Convergence of Mie theory series: criteria for far-field and near-field properties

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We investigate the convergence of the series arising in Mie theory for the solution of electromagnetic scattering by a sphere. In contrast with previous studies that focused only on the scattering cross section, we here consider a wide spectrum of relevant properties, including scattering, extinction, and absorption cross sections, complex scattering amplitudes (i.e., radiation profile), and near-field properties such as surface electric field and average surface field intensity. The scattering cross section is shown to exhibit the fastest convergence, indicating that existing convergence criteria based on this property are not suitable for the majority of other relevant characteristics computed from Mie theory. Criteria are therefore proposed for those properties.

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1. Introduction

The theory of light scattering by a spherically symmetric body is described by Lorenz–Mie theory [1–3]. This theory consists of a rigorous solution of Maxwell equations in spherical coordinates for a spherically symmetric scatterer. This solution finds application in a wide range of fields including atmospheric physics and aerosols [4], three-dimensional graphics rendering [5], general electromagnetic theory [6], optical trapping [7], metamaterials [8], plasmonics [9,10], and surface enhanced Raman spectroscopy [10,11]. It is worth pointing out that for the more recent applications of Mie theory in this list, what is relevant is the computation of the electromagnetic fields in the near field and in particular in the vicinity of the particles; in fact Mie theory codes have been developed to address this specific need [12]. This is in contrast with more traditional application of Mie theory where only far-field, typically scattering, properties are required.

Most of the electromagnetic properties obtained from Mie theory are expressed as infinite sums, which have to be truncated after a finite number of terms in any practical numerical implementation. For the scattering cross section, the number of terms that are needed to be calculated is commonly estimated *a priori* by Wiscombe's criterion [13]. Recently work has been done to extend this to allow one to specify the desired accuracy for the scattering cross section and then estimate the required number of terms to achieve that accuracy [14], possibly beyond the standard floating point accuracy of double precision. Both of these studies have focused exclusively on the scattering cross section, and there is therefore no guarantee that these criteria would apply to other properties, in particular to near field, which may in fact be expected to require more terms in the series for convergence.

We address this issue here by studying explicitly the convergence of the Mie series for several relevant far-field and near-field properties. We show in

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particular that the scattering cross section exhibits the fastest convergence and that existing criteria cannot therefore apply to other properties, even related ones like the complex scattering amplitudes. We then derive alternative criteria that ensure convergence of the series. These criteria will be important in all fields relying on numerical predictions with Mie theory, in particular for the many emerging areas of research requiring near-field calculations. It will also provide a robust basis for further fundamental understanding of the convergence of Mie-type series, which arise in many extensions of Mie theory like generalized Mie theory for multiple scattering [15] and the T-matrix method [16] for nonspherical particles.

2. Expressions for Mie Series

Mie theory is described in great detail in several textbooks [3,10,16], so we will here only summarize for completeness the main series expressions for the electromagnetic properties of interest in this work. We consider a uniform sphere of radius a embedded in a nonabsorbing medium of dielectric constant ϵ_M (real and positive). The optical response of the sphere medium is assumed isotropic and homogeneous and characterized by a (possibly complex) dielectric function ϵ. For scattering at a wavelength λ, the two relevant nondimensional parameters are the size parameter $x = 2\pi\sqrt{\epsilon_M}a/\lambda$ and the relative refractive index $s = \sqrt{\epsilon}/\sqrt{\epsilon_M}$. The optical response of the sphere is then characterized by the electric (a_n) and magnetic (b_n) Mie susceptibilities ($n \geq 1$):

$$a_n(s,x) = \frac{s\psi_n(sx)\psi_n'(x) - \psi_n(x)\psi_n'(sx)}{s\psi_n(sx)\xi_n'(x) - \xi_n(x)\psi_n'(sx)}, \tag{1}$$

$$b_n(s,x) = \frac{\psi_n(sx)\psi_n'(x) - s\psi_n(x)\psi_n'(sx)}{\psi_n(sx)\xi_n'(x) - s\xi_n(x)\psi_n'(sx)}, \tag{2}$$

where ψ_n and ξ_n are Riccati Bessel functions (regular and Hankel of the first kind, respectively).

For an incident monochromatic plane wave, the nondimensional scattering and extinction coefficients (i.e., cross sections normalized to geometric cross section πa^2) are given by the series

$$Q_{\text{Sca}} = \frac{2}{x^2}\sum_{n=1}^{\infty}(2n+1)(|a_n|^2 + |b_n|^2), \tag{3}$$

$$Q_{\text{Ext}} = \frac{2}{x^2}\sum_{n=1}^{\infty}(2n+1)(\text{Re}(a_n) + \text{Re}(b_n)). \tag{4}$$

The absorption coefficient can be computed from the extinction theorem [3] as $Q_{\text{Abs}} = Q_{\text{Ext}} - Q_{\text{Sca}}$.

If we set the direction of incidence as the z axis and that of polarization as the x axis, then the far-field radiation profile is fully determined by two angle-dependent complex scattering amplitudes:

$$S_1(\theta) = \sum_{n=1}^{\infty}\frac{2n+1}{n(n+1)}[a_n\pi_n(\theta) + b_n\tau_n(\theta)], \tag{5}$$

$$S_2(\theta) = \sum_{n=1}^{\infty}\frac{2n+1}{n(n+1)}[a_n\tau_n(\theta) + b_n\pi_n(\theta)], \tag{6}$$

where π_n and τ_n are defined in terms of Legendre polynomials P_n as $\pi_n(\theta) = P_n'(\cos\theta)$ and $\tau_n = d/d\theta(\sin\theta\pi_n)$.

Series expressions can be written for the complex electric field vector $\mathbf{E}(\mathbf{r})$ at any point in space as a function of vector spherical wavefunctions [3,10]. From those we can compute the field intensity enhancement at points on the surface outside the sphere as $M_{\text{Loc}} = |\mathbf{E}|^2/|E_0|^2$, where E_0 denotes the incident field amplitude. One can also analytically express the surface-averaged field intensity enhancement on the surface just outside the sphere, which is an important characteristics for near-field applications like plasmonics, as [10]

$$\begin{aligned}\langle M_{\text{Loc}}\rangle = \frac{1}{4x^4}\sum_{n=1}^{\infty}&(2n+1)[x^2|\psi_n(x) - b_n\xi_n(x)|^2 \\ &+ x^2|\psi_{n'}(x) - a_n\xi_{n'}(x)|^2 \\ &+ n(n+1)|\psi_n(x) - a_n\xi_n(x)|^2].\end{aligned} \tag{7}$$

3. Convergence of Mie Series

All the series given above must be truncated in practice at a maximum $n = N$. Considering the series for the scattering coefficient only and requiring that $|\Gamma_N|^2 + |\Delta_N|^2 \leq 10^{-14}$, Wiscombe proposed the following criterion (for $8 < x < 4200$):

$$N_{\text{Wis}}(x) = x + 4.05x^{1/3} + 2, \tag{8}$$

which is still the most widely used criterion to date. The x term in Eq. (8) is due to the localization principle [2], and this corresponds to the region where the spherical functions contribute the most. The $x^{1/3}$ corresponds to the contribution from the surface waves [17].

Recently, Neves and Pisignano [14] pointed out that a criterion depending explicitly on relative error ε (rather than being based on absolute error as was the Wiscombe criterion) would be more valuable. Using asymptotic properties of the Bessel functions and Mie susceptibilities [18], they suggested the following criterion:

$$N_{\text{AP}}(x,\varepsilon) = x + 0.76x^{1/3}(-\log_{10}\varepsilon)^{2/3} - 4.1, \tag{9}$$

where the coefficients were found by extensive numerical calculations in arbitrary precision arithmetic of the convergence of the series for the scattering coefficient. This criterion is useful for predetermining the number of required terms for calculating the scattering cross section to a given accuracy. No attempt was made, however, to test its validity for other electromagnetic properties of interest, which will now be investigated in more detail. Note that the focus here is not on ultrahigh precision (as was the case in Ref. [14]) but on convergence within standard double-precision arithmetic (with best achievable relative accuracy of the order of 10^{-16}). All calculations are therefore carried out using standard MATLAB double-precision Mie theory codes designed with a special emphasis on near fields for plasmonics applications [12].

The convergence of the series is studied by considering the N dependence of the relative error: $\varepsilon(N) = |U_N - U|/|U|$, where U_N is the truncated series and U is the converged value (calculated for a sufficiently large N). Representative examples of convergence are shown in Fig. 1 for a number of far-field and near-field electromagnetic properties, including

- scattering (Q_{Sca}) and extinction (Q_{Ext}) coefficients;
- back-scattering complex scattering amplitude $S_1(\pi)$ [note that $S_2(\pi)$ and forward scattering amplitudes $S_1(0)$ and $S_2(0)$ are not shown but exhibit a similar dependence];
- average surface electric field intensity outside the sphere $\langle M_{\mathrm{Loc}}\rangle$;
- electric field intensity at point A (defined in Fig. 1);
- the θ-dependent scattering amplitudes $S_1(\theta)$, $S_2(\theta)$, and field intensity on the surface $M_{\mathrm{Loc}}(\theta)$ are also studied for 721 values of $0 \le \theta \le \pi$ to determine the N dependence of the worst relative accuracy for these two properties.

We immediately see from those plots that convergence of all the series only starts once N is of the order of x, as pointed out in previous studies. For $N > x$, the rates of convergence then depend strongly on the properties of interest. Unfortunately, the scattering cross section used in all previous convergence studies converges faster than all other properties studied here. From these plots and additional extensive testing for a range of parameters, we infer the following properties:

- The scattering cross section converges the fastest.
- Next, the extinction (and absorption, not shown) cross sections and all (angle-dependent) complex scattering amplitudes have similar rates of convergence that are slower than scattering.
- Surface field convergence is even slower. In fact, the convergence for the field intensity further away from the sphere for $x = 50$ at a distance of $r = 2a$ from the origin is comparable to that of the extinction (not shown). This suggests that evanescent waves, which tend to require higher order multipoles, are the cause of the slower convergence in the near field. Also, perhaps unexpectedly, the average surface field intensity $\langle M_{\mathrm{Loc}}\rangle$ converges faster than the surface field, in fact as fast as the extinction. This can be understood if errors in the truncated series

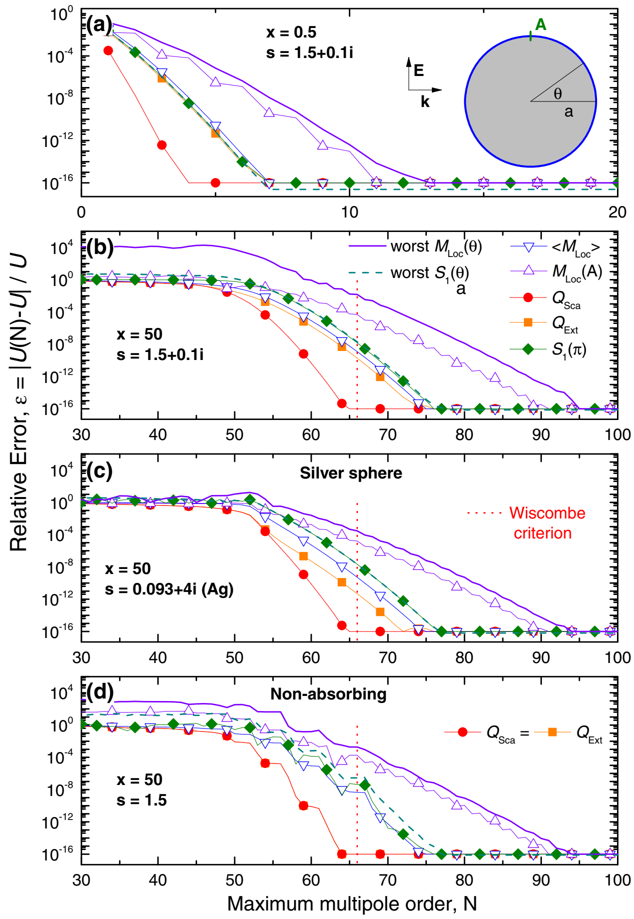

Fig. 1. Convergence of Mie theory calculations computed with the SPlaC package [12] as a function of series truncation (maximum multipole order, N), illustrated here for (a) small and (b) large absorbing dielectric spheres (relative refractive index $s = 1.5 + 0.1i$), (c) a large metallic sphere, and (d) a large nonabsorbing dielectric sphere. A range of far-field and near-field properties are considered: scattering (Q_{Sca}) and extinction (Q_{Ext}) coefficients; back-scattering complex scattering amplitude $S_1(\pi)$; and surface fields intensity enhancements defined as $M_{\mathrm{Loc}} = |E|^2/|E_0|^2$, either at point A or surface-averaged. Also shown are the worst relative accuracy for $S_1(\theta)$, $S_2(\theta)$ and $M_{\mathrm{Loc}}(\theta)$ determined by taking for each N the maximum relative error ε for 721 values of θ between 0 and π. For $x = 50$, the Wiscombe criterion suggests $N_{\mathrm{Wis}} = 66$ (similar to $N_{\mathrm{AP}} = 64$ for $\varepsilon = 10^{-16}$). It is clear that these are appropriate for the scattering coefficients as expected, but not sufficient for any of the other properties.

partially cancel out in the averaging, i.e., regions where the value is overestimated are compensated by regions where it is underestimated. The same remark can be made for the scattering intensities $|S_1(\theta)|^2$ and $|S_2(\theta)|^2$, which converge slower than their angle-averaged property Q_{Sca}.

- The convergence properties of the series are governed almost entirely by the size parameter x and are approximately independent of the sphere optical properties (characterized by s). The only exception is for nonabsorbing sphere [when $\mathrm{Im}(s) = 0$], for which we have trivially $Q_{\mathrm{Sca}} = Q_{\mathrm{Ext}}$ and the extinction then converges as fast as scattering.

• The Wiscombe criterion (or its improved accuracy-dependent version) guarantees in most cases double-precision accuracy for the scattering cross section but is not sufficient for other properties, notably the surface fields, for which the accuracy can be of the order of 1% only in the examples of Fig. 1.

4. Criteria for Truncation

The results of this convergence study indicate the need for criteria adequate for all properties other than the scattering cross section. To this end, we focused on double-precision calculations only as these are sufficient for the vast majority of applications. For a given x and s, we can estimate the number of multipoles $N(x,s)$ required to ensure convergence within double precision. This information can be extracted automatically from convergence plots such as those of Fig. 1. In order to find a convergence criterion for each relevant electromagnetic properties, we computed $N(x,s)$ over a relevant range of values of x and s. Specifically, we here considered

- nine values of x in the small-size regime: $x = 0.1$, 0.2, 0.3, 0.5, 0.7, 1, 1.5, 2, 3 and 20 log-spaced values of $5 \leq x \leq 150$;
- To account for dielectric-type spheres, we consider 10 log-spaced values of $0.01 \leq (\mathrm{Re}(s) - 1) \leq 3$ and 10 linearly spaced values of $0 \leq \mathrm{Im}(s) \leq 4$;
- To account for metallic-type spheres, we considered 10 log-spaced values of $0.1 \leq (1 - \mathrm{Re}(\epsilon)) \leq 20$ and 10 log-spaced values of $0.1 \leq \mathrm{Im}(\epsilon) \leq 10$ from which $s = \sqrt{(\epsilon)}$ is derived.

For each of the 5800 cases, we compute the N dependence of the series for $N \geq x$ and extract from it the limiting relative precision ε for large N and the truncation $N(x,s)$ required for achieving it. The scattering amplitudes $S_1(\theta)$, $S_2(\theta)$ and the surface field intensities $M_{\mathrm{Loc}}(\theta)$ are θ dependent. For those, we determine $N(x,s)$ for 361 values of θ and choose the largest as representative of the worst case convergence. The results are summarized in Fig. 2. Following on Wiscombe's work, we plot $N(x,s) - x$ against $x^{1/3}$. The results of Fig. 2 suggest that criteria that are independent of s and of the same form as originally suggested by Wiscombe are also suitable for other properties, i.e.,

$$N(x) = x + ax^{1/3} + b. \tag{10}$$

It is, however, clear that Wiscombe's criterion ($a = 4.05$ and $b = 2$) is only suitable for the scattering coefficient. To obtain the same accuracy for all electromagnetic properties, we propose to replace it with a set of three criteria based on the results of Fig. 2:

$$N_{\mathrm{SC}}(x,s) = x + 4x^{1/3} \tag{11}$$

for the scattering cross section (note that this is almost unchanged from Wiscombe's criterion);

$$N_{\mathrm{FF}}(x,s) = x + 6.5x^{1/3} \tag{12}$$

for far-field properties such as Q_{Ext}, Q_{Abs}, $S_1(\theta)$, and $S_2(\theta)$ (and as noted earlier also for $\langle M_{\mathrm{Loc}}\rangle$); and

$$N_{\mathrm{NF}}(x,s) = x + 11x^{1/3} + 1 \tag{13}$$

for near-field properties in general. We note that this latter criterion would apply equally to any electromagnetic properties that can be expressed in terms of near-field intensity, including for example

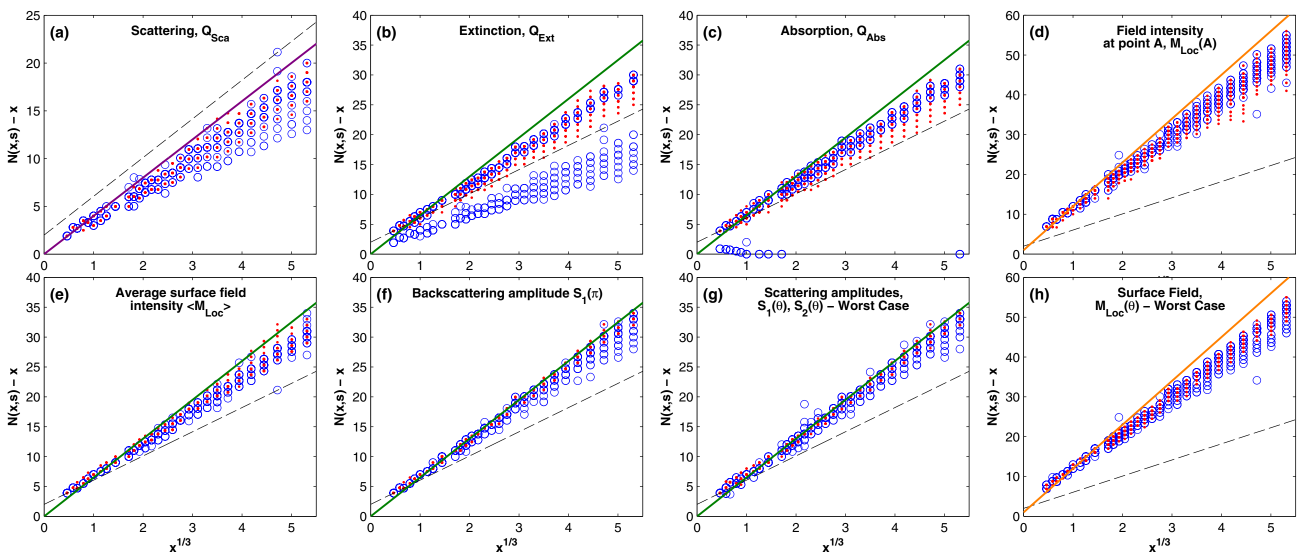

Fig. 2. Number of required multipole $N(x,s)$ to obtain convergence of the Mie series for various far-field and near-field properties of interest. For θ-dependent properties (g), (h), $N(x,s)$ is chosen as the largest among all considered θ to represent the worst case of convergence. All the results are plotted as $N(x,s) - x$ as a function of $x^{1/3}$ for 100 values of s for dielectric-type particles (blue open circles) and 100 values of metallic-type spheres (red solid diamonds). In each plot, we also show the Wiscombe criterion $N_{\mathrm{Wis}}(x)$ (dashed line) and the suggested new criteria (solid lines): $N_{\mathrm{SC}}(x)$ for scattering (a), $N_{\mathrm{FF}}(x)$ for far field (b), (c), (e), (f), (g), and $N_{\mathrm{NF}}(x)$ for near field (d), (h).

nonlinear optical properties. We may expect that this criterion would also be relevant to calculations of scattering by multiple spheres, although further investigations would be needed to confirm this.

These criteria have been chosen such that for $x > 1$ they apply even to the worst possible cases for s, i.e., the solid lines in Fig. 2 are above the majority of points rather than choosing a fit to the data (through the middle). This means that the criteria slightly overestimate the truncation needed in many cases, but this ensures that they do not underestimate it in the more difficult cases. Our choice therefore emphasizes reliability, even if it comes with a small performance cost. Although the criteria are not specifically optimized for smaller sizes ($x < 1$), we will show that they still work well in that region. We also note that those criteria are not unique and that, following the same method as presented here, alternative ones could be derived for specific purposes or over a particular range of size.

5. Discussion and Conclusion

We have seen that the Wiscombe criterion clearly underestimates the number of multipoles required for near-field properties and some far-field properties. Our proposed set of three criteria addresses this issue for most electromagnetic properties of interest in the far and near field. With these criteria established, it is interesting to check how accurate they are at predicting the correct properties. The obtained accuracy (using double-precision computation) is now limited by numerical errors in the floating point arithmetic, not by the early termination of the series. Those relative accuracies, which again depend on the property under study and on both s and x, are summarized in Fig. 3, together with those obtained from the Wiscombe criterion. It is clear that the criteria provide a much better accuracy, simply because of the early truncation of the series with the Wiscombe criterion. Despite this, it is also evident from Fig. 3 that, although this error results in a loss of precision (by several decimal digits) in the final results, the computed far-field properties remain reasonably accurate with better than 10^{-6} accuracy in the range of parameters investigated here. This is probably one of the reasons why this discrepancy has not been noticed before. The error becomes more pronounced for near-field properties where, as suggested in Fig. 3, a wrong result ($\varepsilon \geq 1$) may be obtained in some cases for field calculations on large particles. But again a sufficient accuracy (for most applications) of say 10^{-2} seems to be obtained in the majority of cases. Nevertheless, it is also clear that the criteria proposed here will ensure a much better accuracy (by as much as eight significant digits for near fields), and importantly, this will be achieved for very little extra computing resources, especially at large x where the relative increase in N from N_{Wis} to N_{NF} becomes very small. For example, for $x = 500$, we have $N_{\text{Wis}} = 535$ and $N_{\text{NF}} = 589$ and for $x = 5$, $N_{\text{Wis}} = 14$ and $N_{\text{NF}} = 25$. Given the small extra resources required, the criteria should therefore be used whenever electromagnetic properties other than the scattering cross section are computed.

Finally, this work also highlights how the convergence of Mie series can differ depending on the type

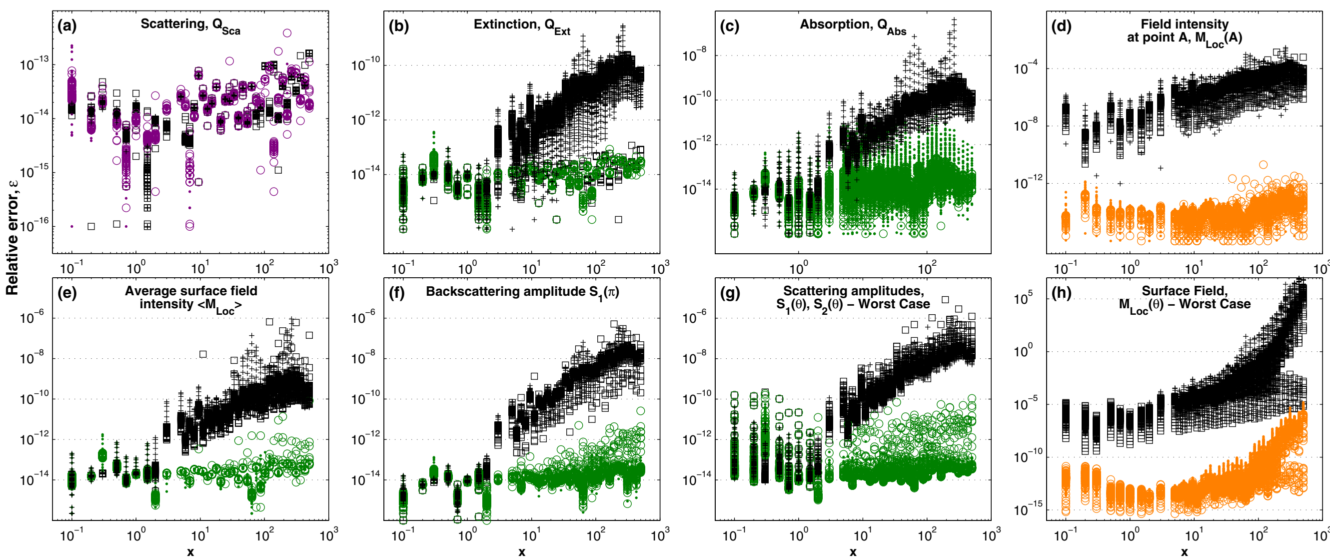

Fig. 3. Estimated accuracy (relative error ε) obtained for double-precision calculations of Mie series for various far-field and near-field properties of interest. For θ-dependent properties (g), (h), we consider the worst accuracy among 361 uniformly distributed θs. For each property, we show the results both for the Wiscombe criterion (black squares and crosses) where the truncation is given by $N_{\text{Wis}}(x)$ and for the proposed criteria (circles and diamonds), $N_{\text{SC}}(x)$ for (a), $N_{\text{FF}}(x)$ for (b), (c), (e), (f), (g), and $N_{\text{NF}}(x)$ for (d), (h). All the plots include 100 values of s for dielectric-type particles (open circles and squares) and 100 values of metallic-type spheres (crosses and diamonds). Note the "splitting" of the plots for large size in (d), (h). Upon inspection, the lower branches correspond to nonabsorbing dielectric sphere while all other cases are in the upper branches (with a larger error).

of properties calculated, with the fastest convergence for scattering cross section and the slowest for near-field properties.

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