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DOI
10.1364/OL.18.001211
Publication date
1993

Published in
Optics Letters

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A.G. Hoekstra and P.M.A. Sloot

Parallel Scientific Computing Group, department of Computer Systems, Faculty of Mathematics and Computer Science, University of Amsterdam, Kruislaan 403, 1098 SJ Amsterdam, the Netherlands, tel. (+31)20-5257463.

Published in
Optics Letters, vol. 18, pp. 1211-1213, 1993.

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Parallel Scientific Computing Group, department of Computer Systems, Faculty of Mathematics and Computer Science, University of Amsterdam, Kruislaan 403, 1098 SJ Amsterdam, the Netherlands, tel. (+31)20-5257463.

The Coupled Dipole method is widely used to calculate the light scattering matrix **S** from arbitrary particles. An important parameter in the model is the size of the dipolar subunits. Usually a size of ~1/10 to ~ 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. Here we will 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 will 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 very powerful method to calculate Elastic Light Scattering from arbitrary particles. The CD method divides a particle in small subvolumes, which are assumed to behave as ideal dipoles. The electric field on each dipole, due to the external field and the field radiated by all other dipoles is calculated. Next the scattered field is obtained by summing the fields radiated by all dipoles in the observation points. By repeating this calculation for a parallel - and a perpendicular polarized incident electric field, the complete (4×4) scattering matrix **S** of the particle can be computed. Although the basic concepts of the model are straightforward, the model possesses many parameters which are topic of active research. An example is the choice of the polarizability of the dipolar subunits. Lakhtakia gives a review of the CD method.[2]

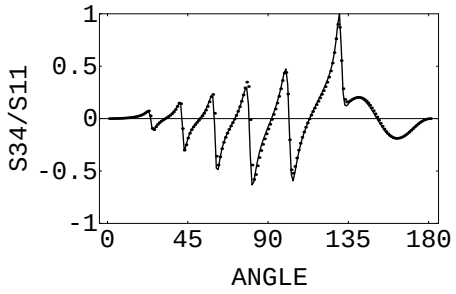
A very important parameter of the CD method is the size of the dipoles. The dipoles are placed on a cubic grid, with grid spacing d. The dipoles therefore are assumed to describe the response of a cube with volume d^3. The computation of the electric field on the dipoles requires solving a set of 3N 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 comparing CD computations on spheres with the exact Mie results, it was concluded that $\lambda/20 \leq d \leq \lambda/10$ gives a good agreement between the simulated and exact differential cross sections.[e.g. 1]

Singham[3] calculated the $\mathbf{S}_{34}$ element with the Coupled Dipole method. By comparing 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. Since N scales as d^{-3}, the total number of dipoles would be 8 to 64 times larger as for accurate $\mathbf{S}_{11}$ calculation. If the system of equations is solved with an $O(N^2)$ iterative method, this would require a factor of 64 to 4096 longer execution times on a computer. This is a very discouraging conclusion. Especially if one realizes that the $\mathbf{S}_{34}$ element is known to be very sensitive for slight changes in structure and optical constants of a particle,[see e.g. 4, 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 α equal to 1.55 and relative refractive index m equal to 1.33. This sphere was simulated with the CD method containing 123 up to 5575 dipoles. The CD results for the $\mathbf{S}_{11}$ elements are already in good agreement with the 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 the 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 require much smaller dipolar subunits.

In order 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 20672 and $d = \lambda/10$. The agreement with the Mie calculation (line) 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 $\lambda/20 \leq d \leq \lambda/10$.



† the calculation was performed with our implementation of the CD method on a 512 node Parsytec GCel computer.

Figure 1: $\mathbf{S}_{34}/\mathbf{S}_{11}$ as a function of the scattering angle, for a sphere with $\alpha = 10.7$ and $m = 1.05$.; the line is the Mie calculation, the dots are the CD calculations with $d = \lambda/10$ (20672 dipoles).

This counter example 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 particle with a rough surface. If the same particle is discretized using 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 show that the decrease of the surface roughness of the discretized particle, as the number of dipoles is increased, obscures the conclusions of Singham.

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

$$(i+1/2)^2 + (j+1/2)^2 + (k+1/2)^2 \le l^2 . \quad [1]$$

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, via $r_{sphere} = (3N/4\pi)^{1/3}d$ (the equal volume sphere[1]). The discretized sphere has a radius $r = r_{sphere}[1 \pm O(\varepsilon)]$ with ε a measure of the surface roughness. In our case the radius is modulated with an amplitude of approximately $d/2$, therefore $\varepsilon = 0.5\ (3N/4\pi)^{-1/3}$.

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 decreases, but at the same time the frequency of the modulation is increased (the cosine term). This is exactly what happens if we increase the number of dipoles in the discretization of the sphere by increasing l in equation 1. Figure 2 shows a cross section of the rough spheres for $l = 3$ and $l = 5$.

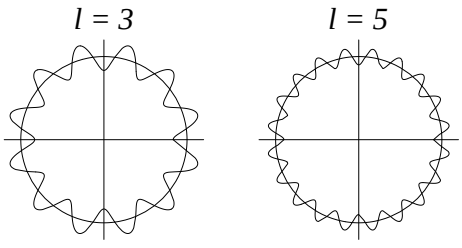


Figure 2: cross section of rough spheres, defined by equation 2, with l equals 3 and 5 respectively.

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

Figure 3 and 4 give the results for $\mathbf{S}_{34}$ and $\mathbf{S}_{11}$ for the l = 3 and l = 5 rough sphere, together with Mie calculation for the α = 1.55 sphere. The l = 17 calculation is indistinguishable from the Mie calculation.

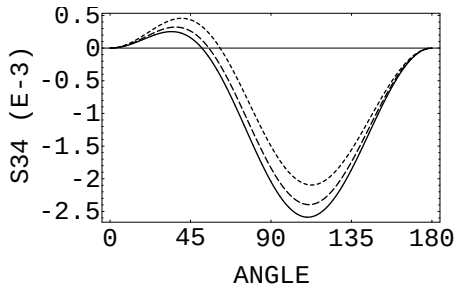


Figure 3: The $\mathbf{S}_{34}$ element as a function of the scattering angle for a sphere with α = 1.55 (line), and of equal volume rough spheres with l = 3 (short dash) and l = 5 (long dash); the refractive index was 1.33.

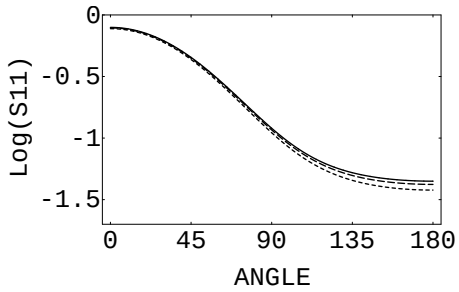


Figure 4: The $\mathbf{S}_{11}$ element as a function of the scattering angle; rest as in figure 3.

The influence of surface roughness is most obvious for the $\mathbf{S}_{34}$ element. The $\mathbf{S}_{11}$ 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 $\mathbf{S}_{12}$ and $\mathbf{S}_{33}$ element (data not shown). However the roughness has a much more pronounced effect on the $\mathbf{S}_{34}$ element, as is obvious from figure 3. Therefore, a coarse discretization of the sphere in the CD method can result in larger errors in the $\mathbf{S}_{34}$ element, compared to errors in the other scattering matrix elements.

If we compare the calculations on the rough sphere with the CD calculations of Singham (figures 1 and 2 in reference 3) we see the same trends. For a small number of dipoles (123, comparable with l = 3), the $\mathbf{S}_{34}$ computation deviates significantly from the exact Mie result, in the same way as the rough sphere (see figure 3). The $\mathbf{S}_{11}$ result of the CD computation already

is very good, with only a deviation from the exact Mie result in the backscattering directions. If the number of dipoles is increased in the CD calculations, the $\mathbf{S}_{11}$ result is in excellent agreement with the exact Mie calculation. The $\mathbf{S}_{34}$ result is approaching the exact results, but the agreement is far from good.

Surface roughness has a strong effect on the $\mathbf{S}_{34}$ element. Therefore, if one wants to exploit the CD method to calculate the $\mathbf{S}_{34}$ 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), this results in relative small dipolar subunits. However, for larger particles (see figure 1) the subunits can be much larger. In that case $\mathbf{S}_{34}$ calculations with comparable accuracy as $\mathbf{S}_{11}$ calculations can be achieved with dipolar subunits with $\lambda/20 \leq d \leq \lambda/10$.

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