a reliable error estimate.

Capabilities of DDA for simulating light scattering by spheres were studied for x up to 160 and m up to 2 [1]. For that we used ADDA v.0.75 [2], which is capable of parallelizing a single DDA simulation. The discretization was chosen according to the standard "rule of thumb" – $y \approx 0.63$ [3], where $y = mkd$ is the discretization parameter (m is the refractive index, k is the free space wavenumber, and d is the size of dipoles). The maximum reachable size parameter x on a cluster of 64 modern processors decreases rapidly with increasing m: it is 160 for $m = 1.05$ and only 20-40 for $m = 2$ (depending on the convergence threshold of the iterative solver ε, see Fig. 1). The limitation is mostly due to the slow convergence of the iterative solver leading to practically unbearable computation times (Fig. 2). The only exception is $m = 1.05$, where x is limited by the available memory. For instance, the simulation for m=1.05 and x=160 used 512^3 computational box, resulting in linear system of $2 \cdot 10^8$ equations. Errors of both integral and angle-resolved scattering quantities show no systematic dependence on x, but generally increase with m. Errors of Q_{ext} and $< \cos\theta >$ range from less than 0.01 % to 6 %. Maximum - and RMS relative errors of $S_{11}(\theta)$ are in the ranges 0.2÷18 and 0.04÷1 respectively. It is important to note that application of the "rule of thumb" does not lead to constant errors in studied cases. Therefore, a more useful approach is to determine computational time required to reach fixed accuracy. We are currently performing such study; the results will be presented at the workshop.

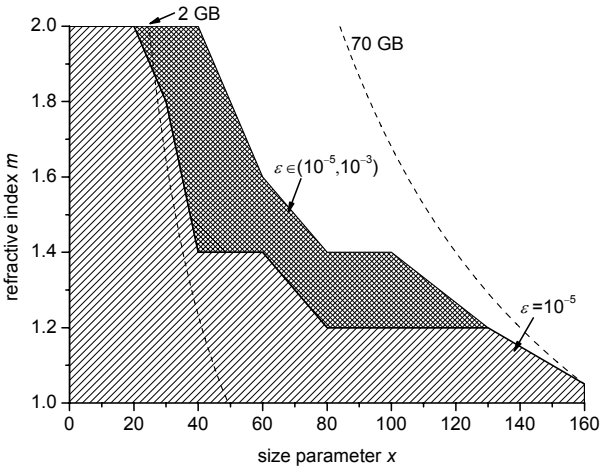

Fig. 1. Current capabilities of ADDA for spheres with different x and m. The striped region corresponds to full convergence and densely hatched region to incomplete convergence. The dashed lines show two levels of memory requirements for the simulation, according to the "rule of thumb".

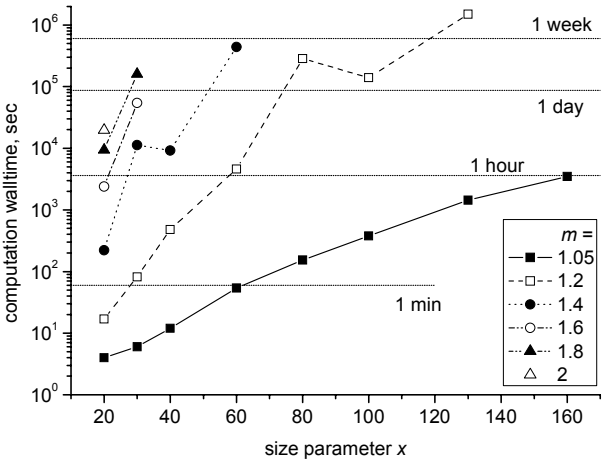

Fig. 2. Total simulation wall clock time (on 64 processors) for spheres with different x and m. Time is shown in logarithmic scale. Horizontal lines corresponding to a minute, an hour, a day, and a week are shown for convenience.

There are few practical issues associated with these simulations. First, if the particle is symmetric for 90° rotation over the propagation direction of the incident light, then only one incident polarization need to be simulated (the results for

the second one can be deduced at very low additional computational cost). Thus computational time, e.g. shown in Fig. 2, is twice less than usual. Although not applicable to complex objects, it is relevant when spheres and other symmetric shapes are used, e.g., for assessment of DDA performance for a particular *x*-*m* region.

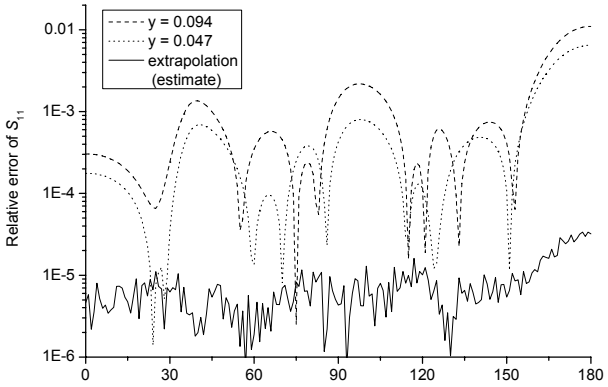

Fig. 3. Errors of $S_{11}(\theta)$ in logarithmic scale for extrapolation using 5 values of y in the interval [0.047,0.094] for $kD = 8$ cube.

Second, an iterative solver is a critical part of a large scale DDA simulation. For instance, at least three of four iterative solvers implemented in ADDA are competitive with each other, i.e. it is not possible to claim the best one [1]. However, it is the iterative solver that limits the reachable x for moderate m. At the workshop, we will discuss different possible improvements: modifications of the existing iterative methods with better numerical properties and preconditioning techniques [4].

Third, the performance steeply depends on m, although it may be alleviated by better numerical algorithms. However, the good side of it is that scattering of visible light by almost all biological cells can be already simulated, if they are placed into liquid medium. Moreover, DDA can naturally simulate scattering by arbitrarily complex and inhomogeneous models of cells.

Finally, the expected convergence of the DDA with decreasing y (keeping geometry and size of the scatterer fixed) will be discussed at the workshop. A rigorous theoretical analysis of DDA errors [5] shows that the error in any measured quantity is bounded by a quadratic function of a discretization parameter y. Moreover, both theoretical consideration and a number of test cases shows that in certain cases, e.g. for cubically shaped particles, the linear term is so small that the convergence is quadratic in common range of y. These results allowed us to propose an extrapolation technique [6]. Its idea is the following: first one performs DDA simulations for several values of y. Then any measured quantity can be extrapolated to $y = 0$, which provides two benefits. First, it allows one to obtain more accurate results at the cost of moderate increase in computational time. For example, Fig. 3 shows the extrapolation results for a cube with size D ($kD = 8$). If we denote the computation time for $y = 0.047$ as t, then total computational time for extrapolation technique is only $2.5t$. The corresponding improvement in accuracy is two orders of magnitude, which is completely unfeasible with "single simulation" approach. However, the improvement of accuracy is significantly less if initial simulations are performed for a larger y, or non-cubically shaped scatterer is used.

Second, the extrapolation technique provides an estimate of the error, even when the accuracy itself is not improved. This estimate is not theoretically robust, however its reliability have been proven for a number of test cases. This estimate is completely internal, and hence can be used for validation of results, which is a long-standing problem of DDA simulations for complex particles. Moreover, an adaptive DDA can be developed, i.e. the code which reaches the prescribed accuracy using minimum computational resources.

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6. M. A. Yurkin, V. P. Maltsev, and A. G. Hoekstra, "Convergence of the discrete dipole approximation. II. An extrapolation technique to increase the accuracy," J. Opt. Soc. Am. A **23**, 2592-2601 (2006).

Discussion with *Maxim Yurkin*
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Hoekstra: What about having absorption in your benchmarks?
Yurkin: Should help a lot for the bigger particles, no real numbers yet.
Lumme: We know from our experience that convergence is much better if you have absorbing particles!

Eremin: For smaller particles errors seem larger? How can this be? And what happens for even smaller particles (smaller then $x = 20$)?
Yurkin: Errors stay in the same order of magnitude.

Okada: Is there a difference between DDSCAT and ADDA?
Yurkin: No, very good agreement between both codes, look at comparison paper by Anti Pentilla et al (JQSRT special issue dedicated to ELS-9)

Eremin: Which numerical method did you use?
Yurkin: QMR.
Eremin: And can you compare QMR with e.g. GMRES?
Yurkin: Rahola did that, GMRES turned out not to be so good.

Lumme: Practical point, you should take several random orientations of a sphere! This improves e.g. the error in the backscattering directions, as was recently demonstrated by Penttilä.
Yurkin: We do only one.

Auguié: What is the best choice for going from one discretization to a next in the extrapolation procedure?
Yurkin: We discussed this in the JOSE paper, we don't know how to do this optimally, but our method as described in the JOSA seems to work good.

Eremin: What does your 'theoretical estimate' mean. Your analysis does not satisfy Maxwell's equations, as divergence in E-field will jump at surfaces.
Yurkin: OK, I see.
Detailed discussion on converge theory followed, no notes taken (sorry).