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Dipolar unit size in coupled-dipole calculations of the scattering matrix elements

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The coupled-dipole method is widely used to calculate the light-scattering matrix $\mathbf{S}$ from arbitrary particles. An important parameter in the model is the size of the dipolar subunits. Usually a size of $\sim 1/10$ to $\sim 1/20$ of the wavelength of the incident light is sufficient for accurate calculations. However, it was noted that accurate $\mathbf{S}_{34}$ calculations require much smaller dipolar subunits. We show that this conclusion is too pessimistic, by examining the sensitivity of the $\mathbf{S}_{34}$ elements on surface roughness of spherical particles. Furthermore we give an example of an accurate $\mathbf{S}_{34}$ calculation with dipolar subunits as large as $1/10$ of the wavelength.

The coupled-dipole (CD) method, originally formulated by Purcell and Pennypacker,¹ is a powerful method with which to calculate elastic light scattering from arbitrary particles. The CD method divides a particle into small subvolumes, which are assumed to behave as ideal dipoles. The electric field on each dipole, caused by the external field and the field radiated by all other dipoles, is calculated. Next the scattered field is obtained by summation of the fields radiated by all dipoles in the observation points. By repeating this calculation for a parallel- and a perpendicular-polarized incident electric field, one can compute the complete (4×4) scattering matrix $\mathbf{S}$ of the particle. Although the basic concepts of the model are straightforward, the model possesses many parameters that are topics of active research. An example is the choice of the polarizability of the dipolar subunits. Lakhtakia² reviewed the CD method.

An important parameter of the CD method is the size of the dipoles. The dipoles are placed on a cubic grid, with grid spacing d . The dipoles are therefore assumed to describe the response of a cube with volume d^3 . The computations of the electric field on the dipoles requires solving a set of $3N$ equations with $3N$ unknowns, where N is the number of dipoles. Therefore it is most advantageous to choose d as large as possible, thus decreasing N . On the other hand, if d becomes too large, the dipole approximation breaks down, and the results of CD simulations will no longer be reliable. By comparison of CD computations on spheres with the exact Mie results, it was concluded that $\lambda/20 \leq d \leq \lambda/10$ gives good agreement between the simulated and exact differential cross sections.¹

Singham³ calculated the $\mathbf{S}_{34}$ element with the CD method. By comparison of the calculations with exact results for a sphere, it was concluded that accurate $\mathbf{S}_{34}$ simulations require much smaller dipoles, with $d \sim \lambda/45$ (depending on the refractive index of the particle), which is two to four times smaller than for accurate $\mathbf{S}_{11}$ simulations. Because N scales as d^{-3} , the total number of dipoles would be 8–64

times larger than for accurate $\mathbf{S}_{11}$ calculations. If the system of equations is solved with an $O(N^2)$ iterative method, a factor of 64–4096 longer execution time on a computer would be required. This is a discouraging conclusion, especially with the realization that the $\mathbf{S}_{34}$ element is sensitive to slight changes in structure and optical constants of a particle (see Refs. 4 and 5) and therefore of main interest. In this Letter we show that Singham's conclusion is too pessimistic.

Singham simulated a sphere with size parameter $\alpha = 1.55$ and a relative refractive index $m = 1.33$. This sphere was simulated with the CD method containing from 123 to 5575 dipoles. CD results for the $\mathbf{S}_{11}$ elements are already in good agreement with Mie results for the model with 123 dipoles ($d \sim \lambda/10$). However, even for 5575 dipoles ($d \sim \lambda/45$), the results of the CD simulation of the $\mathbf{S}_{34}$ element are still not in good agreement with Mie results, although the CD results do approximate the Mie results if the number of dipoles is gradually increased.³ Based on this result and on simulations with $m = 1.1$ and 1.02, it was concluded that accurate $\mathbf{S}_{34}$ computation requires much smaller dipolar subunits.

To verify these results, we conducted CD simulations with a much larger number of dipoles but with $d = \lambda/10$. Figure 1 shows a CD calculation (the dots) of the $\mathbf{S}_{34}$ element of a sphere with $\alpha = 10.7$ and $m = 1.05$; the number of dipoles was 20,672, and $d = \lambda/10$. (The calculation was performed with our implementation of the CD method on a 512-node Parsytec GCel computer.) The agreement with the Mie calculation (the curve) is excellent. This example and other calculations indicate that, if the number of dipoles in the simulation is large enough, $\mathbf{S}_{34}$ can be calculated with the same accuracy as the other matrix elements, with $\lambda/20 \leq d \leq \lambda/10$.

This counterexample shows that another overlooked argument must enter the discussion. The coarseness of the discretization seems to be the key issue. The CD method discretizes a particle with small cubes (assuming dipoles on a cubic grid). This means that we simulate the sphere by a spherical

Fig. 1. S_{34}/S_{11} as a function of the scattering angle for a sphere with $\alpha = 10.7$ and $m = 1.05$. The curve is the Mie calculation, and the dots are the CD calculations, with $d = \lambda/10$ (20,672 dipoles).

particle with a rough surface. If the same particle is discretized by the use of more dipoles, the surface roughness will be smaller and the particle will be more closely approximated. We investigated the influence of surface roughness on the $\alpha = 1.55$ sphere and found that the decrease in surface roughness of the discretized particle as the number of dipoles is increased obscures the conclusions of Singham.

In the CD method we discretize a sphere as follows: place dipoles on grid points with coordinates $(i + 1/2)d$, $(j + 1/2)d$, and $(k + 1/2)d$, with i, j, k integers, demanding that

$$(i + 1/2)^2 + (j + 1/2)^2 + (k + 1/2)^2 \leq l^2. \quad (1)$$

The number l determines the number of dipoles in the discretization; e.g., $l = 3$ results in $N = 136$, and $l = 5$ gives $N = 552$. The size of the dipoles determines the radius of the simulated sphere, through $r_{\text{sphere}} = (3N/4\pi)^{1/3}d$ (the equal-volume sphere¹). The discretized sphere has a radius $r = r_{\text{sphere}}[1 \pm O(\epsilon)]$, with ϵ being a measure of the surface roughness. In our case, the radius is modulated with an amplitude of $\sim d/2$; therefore $\epsilon = 0.5 (3N/4\pi)^{-1/3}$.

Consider a particle with radius

$$r = r_0[1.0 - (2l)^{-1} \cos(4l\theta)], \quad (2)$$

with θ an azimuthal angle. This is a spherical particle with mean radius r_0 and roughness $1/(2l)$. If l is increased, the roughness is decreased, but at the same time the frequency of the modulation is increased (the cosine term). This is what happens when we increase the number of dipoles in the discretization of the sphere by increasing l in relation (1). Figure 2 shows a cross section of the rough spheres for $l = 3$ and $l = 5$.

Note that $(2l)^{-1}$ is approximately equal to the estimated roughness of the discretized sphere. We calculated the S_{11} and S_{34} elements of a random distribution of this rough sphere for $l = 3$, $l = 5$, and $l = 17$ and adjusted r_0 such that the volume of the particle was the same and equal to the test sphere in all cases with $\alpha = 1.55$. We calculated the scattering properties of this axis-symmetric particle with the T-matrix method, using the computer programs of

Barber and Hill.⁶ This calculation serves as a model of the surface roughness of the discretized sphere.

Figures 3 and 4 give the results for S_{34} and S_{11} for the $l = 3$ and $l = 5$ rough spheres, together with Mie calculation for the $\alpha = 1.55$ sphere. The $l = 17$ calculation is indistinguishable from the Mie calculation.

The influence of surface roughness is most obvious for the S_{34} element. The S_{11} element of the rough sphere deviates slightly from the sphere in the backscattering direction. For $l = 5$ the results are almost equal to the sphere. The same is true for the S_{12} and S_{33} elements (data not shown). However,

Fig. 2. Cross section of rough spheres, defined by Eq. (2), with $l = 3$ and $l = 5$.

Fig. 3. S_{34} element as a function of the scattering angle for a sphere with $\alpha = 1.55$ (solid curve) and of equal-volume rough spheres with $l = 3$ (short-dashed curve) and $l = 5$ (long-dashed curve). The refractive index was 1.33.

Fig. 4. S_{11} element as a function of the scattering angle; the rest as in Fig. 3.

the roughness has a much more pronounced effect on the S_{34} element, as seen in Fig. 3. Therefore a coarse discretization of the sphere in the CD method can result in larger errors in the S_{34} element compared with errors in the other scattering matrix elements.

If we compare the calculations on the rough sphere with the CD calculations of Singham (Figs. 1 and 2 in Ref. 3), we see the same trends. For a small number of dipoles (123, comparable with $l = 3$), the S_{34} computation deviates significantly from the exact Mie result in the same way as the rough sphere (see Fig. 3). The S_{11} result of the CD computation already is very good, with only a deviation from the exact Mie result in the backscattering direction. If the number of dipoles is increased in the CD calculation, the S_{11} result is in excellent agreement with the exact Mie calculation. The S_{34} result approaches the exact results, but agreement is far from good.

Surface roughness has a strong effect on the S_{34} element. Therefore, if the CD method is to be used to calculate the S_{34} element of a smooth particle, surface roughness induced by the discretization of

the particle must be very small. This is achieved by using a large number of dipolar subunits (large l). If the particle is small (e.g., the $\alpha = 1.55$ sphere), relatively small dipolar subunits result. However, for larger particles (see Fig. 1), the subunits can be much larger. In that case, S_{34} calculations with accuracy comparable to S_{11} calculations can be achieved with dipolar subunits with $\lambda/20 \leq d \leq \lambda/10$.

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