Application of the discrete dipole approximation to extreme refractive indices: filtered coupled dipoles revived

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Abstract

We compared three formulations of the discrete dipole approximation (DDA) for simulation of light scattering by particles with refractive indices $m = 10 + 10\mathrm{i}$, $0.1 + \mathrm{i}$, and $1.6 + 0.01\mathrm{i}$. These formulations include filtered coupled dipoles (FCD), lattice dispersion relation (LDR) and radiative reaction correction (RRC). We compared number of iterations (proportional to simulation time) and accuracy of final results. We showed that LDR performance for $m = 10 + 10\mathrm{i}$ is especially bad, while FCD, which we have implemented in the ADDA computer code, is a good option for all cases studied. Now these extreme refractive indices can be routinely simulated using modern desktop computers.

1 Introduction

The discrete dipole approximation (DDA) is a well-known method to calculate light scattering by arbitrary shaped inhomogeneous particles [1]. The widespread application of the DDA started with the work of Draine and coworkers [2-4], especially after release of their computer code DDSCAT to the public domain. They also systematically showed that DDA performance deteriorates with increasing refractive index m. Since then it was accepted that application of DDA is limited to a range approximately described as $|m - 1| < 2$, based on the standard formulation of the DDA including the lattice dispersion relation (LDR [4]). Recently, it has been shown that this standard DDA formulation has problems both for $|m| \gg 1$ and $\mathrm{Re}(m) \ll 1$ [5]. Such extreme m-values do appear in spectral resonances of many materials in the infrared range [5]. Accurate predictions of the spectral shape of absorption resonances are of crucial importance for the interpretation of astronomical observations. Moreover, metallic particles in the infrared have very large values of m, hence they might be the dominant source of opacity in many environments [6]. However, currently accurate methods to predict the opacity of metallic particles are lacking.

While the range of $\mathrm{Re}(m) < 1$ is poorly studied, there have been a number of attempts to improve DDA performance for large m. They include filtered coupled dipoles (FCD [7]), weighted discretization (WD [8]), integration of Green's tensor (IT [9]), Rahmani-Chaumet-Bryant formulation (RCB [10]), and surface-corrected LDR (SCLDR [11]). RCB and SCLDR require a preliminary solution of the electrostatic problem for the same particle, and IT requires a numerical evaluation of oscillatory integrals to build up the DDA interaction matrix, which is not trivial to implement and may consume a lot of computer time. WD is an efficient in decreasing shape errors [12] but it causes all boundary dipoles to have different polarizabilities, which is incompatible with current internal data structure of publicly available DDA codes such as DDSCAT and ADDA [13]. The only known drawback of FCD is that it is hard to theoretically analyze its convergence [12]. On the other hand, FCD is a good option since it is easy to implement and it does improve the performance of DDA for large m, as was shown by its authors [7,14]. It seems that the only reason why FCD, proposed 10 years ago, was not adopted by the light scattering community is that it was not included as an option in a publicly available DDA code.

In this paper we endeavor to revive FCD. For that we implement it in the ADDA code and demonstrate its performance for a number of scattering problems in comparison with LDR and radiative reaction correction (RRC [2]) formulations. We also discuss practical feasibility of DDA simulation of light scattering by particles with extreme refractive indices.

2 Methods

FCD is based on application of the sampling theorem to the volume integral equation for the electric field [7], and it effectively modifies the formula for calculation of interaction terms (i.e. off-diagonal terms of the interaction matrix). The new formula requires calculation of sine and cosine integrals, which takes some

time. However, according to our experience, this time is comparable to one iteration of the iterative solver and hence can be neglected in most cases (data not shown). The dipole polarizabilities (i.e. diagonal terms of the interaction matrix) are those of Clausius-Mossotti (CM) with $O((kd)^2)$ corrections [7].

We have implemented FCD in ADDA and used it (v.0.78.2) for all simulations presented in this paper. We tried two extreme refractive indices ($10 + 10i$ and $0.1 + i$, typical for SiC in the infrared [5]) and one moderate one ($1.6 + 0.01i$, typical for silicates in the visible). Three particle shapes were used: a sphere, a cube, and a cubical discretization of a Gaussian random field particle (GRF [15]) using 100 cubes, located on a 8×8×8 grid. We used two different sizes: $kD_x = 8$ ("large") and $kD_x = 10^{-5}$ (Rayleigh regime), where k is the wavenumber and D_x is the particle length along the x-axis. For both cases orientation of the particle was fixed. We used FCD, LDR, and RRC formulations for large particles. For the Rayleigh particles LDR and RRC are both equivalent to CM – so only FCD and CM were used. For all simulations we used the QMR iterative solver [13]. However, we also tried BiCGStab in a few cases (see below). The default threshold of the iterative solver was used (10^{-5}).

For each combination of shape, size, and refractive index we used 18 different discretizations from 8 to 512 dipoles (n_x) per D_x with approximately uniform spacing on a logarithmic scale. For large and Rayleigh particles we use $y = kd|m|$ and $1/n_x$ as discretization parameters respectively. All simulations were run on Dutch compute cluster LISA (http://www.sara.nl/userinfo/lisa/description/). Since only the sphere allows for exact analytical solution, we used the extrapolation technique [16] to infer reference results for the cube and the GRF particle. Using error estimates provided by the extrapolation technique for all formulations applied to the same particle and assuming these errors to be independent, we computed a weighted average and corrected error estimates for each formulation. For spheres we also performed extrapolation to compare its accuracy relative to the exact Mie results.

3 Results and discussion

First we analyze the total number of iterations (N_{iter}) performed by ADDA, which determine the total simulation time. For Rayleigh particles FCD is faster than CM for both extreme refractive indices, while N_{iter} is only weakly dependent on the discretization (see Fig. 1 for example). Results of N_{iter} for the best discretization ($n_x = 512$) are summarized in Table 1: FCD is about 6 and 1.2 times faster for $m = 10 + 10i$ and $0.1 + i$ respectively. For large particles with any of the considered m, as well as for Rayleigh particles with $m = 1.6 + 0.01i$, all formulations show very similar N_{iter} almost independent on y, except for the following. (1) For $m = 10 + 10i$ LDR shows strange dependence of N_{iter} on y for all studied shapes (see Fig. 2 for example). This can be explained by the nature of LDR formulation, which employs corrections of order y^2. When y is not small this correction may be large and wrong, so that it not only decreases the accuracy of simulations (see below) but also strongly increases the condition number of the interaction matrix. This is not so noticeable for very coarse discretizations due to the small dimension of interaction matrix, but become prominent for $y \sim 1$. Other formulations employ corrections given in powers of kd, which is much smaller than y for this m. (2) QMR fails for very fine discretizations of cubes for both RRC and LDR and for both extreme refractive indices (data not shown). However, BiCGStab does converges for these cases showing similar N_{iter} for all formulations (except for LDR in combination with $m = 10 + 10i$).

Due to the space limitations we can not present all the accuracy results in this contribution, and show only a few representative examples. Table 2 summarizes relative errors of absorption efficiency Q_{abs} for all studied cubes, showing errors of different formulations for the best discretization, estimate of the extrapolation error (using the 5 best discretizations), and the corrected estimate of this error. One can see that for cubes with $m = 10 + 10i$ FCD is superior (1-2 orders of magnitude) to other formulations, although for Rayleigh cubes CM yields similar accuracy after extrapolation. For cubes with $m = 0.1 + i$ FCD is 60 times more accurate than CM in the Rayleigh regime and shows similar accuracy for $kD_x = 8$, but is less accurate after extrapolation. The most surprising result is for "very moderate" $m = 1.6 + 0.01i$. FCD is more than 10 times more accurate than both LDR and RRC for cubes, although after extrapolation the accuracies are similar. Such behavior has never been reported for FCD because, to the best of our knowledge, it has never been systematically applied to cubically shaped particles (i.e. those without shape errors [16]). Accuracy results for GRF, simulated only for $m = 10 + 10i$ (data not shown), are similar to the cube results for the same m.

For spheres there is generally a relatively small difference between the accuracies of different DDA formulations, while extrapolation results for FCD have the same or worse accuracy than others (data not shown). There is only one exception, shown in Fig. 3, a large sphere with $m = 10 + 10i$. This figure also

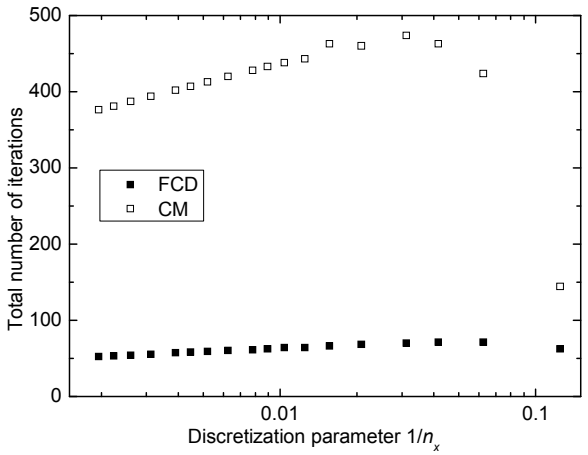

Fig. 1. N_{iter} versus $1/n_x$ for a Rayleigh cube, $m = 10 + 10i$.

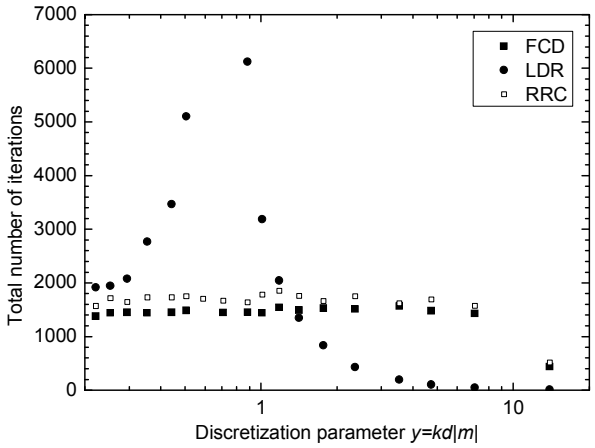

Fig. 2. N_{iter} versus y for $kD_x = 8$ sphere with $m = 10 + 10i$.

Table 1. N_{iter} for Rayleigh particles with $n_x = 512$.

	$m = 10 + 10i$			$m = 0.1 + i$	
formulation	cube	sphere	GRF	cube	sphere
FCD	52	66	82	106	86
CM	376	389	540	121	105

Table 2. Relative errors of Q_{abs} for cubes.

m	kD_x	formulation	$n_x = 512$	extr. est.	cor. est.
$10 + 10i$	$\ll 1$	FCD	8.3×10^{-4}	2.5×10^{-4}	1.2×10^{-4}
		CM	1.4×10^{-2}	1.2×10^{-4}	1.1×10^{-4}
	8	FCD	9.1×10^{-4}	3.6×10^{-5}	3.6×10^{-5}
		LDR	3.0×10^{-1}	1.5×10^{-2}	1.3×10^{-2}
		RRC	2.2×10^{-1}	3.2×10^{-2}	2.3×10^{-2}
$0.1 + i$	$\ll 1$	FCD	1.3×10^{-5}	4.6×10^{-5}	5.9×10^{-5}
		CM	7.7×10^{-4}	4.6×10^{-6}	4.6×10^{-6}
	8	FCD	1.4×10^{-4}	9.0×10^{-4}	1.3×10^{-3}
		LDR	2.4×10^{-4}	2.2×10^{-5}	1.0×10^{-5}
		RRC	1.8×10^{-4}	1.0×10^{-5}	9.7×10^{-6}
$1.6 + 0.01i$	$\ll 1$	FCD	1.7×10^{-7}	8.9×10^{-6}	1.7×10^{-6}
		CM	1.6×10^{-4}	1.4×10^{-6}	1.4×10^{-6}
	8	FCD	1.7×10^{-5}	1.9×10^{-5}	7.8×10^{-6}
		LDR	2.3×10^{-4}	8.7×10^{-6}	7.9×10^{-6}
		RRC	1.5×10^{-4}	5.4×10^{-5}	1.3×10^{-5}

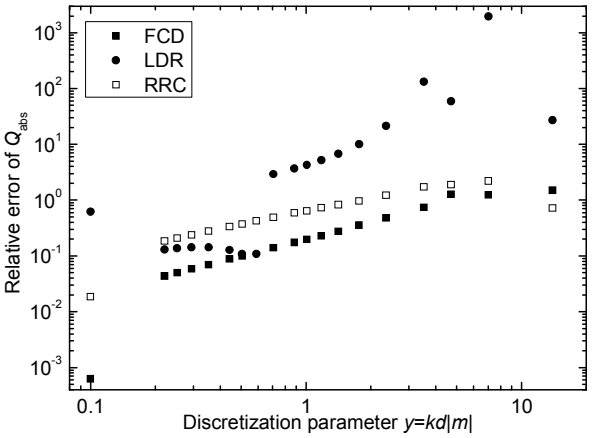

Fig. 3. Relative error of Q_{abs} versus y for $kD_x = 8$ sphere with $m = 10 + 10i$ in log-log scale. Points for $y = 0.1$ depict errors of extrapolated values (using 9 best discretizations) compared to the Mie solution.

shows typical behavior of LDR errors versus y for this m. So we can conclude that LDR is the worst possible option for $m = 10 + 10i$. The general tendency, exemplified in Fig. 3, is that when FCD is superior for $n_x = 512$ it is also superior for almost the whole studied range of FCD, although its superiority for smaller n_x may be smaller, since FCD seems to have a larger exponent in the power dependence of errors on y. The inability of FCD to improve accuracy for spheres in general is probably because shape errors, to which FCD is susceptible to the same extent, contribute most to the total errors for the studied sizes and refractive indices. Further study is required to check this hypothesis. Accuracies of extinction efficiency and angle-resolved S_{11} and $-S_{21}/S_{11}$ show the same trends as that of Q_{abs} (data not shown).

It should be noted that in some cases FCD convergence is oscillatory around the linear trend in log-log scale (data not shown), which explains relatively large errors during extrapolation of its results. However, currently there exists no easy-to-use and robust implementation of DDA extrapolation technique for arbitrary particles, i.e. performance of the extrapolation should first be tested on a class of similar problems, using some reference results. Therefore, for practical applications good accuracy of single DDA simulations seem to be more important than good potential for extrapolation.

FCD makes extreme refractive indices much more feasible for DDA simulations, but they still require extreme computer power. We do not present computational times in this paper, but only give a few guiding values. Requiring moderate accuracy of 10% in Q_{abs} (which is considered sufficient e.g. for computing an absorption spectrum of astrophysical dust), a single DDA simulation will fit into 2 GB of

memory and will take about 10 and 2 hours on 3 GHz single-core processor for single orientation of wavelength-sized particles with refractive index $10 + 10\mathrm{i}$ and $0.1 + \mathrm{i}$ respectively. However, required time can be as small as a few minutes for Rayleigh or cubically shaped particles.

3 Conclusion

We have compared three DDA formulations: FCD, LDR, and RRC for simulations of light scattering by cubes, spheres, and GRF with sizes comparable and much smaller than the wavelength, using three refractive indices: $10 + 10\mathrm{i}$, $0.1 + \mathrm{i}$, and $1.6 + 0.01\mathrm{i}$. FCD improves convergence of the iterative solver for Rayleigh particles and extreme refractive indices: it is about 6 and 1.2 times faster than CM for $m = 10 + 10\mathrm{i}$ and $0.1 + \mathrm{i}$ respectively. FCD significantly decreases discretization errors of the DDA compared to other formulations almost for all studied cases, including moderate value of m. This is clearly visible for cubes and GRF, since their results are not obscured by the presence of large shape errors. The improvement of accuracy is up to a factor 100. The only drawback of FCD is that in some cases the extrapolation technique applied to its results leads to larger errors than for other formulations. If comparing LDR and RRC, our results show that LDR is a “never use” option for $m = 10 + 10\mathrm{i}$, comparable to RRC (and generally to FCD) for $m = 0.1 + \mathrm{I}$, and better than RRC for $1.6 + 0.01\mathrm{i}$ (the latter is well-known in the literature).

FCD has been implemented in the publicly available code ADDA and is ready to be applied by the light scattering community. Although further comparative studies are definitely required, FCD is at least a very good candidate to become a default DDA formulation for day-to-day simulations. Extreme refractive indices, such as considered in this paper, can be routinely (although not quickly) simulated using modern desktop computers.

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