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Testing the accuracy and convergence of scattering calculations using Lorentz reciprocity

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Abstract: We present a simple and versatile approach to test the accuracy of scattering calculations. Based on the Lorentz reciprocity relation, this criterion can be used for any scattering object, especially where a reference solution (e.g. from Mie theory) does not exist. Application examples with arbitrary shape scatterers in plasmonic metals and high-index dielectrics numerically demonstrate the suitability of the technique, which can be utilized with any numerical method to increase the accuracy of the produced results.

1. Introduction

Since the middle of the 20$^{\text{th}}$ century, numerical techniques have become a key driver for science and technology, both in research and industry. A crucial step in the development of a numerical technique is its validation to ensure that it produces accurate results. In optics and electromagnetics, this is done by considering the canonical problem of light scattering by a sphere and comparing the numerical solution for the scattering cross section (SCS) with the analytical reference solution obtained from Mie theory [1]. This approach can be used to test the convergence of the numerical solution toward the reference solution for this generic problem, with the hope that the discrepancy between both solutions decreases as the mesh used for the numerical problem is refined [2].

Unfortunately, there does not exist a generic approach to test the convergence of a numerical technique for an arbitrary scattering problem, short of comparing the solution with that obtained with another numerical approach, which is unsatisfactory and does not provide an absolute accuracy metric.

This letter proposes such a general criterion that can test the convergence of light scattering codes on real, arbitrarily complex, physical problems. This approach is based on the Lorentz reciprocity principle [3,4], which – put in simple terms – says that "if I can see your eyes, so you can see mine". We show that reciprocity can serve as a metric for the convergence of a numerical technique and can be applied to any scattering system, irrespective of its complexity. Furthermore, since this proposition is based on physical considerations, it can be used with any numerical technique for scattering calculations [5–24].

The reciprocity condition holds for an arbitrary linear and time-invariant system possessing loss or gain, but very importantly, not being biased by a time-odd quantity such as a magnetic field and having no spatiotemporal modulations of its parameters. Further details on how reciprocity can be broken can be found in Sec. IV D of Ref. [25] or in Sec. XIX of Ref. [3]. For reciprocal systems, one can find additional useful restrictions imposed on the system by the reciprocity condition. For example, for two co-polarized planewaves propagating along opposite directions, the amount of light scattered in the forward direction should be equal for each wave [26]. From the optical theorem, one can further deduce that the total extinction cross section for these two cases should be equal [26,27]. The reciprocity condition can also serve as a test for periodic systems scattering light in different diffraction orders [28,29].

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To illustrate our point, we use the surface integral equation (SIE) method, a versatile numerical technique for light scattering that solves the integral form of Maxwell's equations [2,6,22,30–42]. The Poggio-Miller-Chang-Harrington-Wu-Tsai (PMCHWT) formulation is used [32,43–45] with Rao-Wilton-Glisson basis functions [46] and a Galerkin scheme with refined singularity subtraction [47]. Reciprocity has also been used to test the convergence of the T-matrix technique Rother and Wauer [48] and the convergence of both the T-matrix technique and the discrete dipole approximation by Schmidt *et al.* [49].

2. Convergence criterion

The reciprocity principle states that in a scattering experiment, the source and receiver can be interchanged without affecting the data acquired by the receiver. This concept can equivalently be written mathematically for two separate sources. Let us consider a scattering problem with two source currents $\mathbf{J}_1$ and $\mathbf{J}_2$ located within two spatially separated volumes V_1 and V_2. The source $\mathbf{J}_1$ produces a scattered electric field $\mathbf{E}_1$ in volume V_2, while the source $\mathbf{J}_2$ produces a scattered electric field $\mathbf{E}_2$ in volume V_1. The Lorenz reciprocity relation states that the currents and the fields are related by [50]:

$$\int_{V_1} \mathbf{E}_2(\mathbf{r}) \cdot \mathbf{J}_1(\mathbf{r}) dV_1 = \int_{V_2} \mathbf{E}_1(\mathbf{r}) \cdot \mathbf{J}_2(\mathbf{r}) dV_2 \,. \tag{1}$$

For two point dipoles $\mathbf{p}_1(\mathbf{r}_1)$ and $\mathbf{p}_2(\mathbf{r}_2)$ serving as electromagnetic sources at positions $\mathbf{r}_1$ and $\mathbf{r}_2$, Eq. (1) takes the form:

$$\mathbf{E}_2(\mathbf{r}_1) \cdot \mathbf{p}_1(\mathbf{r}_1) = \mathbf{E}_1(\mathbf{r}_2) \cdot \mathbf{p}_2(\mathbf{r}_2), \tag{2}$$

as sketched on the top of Fig. 1.

Here, we propose to test the accuracy of the electromagnetic solver by verifying whether the left- and right-hand sides of Eq. (2) are equal. In other words, Eq. (2) is better fulfilled as the numerical solution converges to a more accurate value.

To estimate the error for the reciprocity relation, let us introduce the error parameter Σ_{RCPR} at a fixed wavelength λ as

$$\Sigma_{\text{RCPR}} = \frac{|\mathbf{E}_1(\mathbf{r}_2) \cdot \mathbf{p}_2(\mathbf{r}_2) - \mathbf{E}_2(\mathbf{r}_1) \cdot \mathbf{p}_1(\mathbf{r}_1)|}{|\mathbf{E}_1(\mathbf{r}_2) \cdot \mathbf{p}_2(\mathbf{r}_2)|}, \tag{3}$$

which is estimated to be very small; our simulations indicate that it is in the $10^{-7} - 10^{-3}$ range. Obviously, the exact value of an error estimate for numerical calculations depends on the metric used and cannot be compared with other metrics. For example, the more conventional metric based on the comparison of the numerical SCS, $\sigma_{(\text{DoF})}$, with that obtained from Mie theory $\sigma_{(\text{Mie})}$ [1]:

$$\Delta_{\text{Mie}} = \frac{|\sigma_{(\text{DoF})} - \sigma_{(\text{Mie})}|}{|\sigma_{(\text{Mie})}|} \,. \tag{4}$$

yields errors in the $10^{-4} - 10^{-1}$ range [45,47,51]. In Eq. (4), DoF stands for the number of degrees of freedom of the numerical problem; for SIE, this number corresponds to 3 times the number of triangles used to discretize the scattering object. To be able to compare Σ_{RCPR} and Δ_{Mie} on the same graphs in spite of their different magnitudes, we introduce the arbitrarily scaled error Σ_{Mie} as

$$\Sigma_{\text{Mie}} = \Delta_{\text{Mie}} \cdot 10^{-4}. \tag{5}$$

To study the convergence of the numerical solution for non-spherical objects, where no reference Mie solutions exist, we also introduce another estimate based on a reference solution with a very large number of DoF (i.e. a much refined discretization mesh),

$$\Sigma_{\text{SCS}} = \frac{|\sigma_{(\text{DoF})} - \sigma_{(\text{DoF=max})}|}{|\sigma_{(\text{DoF=max})}|} \cdot 10^{-4} \,. \tag{6}$$

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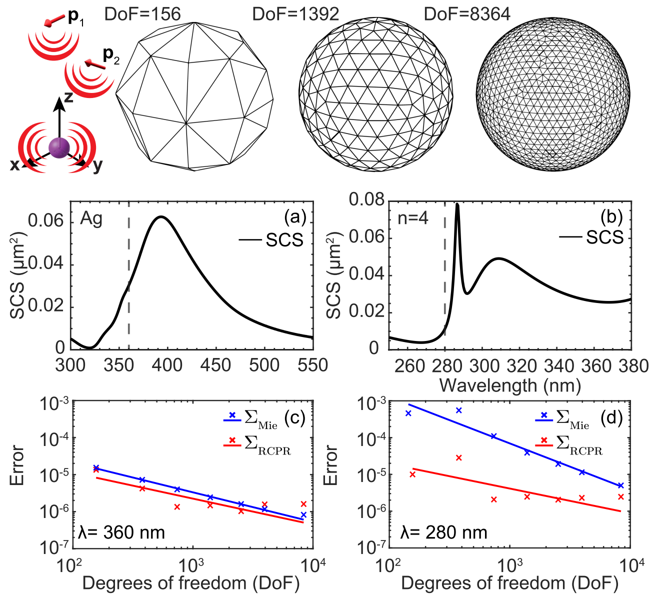

Fig. 1. Light scattering by a 50 nm radius sphere (a), (c) for Ag and (b), (d) for $n = 4$ dielectric: (a) and (b) scattering cross sections computed with Mie theory. (c) and (d) numerical errors for the numerically computed SCS compared to the Mie solution (Σ_{Mie} in blue) or obtained from the Lorentz reciprocity criterion (Σ_{RCPR} in red). The solid lines are fit to the numerical data. Typical meshes are shown at the top with their corresponding DoF and the calculation principle with two dipoles $\mathbf{p}_1$ and $\mathbf{p}_2$ to check Lorentz reciprocity (see text for details).

3. Results and discussion

Let us now compare the different convergence criteria introduced previously and show that Lorentz reciprocity can be used to assess the accuracy of a numerical scheme. To this end, we will consider different geometries and assume that all the scatterers are in vacuum.

3.1. Sphere

To begin, we consider scattering from silver and dielectric spheres with a 50 nm radius. The refractive index for Ag is taken from Johnson and Christy [52], the refractive index for the dielectric is $n = 4$, corresponding to a high dielectric non-lossy material like a semiconductor. The SCSs computed with Mie theory for both objects illuminated by a planewave are shown in Figs. 1(a) and 1(b). We note a simple spectral response, dominated by an electric dipole for the metal [53] and a magnetic dipole plus an electric dipole for the dielectric [54]. To reproduce these data numerically, we simulate the SCS with our home-built SIE code implemented with the PMCHWT formulation [37] using accurate integration of the matrix elements [47]. To study the convergence of the numerical solution, meshes with different numbers of DoF between 156 and 8364 are used, as illustrated at the top of Fig. 1. We first compute the SCS for the Ag sphere at the fixed wavelength $\lambda = 360\,\text{nm}$, and show the values of Σ_{Mie} in blue as a function of the DoF in Fig. 1(c). The convergence rate for the numerical solution $\Sigma_{\text{Mie}} \approx \text{DoF}^{-3/4}$ corresponds to what is reported in the literature, see e.g. Fig. 7 in [42].

To test the convergence with the reciprocity condition, we change the illumination to two dipoles with arbitrary-units magnitudes $\mathbf{p}_1 = (1, 0, 0)$ and $\mathbf{p}_2 = (3, 1, 2)$ and located at positions $\mathbf{r}_1 = (5, 0, 0)$ [μm] and $\mathbf{r}_2 = (40, 75, 32)$[nm], respectively (the same dipoles will be used to test

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reciprocity throughout). The reciprocity error calculations given by Eq. (3) are presented in red for silver in Fig. 1(c). Very importantly, we observe a similar convergence rate for $\Sigma_{\rm RCPR}$ as that of $\Sigma_{\rm Mie}$. The same is true for the dielectric sphere in Fig. 1(d), with the convergence metrics computed for $\lambda = 280\,\rm nm$. These encouraging results indicate that reciprocity can be used to test the convergence of a numerical calculation.

3.2. Cube

Let us now move to geometries for which no reference solutions exist, as is the case for most systems relevant to research and industry. We first consider a cubic scatterer made of Ag and dielectric $n = 4$. Three examples of cubic meshes used in the simulations are shown on the top of Fig. 2. For these cubes, the DoF changes from 36 for a very rough mesh to the mesh with the maximal number of DoF (max=11664). The SCSs for both materials are shown in Figs. 2(a) and 2(b), we note in this case a more complex response, indicating that these structures support several multipoles [55].

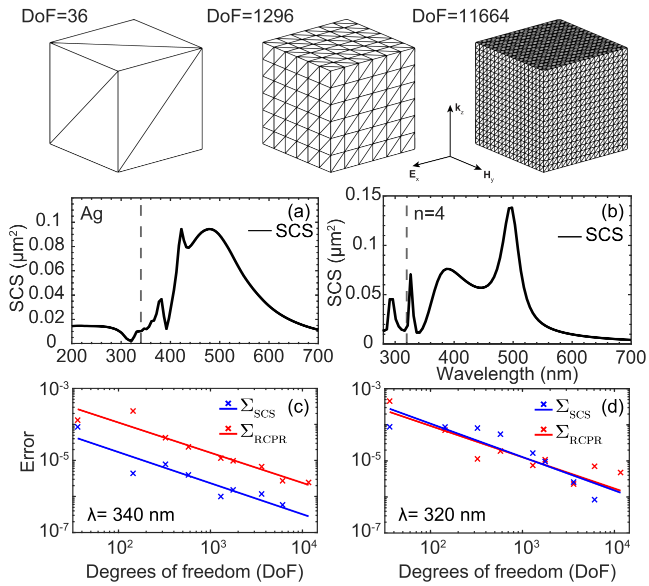

Fig. 2. Light scattering by a $100 \times 100 \times 100\,\rm nm^3$. (a), (c) for Ag and (b), (d) for $n = 4$ dielectric: (a) and (b) scattering cross sections computed with SIE. (c) and (d) numerical errors for the SCS compared to the solution with the maximum DoF=11664 ($\Sigma_{\rm SCS}$ in blue) or obtained from the Lorentz reciprocity criterion ($\Sigma_{\rm RCPR}$ in red). The solid lines are fit to the numerical data. Typical meshes are shown at the top with their corresponding DoF and the illumination conditions. The different convergence metrics are computed for $\lambda = 340\,\rm nm$ for Ag and $\lambda = 320\,\rm nm$ for the dielectric.

While no reference solutions exist for such a system, one can assess the convergence of the numerical simulations by comparing them to an extremely refined model – $\Sigma_{\rm SCS}$ computed with Eq. (6) – as shown in blue in Figs. 2(c) and 2(d). We note a similar convergence for $\Sigma_{\rm SCS}$ as that observed for $\Sigma_{\rm Mie}$ in Fig. 1. Also for those scatterers, the convergence estimate based on reciprocity follows the same power dependence as that observed for $\Sigma_{\rm SCS}$, indicating again that Lorentz reciprocity can be used to test the convergence for such a geometry.

Testing the convergence at different wavelengths provides slightly different convergence rates. Hence, for scatterers that exhibit several spectral features, it might be advantageous to average out the numerical error over the spectrum of interest. Figure 3 shows the corresponding data for the cubes studied in Fig. 2. The average metric $<\Sigma_{RCPR}>$ is obtained by averaging Σ_{RCPR} over 100 equally spaced wavelengths. Again, its value converges smoothly for both materials and can serve as indicator of the convergence of the numerical solution, without resorting to any reference solution.

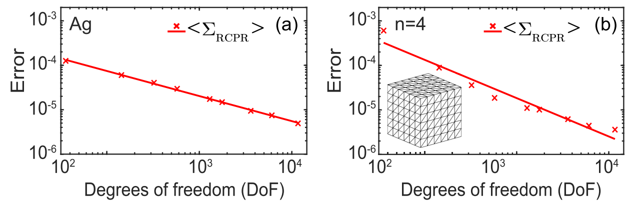

Fig. 3. Convergence estimate averaged over the spectrum, (a) for the Ag cube shown in Figs. 2(a), and (b) for the dielectric cube shown in Fig. 2(b).

3.3. L-shape

Finally, to confirm that the symmetry of the geometry does not affect the results, we perform the same analysis for L-shape structures in Ag and dielectric (n = 4). The simulations are performed with meshes having DoF varying from 132 to 11556, as illustrated on the top of Fig. 4. The scattering cross sections computed with SIE using the finest mesh are shown in Figs. 4(a) and 4(b). The convergences are assessed using either the SCS (Σ_{SCS}) or reciprocity (Σ_{RCPR}). We observe again power laws for these different convergence metrics, which can be well-fitted with a linear function in the log-log scales used in Figs. 4(c) and 4(d).

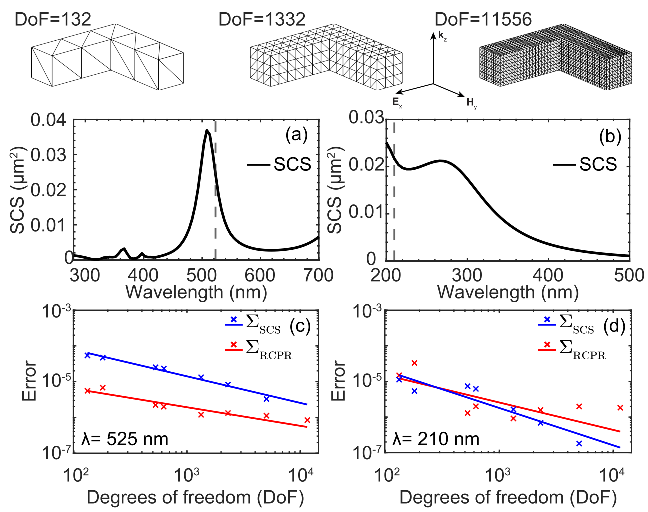

Fig. 4. Light scattering by an L-shape particle with equal arms 100 nm and a 30 nm thickness. (a), (c) for Ag and (b), (d) for $n = 4$ dielectric: (a) and (b) scattering cross sections computed with SIE. (c) and (d) numerical errors for the SCS compared to to the solution with the maximum DoF=11556 (Σ_{SCS} in blue) or obtained from the Lorentz reciprocity criterion (Σ_{RCPR} in red). The solid lines are fit to the numerical data. Typical meshes are shown on the top with their corresponding DoF and the illumination conditions. The different convergence metrics are computed for $\lambda = 525$ nm for Ag and $\lambda = 210$ nm for the dielectric.

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4. Conclusions

We have introduced a simple and versatile metric to assess the convergence of electromagnetic scattering calculations and illustrated its utilization for nanophotonic systems made from plasmonic metals and high-index dielectrics. This criterion relies on the fulfillment of the Lorentz reciprocity principle that states that source and observer can be exchanged in a scattering experiment. It can be used with any numerical method and is extremely simple to implement in practice, as it only requires computing two scattering problems with dipolar sources [56]. The technique can be easily implemented in commercial solvers and works both for time- and frequency-domains calculations.

The validity of this convergence criterion has been carefully assessed on canonical scattering problems where a reference solution exists (Mie scattering by a sphere). Its applicability for scatterers with an arbitrary shape has then been numerically demonstrated, both for plasmonic metals and dielectrics. We trust that this work will contribute to producing robust, quantitative, numerical results that support experiments.

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Data availability. Data underlying the results presented in this paper are not publicly available at this time but may be obtained from the authors upon reasonable request.

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