Scattering by two spheres in contact: comparisons between discrete-dipole approximation and modal analysis

Piotr J. Flatau, Kirk A. Fuller, and Daniel W. Mackowski

This paper applies two different techniques to the problem of scattering by two spheres in contact: modal analysis, which is an exact method, and the discrete-dipole approximation (DDA). Good agreement is obtained, which further demonstrates the utility of the DDA to scattering problems for irregular particles. The choice of the DDA polarizability scheme is discussed in detail. We show that the lattice dispersion relation provides excellent improvement over the Clausius–Mossoti polarizability parameterization.

Key words: Scattering, irregular particles.

1. Introduction

The discrete-dipole approximation (DDA) developed by Purcell and Pennypacker[1] is a flexible and general technique for calculating the scattering and absorptive properties of particles of arbitrary shapes. This method is the subject of active research.[2–4] The DDA is especially suited to scattering by irregular particles characterized by medium values of the size parameter, $x = 2\pi a_{\mathrm{eq}}/\lambda$, where a_{eq} is the radius of a sphere with a volume equivalent to that of the nonspherical scatterer and λ is the wavelength of the electromagnetic wave. There is a need for comparison of the DDA with exact solutions in order (1) to find the number of dipoles needed to model correctly the shape of a particle in the DDA approximation, (2) to decide on numerical convergence criteria, and (3) to find a proper dipole polarizability scheme through modification to the Clausius–Mossoti relationship.

Also, since the DDA solution often involves an iterative solution of a linear problem with matrices of the order of 10^5, it reassuring to see that the method compares well with the exact solution.

P. J. Flatau is with the Scripps Institution of Oceanography, University of California, San Diego, La Jolla, California 92093-0221; K. A. Fuller is with the Department of Atmospheric Science, Colorado State University, Fort Collins, Colorado 80523; and D. W. Mackowski is with the Department of Mechanical Engineering, Auburn University, University, Alabama 36849.

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An arbitrary cluster of spheres[5,6] can be solved exactly by the multipole expansion method. Such a modal analysis provides an independent test of scattering by nonspherical particles. In a recent report, Wiscombe and Mugnai[7] state: "Of great interest, perhaps, is the solution . . . for an arbitrary cluster of spheres; indeed, it seems . . . that sphere clusters would be an excellent archetype for general nonspherical particles. Apparently, however, the solution . . . is nightmarish to put into practice." In agreement with the first part of this quote, we use a cluster of spheres for testing the DDA. It seems that the practical part has been recently improved.[5] Using a modified version of the work by Mackowski[6] we were able to solve for a relatively large cluster of spheres. In this paper, the multipole solution for two spheres is used to test the DDA.

2. Two Spheres

Recent investigations have studied the general solution to Maxwell's wave equation for clusters of spheres.[5,6] The analysis involves a superposition technique, in that the total solution for a scattered electromagnetic field of a particle is constructed from a superposition of individual solutions. To satisfy the boundary conditions on each sphere, addition theorems are used to transform a spherical harmonic from one coordinate to another. Such a formulation leads to a set of linear equations for the expansion coefficients of the scattered fields of the constituent spheres. In matrix form the system of equations is expressed as

$$\mathbf{a}^i + \sum_{j=1, j\neq i}^{N_s} \mathbf{T}^{ji}\mathbf{a}^j = \mathbf{p}^i, \tag{1}$$

where vector $\mathbf{a}$ defines coefficients of the scattered field for sphere i, vector $\mathbf{p}^i$ defines incident field coefficients for a sphere i, $\mathbf{T}^{ji}$ represents the translation matrix from sphere j to i, and N_s is number of spheres. The sizes of $\mathbf{a}$, $\mathbf{p}$, and $\mathbf{T}$ depend on the order of multipole expansion. Far-field scattering and cross sections are determined by $\mathbf{a}$. A detailed account has been given by Mackowski.[6] An exact solution for multiple spheres, which uses multipole expansion, offers a unique opportunity to compare our DDA implementation with an independent solution for nonspherical targets. Figure 1 shows two pseudospheres in contact resolved on $32 \times 32 \times 32$ dipole grid for each of the spheres.

In Fig. 2 we have compared the exact solution for scattering by two spheres (solid curve) in contact with the solution derived from DDA (crosses) for $m = 1.33 + 0.001i$ and a scattering parameter $x = 5$ (results not presented) and $x = 10$. Exact results for S_{11} and S_{22} are compared with S_{11} and S_{22} results, which were computed by the DDA for two perpendicular scattering planes. For $x = 5$, DDA matches the exact solution well, and on a plot scaled as in Fig. 2 it matches exactly and DDA results would overlap. For $x = 10$ and orientation $\alpha = 0$ (Fig. 2) the overall agreement is good although errors can be seen in the side and backscatter directions. In Section 3 we perform a more quantitative error analysis by showing fractional error plots for several values of equivalent size parameter.

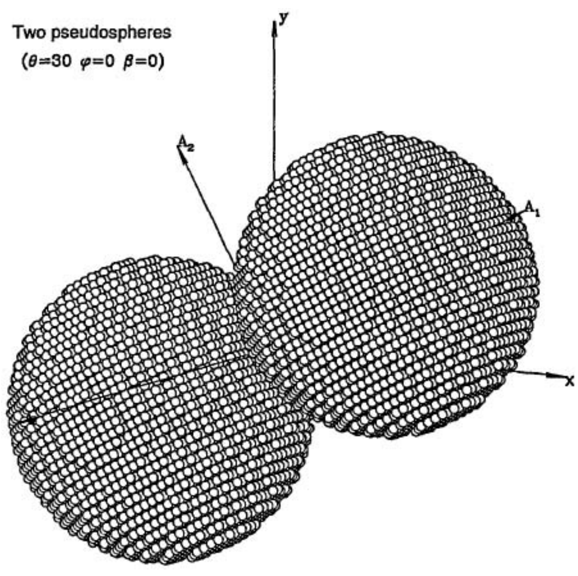

Fig. 1. Two pseudospheres composed of $2 \times 32 \times 32 \times 32$ point dipoles. Light is travelling along the x axis. Spheres are rotated ($\alpha = 30$).

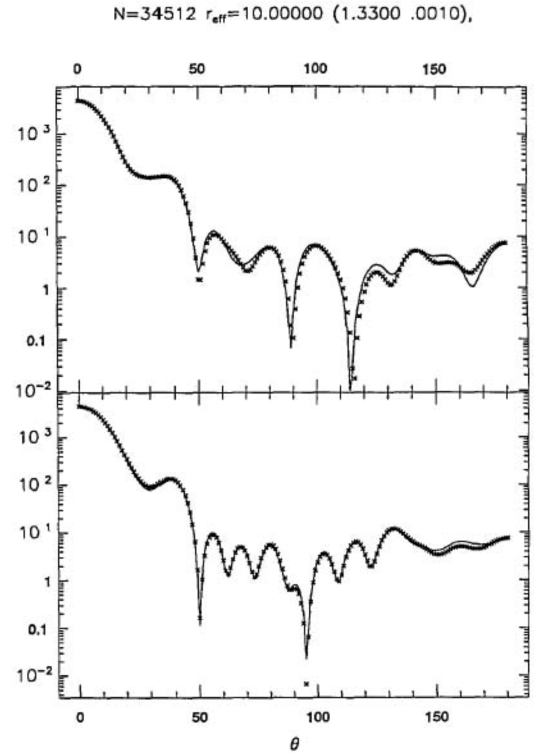

Fig. 2. Scattering by a sphere with refractive index $m = 1.33 + 0.001i$ for $x = ka = 10$ and $\alpha = 0$. Exact results for S_{11} and S_{22} are compared with S_{11} and S_{22} results that were computed by the DDA for $x = 10$.

3. Choice of Polarizability Definition: Comparisons with Two-Sphere Cluster

Since DDA results depend directly upon the dipole polarizabilities, it is important to determine the optimal method for choosing such polarizabilities. Recently Draine and Goodman[4] established the lattice dispersion relation (LDR) method for prescribing the dipole polarizabilities. They solved a closely related problem: choosing the dipole polarizabilities such that an infinite lattice of point dipoles will propagate electromagnetic plane waves with the same dispersion relation as a medium of specified dielectric function ϵ.

In order to compare their new prescription for polarizability with those proposed previously, they report the results of extensive DDA calculations for absorption and scattering by single spheres, and compare exact Lorenz–Mie theory results with DDA calculations. They find that for moderate $|\epsilon - 1|$ their prescription for the dipole polarizabilities generally provides more accurate results for scattering and absorption by spheres; this superiority is presumed to extend to nonspherical targets.

The unique aspect of this prescription, which they were not able to test thoroughly, is that it depends not only on refractive index m but also on the direction of propagation and the polarization state of the incident radiation. In this section we extend their analysis to include comparisons with the exact solution for nonspherical particles composed of two spheres in contact. We conclude that, indeed, the DDA calculations of absorption and scattering should be based on the LDR prescription for the dipole polarizabilities.

The Draine and Goodman[4] polarizability can be written as

$$\alpha = \frac{\alpha^{(nr)}}{1 - (2/3)i[\alpha^{(nr)}/d^3](k_0 d)^3}, \tag{2}$$

with

$$\alpha^{(nr)} \approx \frac{\alpha^{(0)}}{1 + [\alpha^{(0)}/d^3](b_1 + m^2 b_2 + m^2 b_3 S)(k_0 d)^2}, \tag{3}$$

$$b_1 = c_1/\pi = -1.8915316, \tag{4}$$

$$b_2 = c_2/\pi = 0.1648469, \tag{5}$$

$$b_3 = -(3c_2 + c_3)/\pi = -1.7700004, \tag{6}$$

where $\alpha^{(0)}$ is the Clausius–Mossotti polarizability:

$$\alpha_{\mathbf{i}}^{(0)} \equiv \frac{3d^3}{4\pi}\left(\frac{m_{\mathbf{i}}^2 - 1}{m_{\mathbf{i}}^2 + 2}\right). \tag{7}$$

Here, $m_{\mathbf{i}}$ is the refractive index at lattice site $\mathbf{i}$, and the dependence on direction and polarization enters solely through the quantity S. There are two other choices of polarizability used in the current literature on the subject. Goedecke and O'Brien[8] and Hage and Greenberg[9] showed that the fundamental DDA equation can be derived from a simple discretization of an integral formulation of the scattering problem, the digitized Green's function/volume integral equation formulation (DGF/VIEF) method. Using the optical theorem, Draine[10] showed that when $k_0 d$ was finite the polarizabilities $\alpha_{\mathbf{i}}$ should include a radiative reaction correction [the Clausius–Mossoti plus radiative reaction (CMRR) method].

Figure 3 presents the comparison of a two-sphere, multipole solution with the DDA for $\alpha = 30$, which corresponds to the configuration in Fig. 1. Results are shown for three different prescriptions for the dipole polarizabilities: CMRR, DGF/VIEF, and LDR as functions of size parameter $x = k_0 a_{\text{eff}}$. Refractive index $m = 1.33 + 0.01i$ is used and the dipoles are placed on a $2 \times 32 \times 32 \times 32$ cubic lattice. For the calculations light propagates along the x axis and is unpolarized. The LDR method is superior to DGF/VIEF and CMRR for a broad range of size parameter values. For $\alpha = 30$, the LDR method gives excellent agreement, which indicates that the directional corrections in Eq. (2) are indeed an improvement.

Figure 4 presents a comparison of a two-sphere multipole solution with the DDA for the same physical parameters as in Fig. 3 but for fixed $x = 5$ with α as a function of orientation. Again the LDR is consistently better in comparison with the other two schemes. The fractional error for scattering efficiency (Fig. 4) is close to 1% in comparison with the multipole solution, and for absorption efficiency (results not presented) the error is less than 3%.

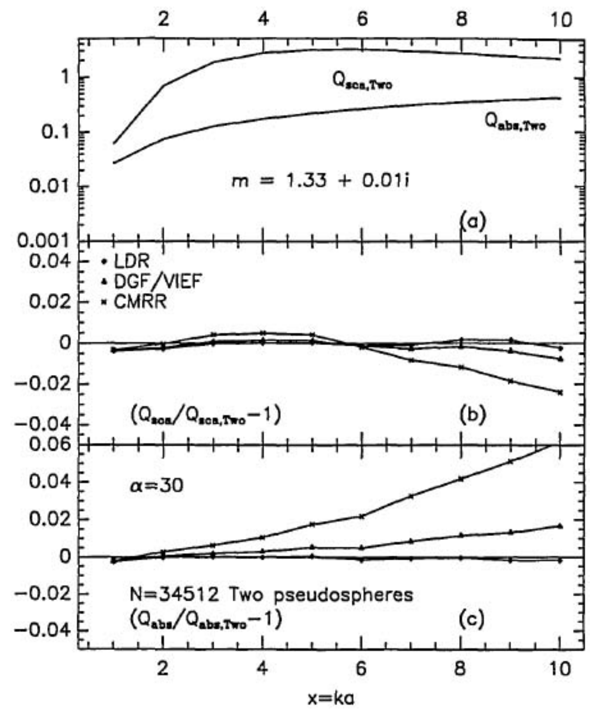

Fig. 3. (a) Q_{sca} and Q_{abs} for two spheres of refractive index $m = 1.33 + 0.01i$ in contact, (b) fractional error in computed value of Q_{sca}, (c) Q_{abs} for the $N = 2 \times 34{,}512$ two pseudospheres of Fig. 1. Results are shown for three different prescriptions for the dipole polarizabilities: CMRR, VIEF, and LDR as functions of $x = k_0 a_{\text{eff}}$, $\alpha = 30$.

4. Summary

This paper presents further evidence that DDA is a sound method for the study of electromagnetic scatter-

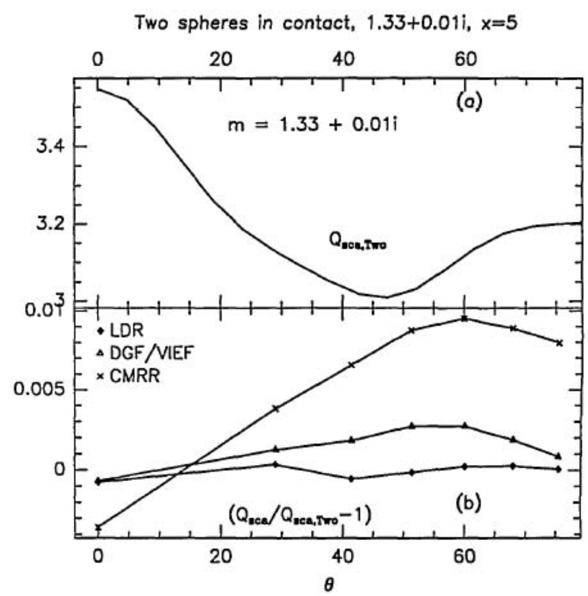

Fig. 4. (a) Dependence of Q_{sca} on orientation for the two spheres of Fig. 3 with $x = 5$, (b) fractional error in computed value of Q_{sca} as a function of α for the two pseudospheres of Fig. 1.

ing by irregular particles.[11,12] The choice of the polarizability scheme is justified on the basis of the multipole solution for a cluster of two spheres in contact. Results show that the DDA, together with the conjugate-gradient fast-Fourier-transform algorithm, makes possible accurate calculations of scattering and absorption by dielectric targets for a medium range of size parameters. It is shown that the LDR polarizability works well in the case of nonspherical particles. This extends recent results of Draine and Goodman,[4] wherein only spherical targets were tested.

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