

Convergence of the discrete dipole approximation. II. An extrapolation technique to increase the accuracy

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We propose an extrapolation technique that allows accuracy improvement of discrete dipole approximation computations. The performance of this technique was studied empirically on the basis of extensive simulations for five test cases using many different discretizations. The quality of the extrapolation improves with refining discretization, reaching extraordinary performance especially for cubically shaped particles. A 2-order-of-magnitude decrease of error is demonstrated. We also propose estimates of the extrapolation error, which are proven to be reliable. Finally, we propose a simple method to directly separate shape and discretization errors and illustrate this for one test case. © 2006 Optical Society of America

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1. INTRODUCTION

The discrete dipole approximation (DDA) is a well-known method to solve the light-scattering problem for arbitrary shaped particles. Since its introduction by Purcell and Pennypacker,¹ it has been improved constantly. The formulation of the DDA summarized by Draine and Flatau² more than ten years ago is still the one most widely used for different applications,³ partly owing to the publicly available high-quality and user-friendly code DDSCAT.⁴

DDA directly discretizes the volume of the scatterer and hence is applicable to arbitrarily shaped particles. However, the drawback of this discretization is the extreme computational complexity of DDA of $O(N^2)$, where N is the number of dipoles. This complexity is decreased to $O(N \log N)$ by advanced numerical techniques.^{2,5} Still, the usual application strategy for DDA is single computation, where a discretization is chosen on the basis of available computational resources and some empirical estimates of the expected errors.^{3,4} These error estimates are based on a limited number of benchmark calculations³ 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 N), e.g., Refs. 2 and 6. Only several pa-

pers directly present errors versus discretization parameter (e.g., d —the size of a single dipole).^{7–15} The range of d typically studied in those papers is limited to a five-times difference between minimum and maximum values (with the exception of two papers^{9,10} where it is 15 times). Only two papers^{7,15} 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 or discussion of its capabilities.

It has been acknowledged for a long time that DDA errors are due to two different factors: shape (it is not always possible to describe the particle shape exactly by a collection of cubical cells) and discretization (finite size of each cell).⁶ However, the question of which of them is more important in different cases is still open. A discussion on this issue spanned through several papers^{16–20} that have not reached any definite conclusions yet. The uncertainty is due to the indirect methods used that have inherent interpretation problems.

In our accompanying paper,²¹ which from now on we will refer to as Paper 1, we performed a theoretical analysis of DDA convergence when refining the discretization. It provides the basis for this paper, where an extrapolation technique is introduced (Section 2) to improve the accuracy of DDA computations. We thoroughly discuss all free parameters that influence extrapolation performance

and provide a step-by-step prescription, which can be used with any existing DDA code without any modifications. It is important to note that, although Paper 1 provides a firm theoretical background, it is not necessary to go through all theoretical details to understand and apply the extrapolation technique that we introduce here. In Section 3 we present extensive numerical results of DDA computations for five different scatterers using many different discretizations. These results are discussed in Section 4 in evaluating the performance of the extrapolation technique. We also propose a method (new to our knowledge) to directly separate shape and discretization errors of DDA (described and illustrated in Subsection 3.B). The results and possible applications are discussed in Section 4. We formulate the conclusions of the paper in Section 5.

2. EXTRAPOLATION

In this section we describe a straightforward technique to significantly increase the accuracy of a DDA simulation with a relatively small increase of computation time. This technique does not require any modification of a DDA program but only postprocessing of computed data. Therefore it can be easily implemented in any existing DDA code.

In Paper 1 we have proven that the error of any measured quantity is bounded by a quadratic function of the discretization parameter $y = kd|m|$ (k is a free-space wave vector, m is the 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 ϕ^y is some measured quantity [e.g., extinction efficiency Q_{ext} , Mueller matrix elements at some scattering angle $S_{ij}(\theta)$, etc.] and $\delta\phi^y$ is 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), which are described in detail in Paper 1.

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). The applicability of this assumption will be tested empirically in Subsection 3.B. Introduction of higher-order terms is possible but not necessary (contrary to the quadratic term), and we avoid it in order to keep our technique as simple and robust as possible. We can now write

$$\phi^y = a_0 + a_1y + a_2y^2 + \zeta^y, \quad (2)$$

where a_0, a_1, a_2 are constants that are chosen such that ζ^y —the error of the approximation—is minimized, a_0 is then an estimate for the exact value of the measured quantity ϕ^0 . A procedure to determine a_0 is basically fitting a quadratic function over several points $\{y, \phi^y\}$, which are obtained by a standard DDA simulation. In the ideal case of $\zeta^y = 0$, one can use any three values of y to obtain the exact value of ϕ^0 . However, in practice, different fits will always give different results. We limit ourselves to the usual least-squares polynomial fit of the data. There are three questions one should answer before conducting such a fit.

- (1) How many and which values of y to use?
- (2) How to weight the influence of different calculated values used in the fitting; i.e., what is the behavior of expected errors ζ^y ? (Note that in the polynomial fit we minimize χ^2 , the summation of the squared difference between computed values and the fitting function weighted by the inverse of the expected error ζ^y .)
- (3) How to estimate the difference between a_0 and ϕ^0 , i.e., the error of the final result?

It is important to note that, although there are some theoretical hints, answers to these questions are mainly empirical and should be tested. Our approach is based on the test cases presented in Subsection 3.B. These may not be representative for all scattering problems, but they do show the potential power of our approach. We do not attempt to choose the most suitable fit options but merely demonstrate the applicability of the technique.

We start by analyzing the second question: what is the expected deviation from the quadratic model; i.e., what is the functional dependence of ζ^y on y , to be used as a weighting function in the polynomial-fitting procedure? For cubically shaped particles, defined in Paper 1 as particles whose shape can be exactly discretized using cubical subvolumes, one expects a smooth variation of the function ϕ^y , and the error can be attributed as a model error, i.e., coming mainly from neglecting higher-order terms in the convergence analysis of Paper 1. In that case the error ζ^y is expected to be a cubical function of y . We have tried cubical, quadratic, and linear error functions when fitting results for cubically shaped particles and found that, although the differences are small, cubical errors generally lead to the best fits (data not shown).

Shape errors, which are present for noncubically shaped particles, are expected to be very sensitive to y because they depend on the position of the particle surface inside the boundary dipole that changes considerably by a small variation of y (for details, see Paper 1). Therefore shape errors can be viewed as random noise superimposed on a smooth variation of ϕ^y . The asymptotic behavior of shape errors is linear in y (see Paper 1). Indeed, in certain cases we found that using linear errors ζ^y results in significantly better fits than when using cubical errors. However, in other cases, linear errors performed significantly worse. In our experience, using a cubical error function is, in general, always more reliable, even in the presence of shape errors, because it decreases the influence of points with high values of y , where the error is larger and less predictable. Since we want the procedure to be as robust as possible and not to use more complex error functions than strictly needed (e.g., polynomial), we take a cubical dependence of the error ζ^y , for both cubically and noncubically shaped scatterers.

The choice of values of y for computation can be described by the interval $[y_{\min}, y_{\max}]$, the number of points, and their spacing. y_{\min} is usually determined by available computer hardware (time or memory bounds), which is the best discretization that can be computed for a given resource. The goal of the extrapolation procedure is to increase the accuracy beyond this single DDA boundary. We will show in Subsection 3.B that the overall performance of this technique strongly depends on y_{\min} .

The choice of y_{\max} is governed by two notions: a larger interval of data points generally leads to better extrapolation, but errors for high values of y are more random and their significance is anyway much smaller (since we use a cubical error function). We have found that for cubically shaped scatterers a good choice is $y_{\max}=2y_{\min}$, while for noncubically shaped scatterers increasing the interval to $y_{\max}=4y_{\min}$ does improve the fits. Probably that is due to the fact that the quality of fit for noncubically shaped scatterers is determined by quasi-random shape errors and increasing the range leads to larger statistical significance of the result. We will also demand that y_{\max} be less than 1, since otherwise DDA is definitely far from its asymptotic behavior.

Spacing of the sample points depends partly on the problem, especially for cubically shaped scatterers (in that case an arbitrary number of dipoles cannot be used). We space computational points approximately uniform on a logarithmic scale, acknowledging the fact that a relative difference in y is more significant than an absolute. The total number of points should be large enough for statistical significance. However, a large number of points increases computational time. We have used five points for cubically shaped particles (the ratio of $1/y$ values is 8:7:6:5:4) and nine points for noncubically shaped particles (the ratio of $1/y$ values is 16:14:12:10:8:7:6:5:4) or less if $y_{\max} < 4y_{\min}$.

The estimation of the error of the final result is difficult, since this error is due to model imperfection and not to some kind of random noise. The standard least-squares-fitting technique²² provides a standard error (SE) for the parameter a_0 , which we use as a starting point. Numerical simulations (Subsection 3.B) show that for spheres (the only noncubical shape we studied) real errors are less than 2(SE) in most cases. That is what one would expect if ζ^y is considered completely random (which is similar to the expected behavior of the shape errors). For cubical shapes, on the contrary, we have to estimate the error as 10(SE) to reliably describe the real errors. It is important to note that an error estimate based on the SE is the simplest one can use. Its drawback is that we have to use a large multiplier (based on the real errors obtained in some of our simulations), which may lead to significant overestimation of real errors in certain cases.

We can now formulate the step-by-step extrapolation technique. We use abbreviations (c) and (nc) for cubically and noncubically shaped scatterers, respectively.

- (1) Select y_{\min} on the basis of your computational resources.
- (2) Take y_{\max} to be 2 (c) or 4 (nc) times y_{\min} but not larger than 1.
- (3) Choose five (c) or nine (nc) points over the interval $[y_{\min}, y_{\max}]$ 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 ϕ^0 .
- (6) Multiply the 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 Section 3, together with computational costs.

The extrapolation procedure is similar to a Romberg integration method,²² 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.

3. NUMERICAL SIMULATIONS

A. Discrete Dipole Approximation

The basics of the DDA method were summarized by Draine and Flatau.² In this paper we use the lattice dispersion relation prescription for dipole polarizability,²³ which is most widely used nowadays, e.g., in the publicly available code DDSCAT 6.1.⁴ We also employ dipole size correction⁶ for noncubically shaped scatterers to ensure that the cubical approximation of the scatterer has the correct volume; this is believed to diminish shape errors, especially for small scatterers.² We use a standard discretization scheme without any improvements for boundary dipoles.

The main numerical challenge of DDA is to solve a large system of $3N$ linear equations. This is done iteratively using a Krylov-subspace method,²² while the matrix-vector products are computed using a fast Fourier transform (FFT)-based algorithm.⁵ Our code—AMSTERDAM DDA²⁴—is capable of running on a cluster of computers (parallelizing a single DDA computation), which allows us to use a practically unlimited number of dipoles, since we are not limited by the memory of a single computer.^{25,26} We used a relative error of residual $< 10^{-8}$ as a stopping criterion. Tests suggest that the relative error of the measured quantities due to the iterative solver is then $< 10^{-7}$ (data not shown) and hence can be neglected (total relative errors in our simulations are $> 10^{-6} \div 10^{-5}$ —see Subsection 3.B). All DDA simulations were carried out on the Dutch national computer cluster LISA.²⁷

The execution time of one iteration depends solely on N ; it consists of an arithmetic part that scales linearly with N and an FFT part that scales as $N \ln N$. The number of iterations only slightly depends on the discretization parameter y for fixed geometry of the scatterer. Rahaola proved this theoretically for any Krylov-subspace method,²⁸ and our own experience agrees with this conclusion. Therefore the total computational time scales linearly with $N(\propto y^{-3})$ or slightly faster (considering logarithm and imperfect optimization), which is consistent with our timing results (data not shown).

We can now estimate the computational overhead of the extrapolation technique compared with a single DDA computation for y_{\min} [$\text{time} - t(y_{\min})$]. Considering the spacing of points we used (described in Section 2), the execution time needed for the five-point computation is $t_5 < 2.5t(y_{\min})$ and that for the nine-point computation is $t_9 < 2.7t(y_{\min})$. Memory requirements are the same as for a single computation. For comparison, one should note that an eight-times increase in computational time and

memory requirements (for a single DDA computation with $y=y_{\min}/2$) gives only a two- to four-times increase in accuracy (depending in which error regime—linear or quadratic— y_{\min} is located).

B. Results

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 (total 2176 dipoles, see Fig. 1, x equal to that of a sphere). By D we denote the diameter of a sphere or the edge size of a cube. All scatterers are homogenous with $m=1.5$. Although DDA errors significantly depend on m (see, e.g., Ref. 12), we limit ourselves to one single value and study the effects of size and shape of the scatterer.

The maximum number of dipoles per D (n_D) was 256. The values of n_D that we used are of the form $\{4, 5, 6, 7\}$ (2^p) (p is an integer), except for the discretized sphere, where all n_D are multiples of 16 (this is required to exactly describe the shape of the particle composed from a number of cubes—see Fig. 1). The minimum values for n_D were 8 for the $kD=3$ sphere; 16 for the cube, the $kD=10$ sphere, and the discretized sphere; and 40 for the $kD=30$ sphere.

Typical computation time for the finest discretization (for the cube with $y=0.047$, resulting in $N=1.7 \times 10^7$) currently is 2.5 h on a cluster of 64 P4 3.4 GHz processors. We expect that it can be improved by an order of magnitude by using modern FFT routines (e.g., Fastest Fourier Transform in the West²⁹) and faster iterative solvers (biconjugate gradient stabilized and quasi-minimal residual, which were shown to be clearly superior to conjugate gradient applied to the normalized equations with minimization of the residual norm,^{30,31} which we still use). We are currently improving our code along these lines.

All computations use a direction of incidence parallel to one of the principal axes of the cubical dipoles. The scat-

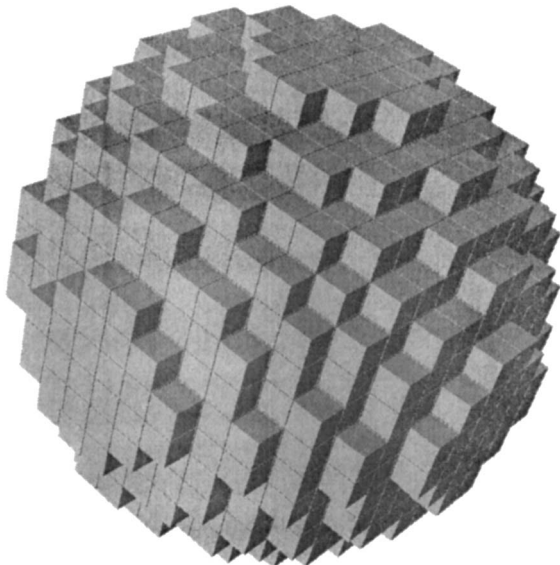


Fig. 1. Cubical discretization of a sphere using 16 dipoles per diameter (total 2176 dipoles).

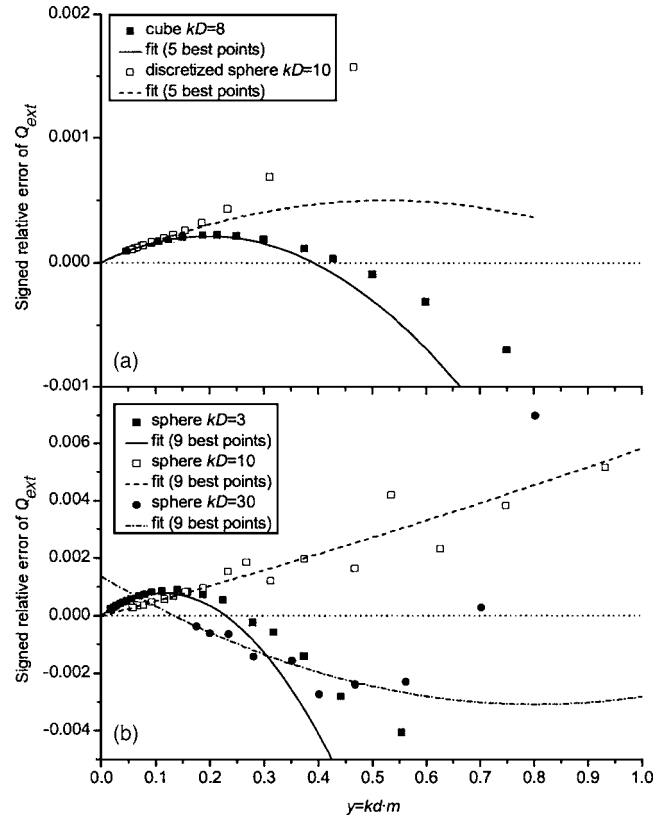


Fig. 2. Signed relative errors of Q_{ext} versus y and their fits by quadratic functions for (a) the $kD=8$ cube and discretized $kD=10$ sphere, (b) three spheres. Five and nine best points are used for fits in (a) and (b), respectively.

tering plane is parallel to one of the faces of the cubical dipoles. In this paper we show results only for the extinction efficiency Q_{ext} (for incident light polarized parallel to one of the principal axes of the cubical dipoles) and phase function $S_{11}(\theta)$ as the most commonly used in applications. However, the extrapolation technique is equally applicable to any measured quantity. For instance, we have also applied it to other Mueller matrix elements (data not shown).

Reference (exact) results of $S_{11}(\theta)$ and Q_{ext} for spheres are obtained by Mie theory (the relative accuracy of the code we use³² is at least $<10^{-6}$). Unfortunately, no analytical theory is available for the cube and the discretized sphere, which could provide us with exact results. Instead, we use extrapolation over the five finest discretizations as reference results for these shapes.

To justify this choice, we discuss, as an example, simulation results of Q_{ext} for the cube. Instead of showing values of Q_{ext} itself, we show in Fig. 2(a) ($Q_{ext}/a_0 - 1$), with a_0 obtained through fitting the five finest discretizations. The extrapolation through these five best points ($y_{\min}=0.047$, $y_{\max}=0.094$) is also shown. The deviation of the fit from the five best points [that overlap on Fig. 2(a)] is very small indeed. This is also characterized by a small estimate of the extrapolation error 1.8×10^{-6} (see Table 1). In Paper 1 we proved that the DDA converges to the exact solution; therefore the result of the best extrapolation should be close to the exact result. The relative difference between the best discretization and the best extrapolation

is only 9.0×10^{-5} ; therefore it does not make a big difference which one to use as a reference when evaluating, for instance, the error of the extrapolation through the five worst discretizations ($y_{\min}=0.38, y_{\max}=0.75$). Hence all conclusions with respect to the reliability of the error estimates (as discussed in Section 4) do not depend on the choice of reference if y_{\max} is large enough. We also apply this reasoning to smaller y_{\min} and assume that using the reference value obtained by extrapolation of the finest discretizations is a good enough estimate of the exact value.

The same justification is valid for the discretized sphere (see Table 1 for Q_{ext} results). Comparison of errors of different extrapolation results of $S_{11}(\theta)$ (shown in Figs. 3 and 4) is even more convincing. Reference results themselves [both of Q_{ext} and $S_{11}(\theta)$] can be found in Paper 1.

Next, we show the results obtained by the extrapolation technique. The dependence of the signed relative errors of Q_{ext} on y for all five test cases is shown in Fig. 2. Figure 2(a) depicts results for the cube and the discretized sphere. The five best points for each scatterer are fitted by a quadratic function, using the method described in Section 2. Figure 2(b) depicts extrapolation results for spheres, using the nine best points for each of them (cf. Section 2). Since the exact Mie solution is available, the intersection of a fit with a vertical axis is a measure of the accuracy of the extrapolation result. Table 1 summarizes

Table 1. Extrapolation Errors of Q_{ext} ^a

y_{\min}	y_{\max}	p	Error of y_{\min}	Extrapolation	
				Estimate	Real
<i>kD=8 Cube</i>					
0.047	0.094	5	9.0×10^{-5}	1.8×10^{-6}	—
0.094	0.19	5	1.6×10^{-4}	6.6×10^{-6}	4.6×10^{-6}
0.19	0.38	5	2.2×10^{-4}	5.3×10^{-5}	4.0×10^{-5}
0.38	0.75	5	1.1×10^{-4}	3.7×10^{-4}	3.2×10^{-4}
<i>Discretized $kD=10$ Sphere</i>					
0.058	0.12	5	1.0×10^{-4}	2.4×10^{-5}	—
0.12	0.23	5	2.0×10^{-4}	9.0×10^{-6}	7.9×10^{-6}
0.23	0.93	4	4.3×10^{-4}	1.2×10^{-3}	5.9×10^{-4}
<i>$kD=3$ Sphere</i>					
0.018	0.070	9	2.2×10^{-4}	1.0×10^{-5}	4.1×10^{-6}
0.035	0.14	9	4.0×10^{-4}	5.9×10^{-5}	4.8×10^{-5}
0.070	0.28	9	6.8×10^{-4}	8.7×10^{-5}	5.7×10^{-6}
0.14	0.54	9	9.0×10^{-4}	3.7×10^{-4}	7.0×10^{-4}
0.28	0.54	5	2.4×10^{-4}	4.3×10^{-3}	1.8×10^{-3}
<i>$kD=10$ Sphere</i>					
0.059	0.23	9	2.7×10^{-4}	2.0×10^{-4}	2.7×10^{-5}
0.12	0.47	9	5.5×10^{-4}	5.5×10^{-4}	3.7×10^{-4}
0.23	0.93	9	1.5×10^{-3}	3.1×10^{-3}	2.1×10^{-3}
<i>$kD=30$ Sphere</i>					
0.18	0.70	9	3.8×10^{-4}	1.3×10^{-3}	1.4×10^{-3}
0.18	0.35	5	3.8×10^{-4}	3.3×10^{-3}	6.9×10^{-4}

^a p is number of points used. Estimate of the extrapolation errors is 10(SE) for first two particles and 2(SE) for spheres.

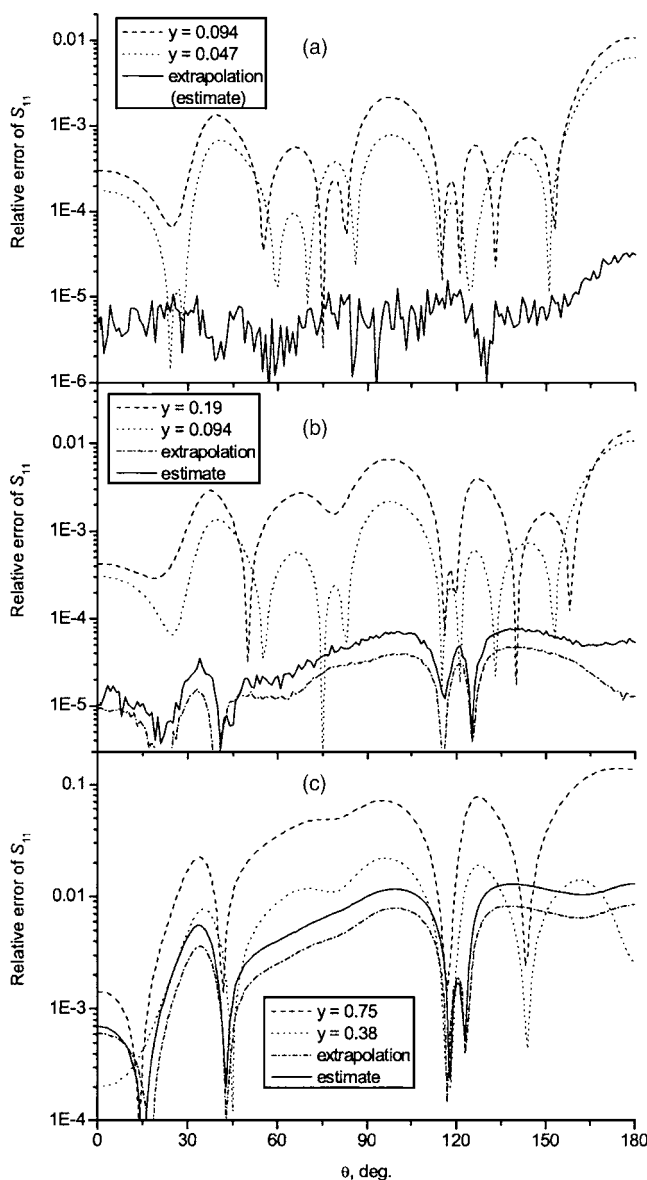


Fig. 3. Errors of $S_{11}(\theta)$ in logarithmic scale for extrapolation using five values of y in the intervals (a) [0.047,0.094], (b) [0.094,0.19], and (c) [0.38,0.75] for the $kD=8$ cube. Estimate of the extrapolation error is 10(SE).

the parameters (y_{\min}, y_{\max} , number of points) of all the extrapolations that were carried out and their performance for Q_{ext} .

Next, we present some of the extrapolation results for $S_{11}(\theta)$. Results for the cube are shown in Fig. 3. Each subfigure shows real (compared with the best extrapolation—reference) and estimated errors together with the errors of the finest and crudest discretizations used. Only the estimate of the error is shown for the best extrapolation—Figs. 3(b) and 3(c) show extrapolation results using five points in the intervals [0.094,0.19] and [0.38,0.75], respectively. The performance of the extrapolation for the discretized sphere is shown in Fig. 4: Fig. 4(a) shows the best extrapolation, and Figs. 4(b) and 4(c) show results for extrapolation using five and four points in the intervals [0.12,0.23] and [0.23,0.93], respectively. The broad spacing of points for extrapolation depicted in Fig. 4(c) is, as

was noted above, due to the complex shape of the discretized sphere that limits possible values of y to be 0.93 divided by an integer [total time for computing these four points is $<1.6t(y_{\min})$]. It is important to note once more that we use $10(SE)$ an estimate of extrapolation error for the cube and discretized sphere and $2(SE)$ for spheres (cf. Section 2).

Extrapolation results for the $kD=3$ sphere are summarized in Fig. 5: Fig. 5(a) shows the best extrapolation (using nine points in the interval $[0.018, 0.070]$), and Fig. 5(b) shows the worst, but still satisfactory, result, i.e., one that shows definite improvement of accuracy over most of the θ range. The extrapolation using five points from the interval $[0.28, 0.54]$ is no longer satisfactory (data not shown). Errors of the two best extrapolations for the

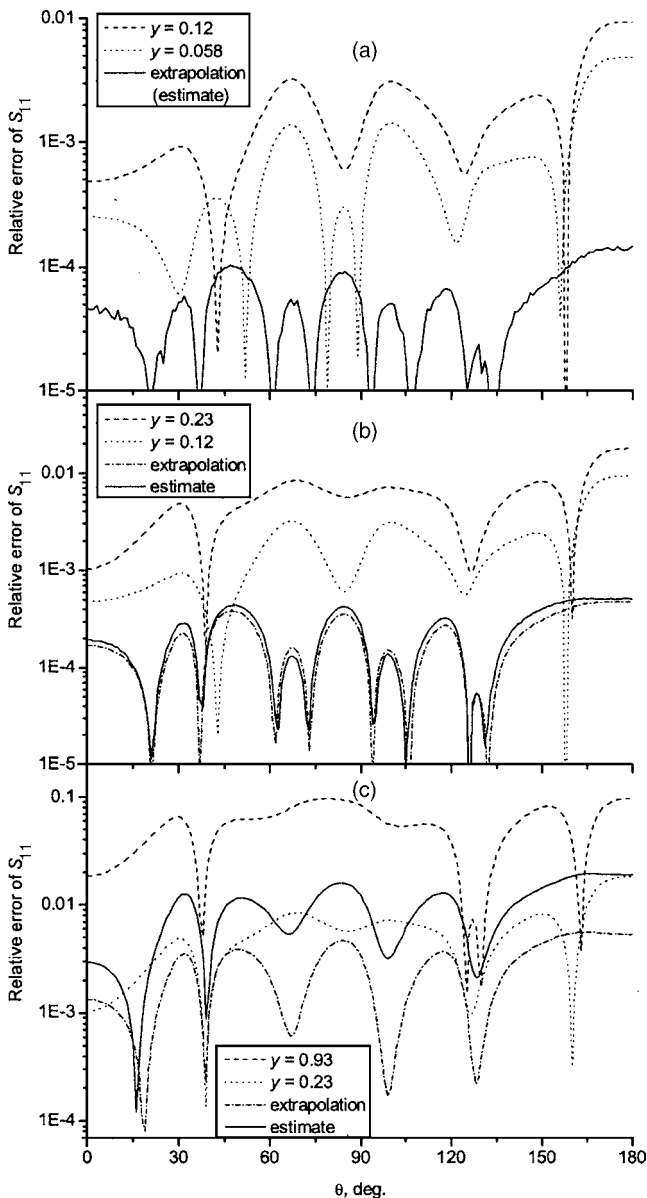


Fig. 4. Errors of $S_{11}(\theta)$ in logarithmic scale for extrapolation using five values of y in the intervals (a) $[0.058, 0.12]$, (b) $[0.12, 0.23]$ and using four values of y in the interval (c) $[0.23, 0.93]$ for the discretized $kD=10$ sphere. Estimate of the extrapolation error is $10(SE)$.

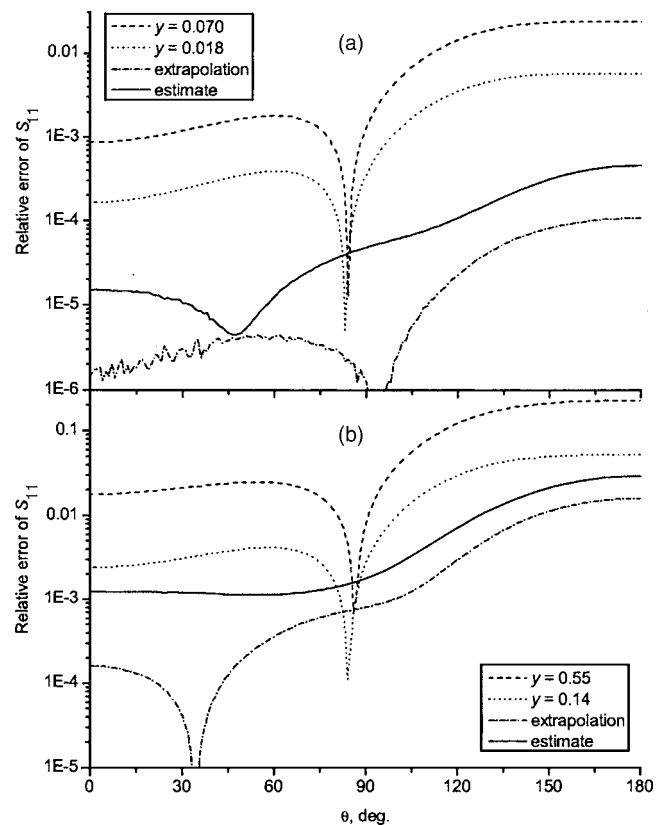


Fig. 5. Errors of $S_{11}(\theta)$ in logarithmic scale for extrapolation using nine values of y in the intervals (a) $[0.018, 0.070]$, (b) $[0.14, 0.55]$ for the $kD=3$ sphere. Estimate of the extrapolation error is $2(SE)$.

$kD=10$ sphere (using nine points from the intervals $[0.059, 0.23]$ and $[0.12, 0.47]$) are shown in Figs. 6(a) and 6(b), respectively. A third extrapolation for the $kD=10$ sphere is not satisfactory (data not shown). Both extrapolations for the $kD=30$ sphere show similar controversial results; only one of them (nine points from the interval $[0.18, 0.70]$) that is overall slightly better is shown in Fig. 7. The estimate of the extrapolation error is overall slightly higher than the real errors of the extrapolation (data not shown).

Results of $S_{11}(\theta)$ for all extrapolations (see Table 1) support the following trend: the quality of the extrapolation (defined as decrease of error compared with a single DDA computation for y_{\min}) rapidly degrades with increasing y_{\min} . The ratio of estimated to real errors increases with increasing y_{\min} (that can be considered a degradation of the estimate quality).

Computation of exact results for both the $kD=10$ sphere and its cubical discretization ($y=0.93$) allows us for the first time, to our knowledge, to directly separate and compare shape and discretization errors of single DDA computations. The shape error is the difference between some measured quantity for a discretized sphere (calculated to a high accuracy) and that for the exact sphere. The discretization error is the difference between a calculation using a limited number of dipoles (2176) and an exact (very accurate) solution for the cubical discretization of the sphere [dashed curve in Fig. 4(c)]. The total error is just the sum of the two. These three types of error

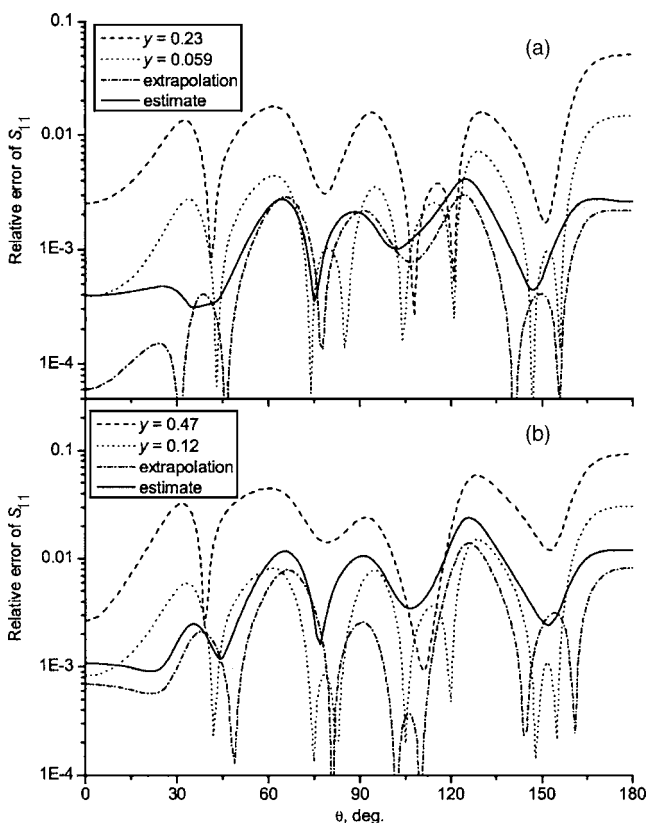


Fig. 6. Errors of $S_{11}(\theta)$ in logarithmic scale for extrapolation using nine values of y in the intervals (a) [0.059,0.23], (b) [0.12,0.47] for the $kD=10$ sphere. Estimate of the extrapolation error is 2(SE).

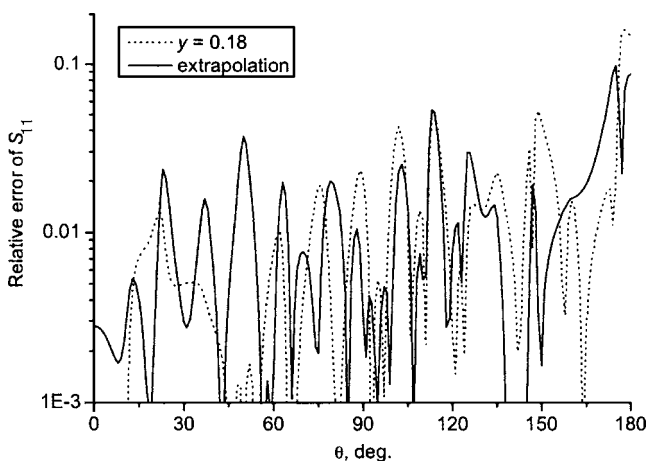


Fig. 7. Errors of $S_{11}(\theta)$ in logarithmic scale for extrapolation using nine values of y in the interval [0.18,0.70] for the $kD=30$ sphere.

for $S_{11}(\theta)$ are shown in Fig. 8, all relative to the exact value for the discretized sphere. Errors of Q_{ext} are shown in Table 2.

4. DISCUSSION

In their review Draine and Flatau² gave the condition $y < 1$ for applicability of the DDA. Usually $y=0.6$ (ten dipoles per wavelength in the medium) is used in

applications.³ Smaller y are used only in studies of DDA errors^{2,12,13} or of light scattering by particles much smaller than a wavelength (then d is determined by a shape of a scatterer, and y , being proportional to scatterer size, can be arbitrarily small).³³ However, if one wishes to achieve better (than usual) accuracy of a DDA simulation, smaller y must be used.

The best extrapolation for the cube [Fig. 3(a)] shows a large improvement compared with the best single DDA calculation (it should be noted, however, that this result is based on the empiric error estimate). Maximum errors are decreased more than 2 orders of magnitude. This would be impossible to reach by a single DDA calculation as it will require over 6-order-of-magnitude increase in execution time and memory, since there is only linear convergence for such small y . Even for $y_{min}=0.38$ the extrapolation can be called satisfactory because the maximum error is decreased almost two times when the estimate of the error is considered (the real errors are even less). It is important to note that an estimate of the error is important by itself (even when it is not less than the error of a single DDA computation) because it does not require an exact solution (which is usually unavailable in real applications). In general, the extrapolation decreases large errors better than those that are already small; i.e., it may significantly decrease maximum errors but prove less satisfactory for certain measured quantity (e.g., S_{11} for certain θ). This conclusion holds true for all the extrapolations we performed (Figs. 3–7 and those not shown).

Extrapolation results for the discretized sphere (Fig. 4) are similar to those for the cube. Extrapolations for

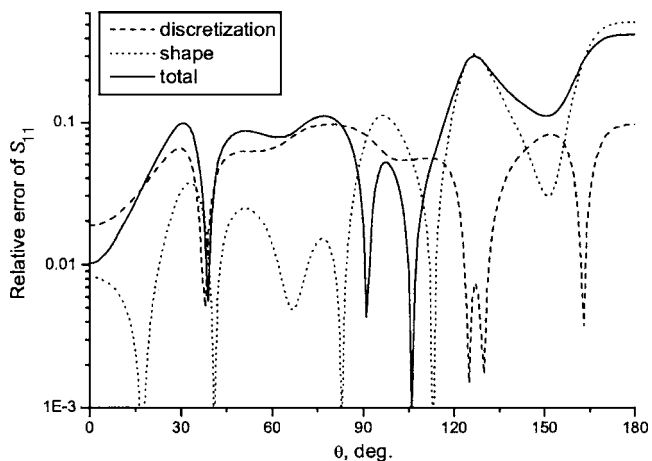


Fig. 8. Comparison of discretization and shape errors of $S_{11}(\theta)$ for the $kD=10$ sphere discretized using 16 dipoles per D ($y=0.93$).

Table 2. Comparison of Shape and Discretization Errors of Q_{ext} for the $kD=10$ Sphere Discretized with $y=0.93^a$

Type	Shape	Discretization	Total
Error	3.1×10^{-3}	8.3×10^{-3}	5.2×10^{-3}

^aAll errors are relative to the best extrapolation result for the discretized sphere.

$y_{\min}=0.058$ and 0.12 are very good (more than an order-of-magnitude decrease of maximum errors), while for $y_{\min}=0.23$ the extrapolation is on the edge of being satisfactory. The latter is strongly influenced by the fact that only four points in a broad interval are used (hence it does not fully comply with the procedure specified in Section 2).

The best extrapolation for the $kD=3$ sphere [Fig. 5(a)] shows results comparable with cubically shaped scatterers; however, it uses an extremely small $y_{\min}=0.018$. Already for $y_{\min}=0.14$ [Fig. 5(b)], it decreased the maximum errors only by a factor of 2. A similar boundary value of y_{\min} for satisfactory extrapolation is observed for the $kD=10$ sphere [Fig. 6(b)], while the best extrapolation [Fig. 6(a)] does show good results (four-times decrease of maximum error), although significantly worse than the analogous results for cubically shaped scatterers. Unfortunately, we are currently not able to reach sufficiently small y for the $kD=30$ sphere, and the best extrapolation (Fig. 7) uses rather large $y_{\min}=0.18$, resulting in almost negligible improvement of accuracy.

We have also studied a $kD=8$ porous cube that was obtained by dividing a cube into 27 smaller cubes and then removing randomly nine of them. All the conclusions are the same as those reported for the cube but with slightly higher overall errors (data not shown).

Extrapolation of Q_{ext} (Table 1) shows results similar to those discussed above; however, the improvement of accuracy is generally less than for maximum errors in $S_{11}(\theta)$ (which is in agreement with what we stated above, since errors in Q_{ext} are already small). Moreover, one should take into account that errors of a single DDA calculation for some y_{\min} are unexpectedly small (e.g., the last extrapolations for the cube and the $kD=3$ sphere), but these are just lucky hits near the points where the function $\delta Q_{ext}(y)$ crosses the horizontal axis (cf. Fig. 2).

Summarizing all results, we can conclude that shape errors significantly degrade the extrapolation performance because of its abrupt behavior, and therefore the extrapolation technique is much more suited for cubically shaped particles. One may expect satisfactory extrapolation for noncubically shaped particles only when $y_{\min} < 0.15$, whereas for cubically shaped particles the condition is $y_{\min} < 0.4$. It is important to note, though, that extrapolation can be used for any y_{\min} . The estimate of the error coming from the fitting procedure (SE) can then be used to decide whether this extrapolation was satisfactory. The quality of the extrapolation significantly increases with decreasing y_{\min} ; hence extrapolation is of biggest value for obtaining (very accurate) benchmark results. The size of the particle for which the extrapolation technique provides significant improvement is mainly determined by available computational resources that are required to reach small enough y_{\min} . However, further testing is required to evaluate the quality of extrapolation for scatterers large compared with the wavelength.

It is important to note that the linear extrapolation that was applied in two papers^{7,15} may lead to completely erroneous results (e.g., if points on the right branch of the parabolas for the cube and the $kD=3$ sphere in Fig. 2 are used). Quadratic extrapolation, as proposed in this paper, is much more reliable.

Throughout all the extrapolations we have used error estimates as specified in Section 2: 10(SE) and 2(SE) for cubically and noncubically shaped scatterers, respectively. All the results show that these estimates are reliable; i.e., in most cases real errors are less than the estimates. There are only two exceptions, both for the $kD=3$ sphere: for the fourth extrapolation of Q_{ext} (Table 1) the real error is 1.8 times larger than the estimate, and for the second of S_{11} the real error is 1.5–2 times larger than the estimate for a broad range of θ (data not shown). The existence of such exceptions is acceptable, since the estimates have a statistical nature of a confidence interval. However, these estimates, though reliable, are definitely not optimal: i.e., they often significantly overestimate the real errors [e.g., Fig. 5(a)]. The quality of the estimate also seems to be sensitive to the spacing of y values used for extrapolation—cf. Fig. 4(c), where unusually broad spacing was used. Generally, the overestimation increases with increasing y_{\min} . We can conclude that the error estimate should be improved, and this is the subject of future research. However, the current estimate is already suitable for practical applications, since they mainly require reliability of the error estimate, which is demonstrated empirically in this paper.

It is important to note that we limited ourselves to a single value of m . Although bounds of y_{\min} to obtain satisfactory extrapolation are definitely dependent on m , other conclusions, such as the reliability of the error estimate, are expected to hold true for a broad range of m . This can be easily tested for specific values of m of interest using the methodology put forward in this paper.

Finally, we discuss the results presented in Fig. 8. One cannot conclude that shape errors dominate over discretization errors (or the other way around): for some θ , shape errors are much larger than discretization errors and, for others, vice versa. However, maximum errors occurring in backscattering directions are definitely due to shape errors (the ratio of maximum shape to maximum discretization errors is about 4). Errors in Q_{ext} (Table 2) are, on the contrary, mostly due to discretization (although they are almost 2 orders of magnitude smaller than maximum errors of S_{11}). One may expect shape errors to become even more important for smaller values of y , since the linear component of discretization errors is significantly smaller than that of shape errors (hence, for large values of y , shape errors scale linearly and discretization errors scale almost quadratically). Our single result principally shows different angle dependence of shape and discretization errors of S_{11} : shape errors have a clear tendency to significantly increase toward backscattering, while the general trend of discretization errors is uniform over the whole θ range.

We have presented a simple method to directly separate shape and discretization errors and only one result for illustration. All previous comparisons of shape and discretization errors had significant inherent interpretation problems that caused a lot of discussions about their conclusions.^{16–20} Our method is free of such problems and therefore can be used for rigorous study of shape errors in the DDA. For instance, it can help to directly evaluate the performance of different techniques to reduce such errors, e.g., weighted discretization⁹ (WD). Discretization errors

are then the limit one can achieve by drastically reducing shape errors.

We have used a traditional DDA formulation² to show that the extrapolation technique can be used with current DDA codes (e.g., DDSCAT⁴ and ADDA²⁴) without any modifications. However, as we showed in Paper 1, several modern improvements of the DDA [namely, integration of Green's tensor³⁴ (IT) and WD] should significantly change the convergence behavior of DDA computations and hence influence the performance of the extrapolation technique. IT should completely eliminate the linear term for cubically shaped scatterers. This will improve the accuracy especially for small γ and probably also improve the quality of the extrapolation for such scatterers. WD should significantly decrease shape errors and hence total errors for noncubically shaped particles; moreover, it should significantly decrease the amplitude of quasi-random error oscillations because it takes into account the location of the interface inside the boundary dipoles. Therefore WD should improve the quality of the extrapolation for noncubically shaped scatterers. Testing of extrapolation performance of DDA using IT and WD is a subject of a future study.

5. CONCLUSION

On the basis of the theoretical convergence analysis as presented in Paper 1, 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 noncubically 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 a 2-order-of-magnitude decrease of error when $y_{\min} \approx 0.05$ for wavelength-sized scatterers with $m = 1.5$ (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 an adaptive DDA—a code that will automatically refine discretization to reach a required accuracy.

We also proposed a simple method to directly separate shape and discretization errors. Maximum errors of $S_{11}(\theta)$ for the $kD = 10$ sphere with $m = 1.5$, discretized using 16 dipoles per diameter ($\gamma = 0.93$), are mostly due to shape errors; however, the same is not true for all measured quantities. This method can be employed to rigorously study fundamental properties of these two types of error and to directly evaluate the performance of different techniques aimed at reducing shape errors.

Our theory predicts that modern DDA improvements (namely, IT and WD) should significantly change the performance of the extrapolation technique; however, numerical testing of these predictions is left for future research.

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