

# An extrapolation technique to increase the accuracy of the Discrete Dipole Approximation

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## Abstract

We propose an extrapolation technique that allows accuracy improvement of Discrete Dipole Approximation computations. The performance of this technique was studied empirically based on extensive simulations for 5 test cases using many different discretizations. The quality of the extrapolation improves with refining discretization reaching extraordinary performance especially for cubically shaped particles. A two order of magnitude decrease of error was demonstrated. We also propose estimates of the extrapolation error, which were proven to be reliable.

## 1 Introduction

The Discrete Dipole Approximation (DDA) is a well-known method to solve the light scattering problem for arbitrary shaped particles [1]. Since DDA has an extreme computational complexity, the usual application strategy for DDA is “single computation”, where a discretization is chosen based on available computational resources and some empirical estimates of the expected errors [2]. These error estimates are based on a limited number of benchmark calculations [2] and hence are external to the light scattering problem under investigation. Such error estimates have evident drawbacks, however no better alternative is available.

Usually, errors in DDA are studied as a function of the size parameter of the scatterer  $x$  (at a constant or few different values of number of dipoles  $N$ , see, e.g. [1]). Few papers directly present errors versus discretization parameter (e.g.  $d$  – the size of a single dipole). The range of  $d$  typically studied in those papers is typically limited to a 5 times difference between minimum and maximum values. Only two of these papers [3, 4] use extrapolation (to zero  $d$ ) to get an exact result of some measured quantity, however they use the simplest linear extrapolation without any theoretical foundation nor discussion of its capabilities.

In this study we introduce an extrapolation technique (Sect. 2) to improve the accuracy of DDA computations with a relatively small increase of computation time. We provide a step-by-step prescription, which can be used with any existing DDA code without any modifications. In Sect. 3 we present few numerical results of DDA computations for 5 different scatterers using many different discretizations. These results are discussed to evaluate the performance of the extrapolation technique. We formulate the conclusions of the study in Sect. 4.

## 2 Extrapolation

We have submitted a paper [5], in which we performed a theoretical analysis of DDA convergence when refining the discretization. There we proved that the error of any measured quantity is bounded by a quadratic function of the discretization parameter  $y = kd|m|$  ( $k$  – free space wave vector,  $m$  – refractive index of the

scatterer):

$$|\delta\phi^y| \leq (a_2^\phi - b_2^\phi \ln y)y^2 + (a_1^\phi - b_1^\phi \ln y)y, \quad (1)$$

where  $y$  is some measured quantity (e.g. extinction efficiency  $Q_{\text{ext}}$ , Mueller matrix elements at some scattering angle  $S_{ij}(\theta)$ , etc.) and  $\delta\phi^y$  its error (difference between a result of the numerical simulation and an exact value).  $a_{1,2}^\phi, b_{1,2}^\phi$  are constants (independent of  $y$ ).

Here, we proceed and assume that for sufficiently small  $y$ ,  $\delta\phi^y$  can in fact be approximated by a quadratic function of  $y$  (taking the logarithmic term as a constant):

$$\phi^y = a_0 + a_1 y + a_2 y^2 + \zeta^y, \quad (2)$$

where  $a_0, a_1, a_2$  are constants that are chosen such that  $\zeta^y$  – the error of the approximation – is minimized.  $a_0$  is then an estimate for the exact value of the measured quantity  $\phi^0$ ; it is determined by a least-square quadratic fit over several points  $\{y, \phi^y\}$ , which are obtained by a standard DDA simulation.

Practical implementation of such fit has several free parameters. Below, we present our choice, which is not necessarily optimal and may be improved. However, it does work well for several test cases, thus demonstrating the potential power of our approach. We select computational points  $y$  in the range  $[y_{\text{min}}, y_{\text{max}}]$  and space them uniformly in logarithmic scale.  $\zeta^y$  is considered to be proportional to  $y^3$ , and the weights in definition of the  $\chi^2$ , which is minimized during the fit, are the inverse. The Standard Error (SE) of  $a_0$  that is obtained during the least-square fit [6] is multiplied by an empiric constant to estimate the error of the extrapolation. This constant is based on the test cases that we have studied (to make this estimate reliable).

The performance of extrapolation technique significantly differs for particles, which shape can or can not be described by a set of cubical dipoles. We call it cubically (c) and non-cubically (nc) shaped scatterers, respectively. We can now formulate the step-by-step extrapolation technique:

1. Select  $y_{\text{min}}$  based on your computational resources.
2. Take  $y_{\text{max}}$  to be 2 (c) or 4 (nc) times  $y_{\text{min}}$  but not larger than 1.
3. Choose 5 (c) or 9 (nc) points over the interval  $[y_{\text{min}}, y_{\text{max}}]$  approximately uniformly spaced on a logarithmic scale.
4. Perform DDA computations for each  $y$ .
5. Fit the quadratic function (Eq. (2)) over the points  $\{y, \phi^y\}$  using  $y^3$  as errors of data points;  $a_0$  is then the estimate of  $\phi^0$ .
6. Multiply SE of  $a_0$  by 10 (c) or 2 (nc) to obtain an estimate of the extrapolation error.

Results of using this procedure are presented in Sect. 3, together with computational costs.

The extrapolation procedure is similar to a Romberg integration method [6], which is adaptive. The error estimate, obtained by extrapolation, is an internal accuracy indicator of DDA computations that is just as important as the increase in the accuracy itself. Our error estimate opens the way to adaptive DDA, i.e. a code that will reach a required accuracy, using minimum computational resources.

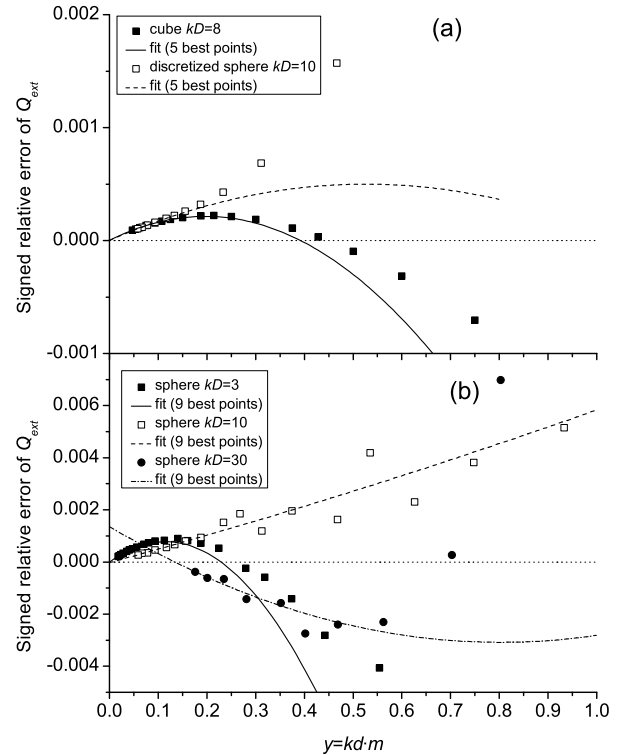


Figure 1: Signed relative errors of  $Q_{\text{ext}}$  versus  $y$  and their fits by quadratic functions for (a)  $kD = 8$  cube and discretized  $kD = 10$  sphere, (b) 3 spheres.

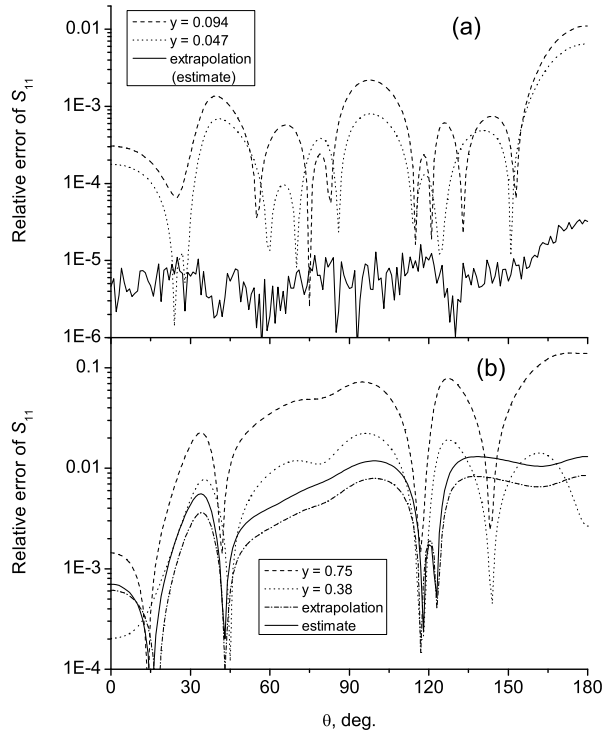


Figure 2: Errors of  $S_{11}(\theta)$  in logarithmic scale for extrapolation using 5 values of  $y$  in the intervals  $[0.047, 0.094]$  (a) and  $[0.38, 0.75]$  (b) for  $kD = 8$  cube. Estimate of the extrapolation error is  $10 \times SE$ .

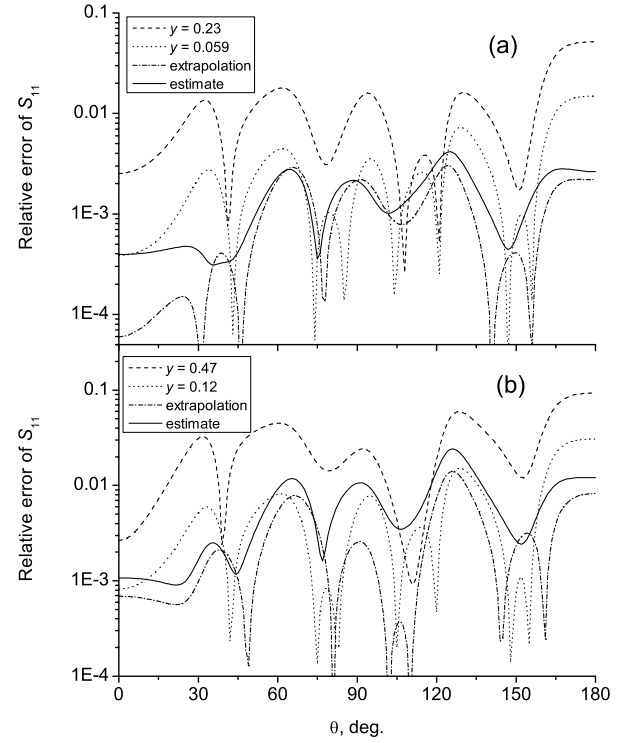


Figure 3: Errors of  $S_{11}(\theta)$  in logarithmic scale for extrapolation using 9 values of  $y$  in the intervals  $[0.059, 0.23]$  (a) and  $[0.12, 0.47]$  (b) for  $kD = 10$  sphere. Estimate of the extrapolation error is  $2 \times SE$ .

### 3 Simulation results

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 an unlimited number of dipoles, since we are not limited by the memory of a single computer [7, 8]. The execution time of extrapolation is by a constant factor higher than time of a single simulation with discretization  $y_{\min}$ :  $t_5 < 2.5t(y_{\min})$  and  $t_9 < 2.7t(y_{\min})$  for 5 and 9 points, respectively. Memory requirements are the same as for a single  $y_{\min}$  computation. All DDA simulations were carried out on the Dutch national compute cluster LISA [9].

We study five test cases: one cube with  $kD = 8$ , three spheres with  $kD = 3, 10, 30$ , and a particle obtained by a cubical discretization of the  $kD = 10$  sphere using 16 dipoles per  $D$ . By  $D$  we denote the diameter of a sphere or the edge size of a cube. All scatterers are homogenous with  $m = 1.5$ . The maximum number of dipoles per  $D$  ( $n_D$ ) was 256 — other points were chosen according to the technique described in Sect. 2.

Figure 1 shows simulation results of  $Q_{\text{ext}}$  for all the test cases and extrapolation through the best points. The reference values for the cube and discretized sphere are obtained by the best extrapolation, and for spheres — by the Mie theory.

Extrapolation results of  $S_{11}(\theta)$  for the cube are shown in Fig. 2. When  $y_{\min} = 0.047$ , maximum (over the scattering angle) errors are decreased by more than two orders of magnitude. The extrapolation gives significant improvement of the accuracy even when  $y_{\min} = 0.38$ .

Extrapolation performance for non-cubically shaped particles is not that exciting, which is illustrated in Fig. 3, however accuracy is improved by almost an order of magnitude when  $y_{\min} = 0.059$ . Estimates of the errors do enclose the real errors (Figs. 2 and 3), which is also supported by all the test cases.

## 4 Conclusion

Based on the theoretical convergence analysis as presented in [5], we proposed an extrapolation technique together with a step-by-step prescription, which allows accuracy improvement of DDA computations. The performance of this technique was studied empirically and we showed that it significantly suppresses maximum errors of  $S_{11}(\theta)$  when  $y_{\min} < 0.4$  and 0.15 for cubically and non-cubically shaped scatterers, respectively (for  $m = 1.5$ ). The quality of the extrapolation improves with decreasing  $y_{\min}$  reaching extraordinary performance, especially for cubically shaped particles – more than two order of magnitude decrease of error when  $y_{\min} \approx 0.05$  for wavelength-sized scatterers (total computational time for extrapolation is less than 2.7 times that for a single DDA computation).

The proposed estimates of the extrapolation error were proven to be reliable, although they can be improved to decrease overestimation of the errors in some cases. This error estimate is completely internal, and hence can be used to create adaptive DDA – a code that will automatically refine discretization to reach a required accuracy.

The extrapolation technique is more suited for benchmark calculations to increase the accuracy of already accurate results (compare the limitations above with the usual DDA discretization  $y = 0.6$  [2]), however even for large  $y_{\min}$  it can provide an useful error estimate. However, further investigation on other test scatterers is required to evaluate the performance of the technique.

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