

Light scattering by rectangular solids in the discrete-dipole approximation: a new algorithm exploiting the Block-Toeplitz structure

Piotr J. Flatau and Graeme L. Stephens

Department of Atmospheric Science, Colorado State University, Fort Collins, Colorado 80523

Bruce T. Draine

Princeton University Observatory, Peyton Hall, Princeton, New Jersey 08544

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The discrete-dipole approximation is used to study the problem of light scattering by homogeneous rectangular particles. The structure of the discrete-dipole approximation is investigated, and the matrix formed by this approximation is identified to be a symmetric, block-Toeplitz matrix. Special properties of block-Toeplitz arrays are explored, and an efficient algorithm to solve the dipole scattering problem is provided. Timings for conjugate gradient, Linpack, and block-Toeplitz solvers are given; the results indicate the advantages of the block-Toeplitz algorithm. A practical test of the algorithm was performed on a system of 1400 dipoles, which corresponds to direct inversion of an 8400×8400 real matrix. A short discussion of the limitations of the discrete-dipole approximation is provided, and some results for cubes and parallelepipeds are given. We briefly consider how the algorithm may be improved further.

INTRODUCTION

The discrete-dipole approximation (DDA) developed by Purcell and Pennypacker¹ 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 in several diverse fields: for example, Draine² examines the ultraviolet optical properties for interstellar dust composed of extremely anisotropic graphite particles. Flatau *et al.*^{3,4} apply the method to study scattering by hexagonal ice crystals, which are common in upper tropospheric cirrus clouds and may occur in polar stratospheric clouds. O'Brien and Goedecke⁵⁻⁷ are concerned with scattering of millimeter waves by snow crystals. Keller and Bustamante⁸ describe the application to spectroscopy of large, internally inhomogeneous, molecular aggregates of chromophores (e.g., viruses and chromosomes) bound together in a rigid structure. The DDA is especially suited to scattering characterized by small values of the size parameter x , defined as $x = 2\pi a_{eq}/\lambda$, where a_{eq} is the equivalent radius (the radius of a sphere of equal volume) and λ is the wavelength of the electromagnetic wave. It shares many of the conceptual features of the well-known Rayleigh-Gans-Debye approximation (see Ref. 9 for an application of Rayleigh scattering developed in a way similar to the DDA ideas) but demands much more computational effort.

Various methods of dealing with the problem of scattering by nonspherical particles are reviewed by Wiscombe and Mugnai¹⁰ and Pollack and Cuzzi.¹¹ Singham and Bohren¹² recently discussed the virtues of some of the different methods used to solve the DDA. A direct solver method was used

by Singham and Salzman,¹³ an iterative method of the (complex) conjugate-gradient (CCG) type was introduced by Yung¹⁴ and used in an improved form by Draine,² and Born-type expansions have been proposed by several authors.^{8,12,15}

In this paper we introduce a different method of solution for the specific case of light scattering by homogeneous rectangular solid particles. Such particles were studied theoretically^{1,16-18} as well as experimentally¹⁹⁻²⁴ and occur in nature at low temperatures in the atmosphere; examples are the diamond-dust^{25,26} particles collected in Antarctica. Whalley²⁷ suggested that Scheiner's halo may be due to cubic ice (but compare Weinheimer and Knight²⁸ for the opposite point of view). In a review paper, Hallet²⁹ mentions materials that could crystallize as a hydrate in the cubic system. Mother-of-pearl clouds³⁰ and polar stratospheric clouds may contain cubic particles.

For the particle geometry under consideration, we identify the DDA matrix as a symmetric block-Toeplitz (BT) matrix and use the special properties of such arrays to develop a new algorithm. The special features of rectangular solids that give rise to the particular mathematical structure exploited in this study also exist to a considerable degree for particles of less regular shape. We suspect that this is the reason why iterative schemes (such as the CCG algorithm) are so remarkably efficient in DDA applications.

The paper is organized as follows: in the next section we present the formulation of the DDA,^{1,2} and the BT structure³¹⁻³³ is introduced in the subsequent section. Next the generalized Levinson³² algorithm for the direct solution of the BT matrix is presented, and its implementation³³ is discussed. The role of the Gohberg-Semencul-Heinig³⁴

theorem is described, and results are shown for cubic particles.

DISCRETE-DIPOLE APPROXIMATION

The DDA replaces the solid particle by an array of N point dipoles (Fig. 1), with the spacing between the dipoles small compared with the wavelength. The dipoles are assumed to occupy positions on a cubic lattice. Each dipole has an oscillating polarization in response to both an incident plane wave and the electric fields that are due to all the other dipoles in the array. The self-consistent solution for the dipole polarizations can be obtained as the solution to a set of coupled linear equations^{1,2}:

$$\tilde{\mathbf{A}}\tilde{\mathbf{P}} = \tilde{\mathbf{E}}_{\text{inc}}, \quad (1)$$

where $\tilde{\mathbf{A}}$ is a $3N \times 3N$ symmetric complex matrix that depends on particle shape (i.e., on the geometry of the N -point array), the dielectric constant, and the ratio of the incident wavelength to the interdipole spacing; $\tilde{\mathbf{P}}$ is a $3N$ -dimensional unknown vector of dipole polarizations; $\tilde{\mathbf{E}}_{\text{inc}}$ is a $3N$ -dimensional known vector of the incident electric field. We will refer to $\tilde{\mathbf{A}}$ as the DDA matrix. The inverse of $\tilde{\mathbf{A}}$ is of fundamental importance. For example, the extinction cross section is given by²

$$C_{\text{ext}} = \frac{4\pi k}{|\tilde{\mathbf{E}}_{\text{inc}}|^2} \text{Im}[\tilde{\mathbf{E}}_{\text{inc}}^* \cdot (\tilde{\mathbf{A}}^{-1} \tilde{\mathbf{E}}_{\text{inc}})], \quad (2)$$

where $\tilde{\mathbf{E}}_{\text{inc}}$ is a three-dimensional vector, the scalar product is between two $3N$ -dimensional vectors $\tilde{\mathbf{E}}_{\text{inc}}^*$ and $\tilde{\mathbf{A}}^{-1} \tilde{\mathbf{E}}_{\text{inc}}$, and an asterisk indicates a complex conjugate. Equation (2) can be rewritten⁸ as

$$C_{\text{ext}} = \frac{4\pi k}{|\tilde{\mathbf{E}}_{\text{inc}}|^2} \text{Im}(\tilde{\mathbf{E}}_{\text{inc}}^* \tilde{\mathbf{E}}_{\text{inc}} : \tilde{\mathbf{A}}^{-1}), \quad (3)$$

where the colon indicates contraction³⁵ of two matrices, $\mathbf{a}$ and $\mathbf{b}$. Equation (3) indicates that the shape information contained in the matrix $\tilde{\mathbf{A}}^{-1}$ is effectively decoupled from the orientational information contained in the matrix $\tilde{\mathbf{E}}_{\text{inc}}^* \tilde{\mathbf{E}}_{\text{inc}}$. Thus, by holding the particle fixed and summing over incident directions to find $\langle \tilde{\mathbf{E}}_{\text{inc}}^* \tilde{\mathbf{E}}_{\text{inc}} \rangle$, we can get any

desired orientational average^{8,9,36} of the extinction cross section $\langle C_{\text{ext}} \rangle$.

The notation here follows that of Draine,² and for convenience we define $K = 3N$. Direct methods of solving Eq. (1) require computational effort proportional to $O(K^3)$ multiplications and storage of $O(K^2)$ numbers. In order to obtain a satisfactory approximation to the actual particle, one typically requires a large number of dipoles (say, $>10^3$) for particles with dimensions comparable with the wavelength.² Thus the direct solution of Eq. (1) becomes intractable under such conditions. Iterative schemes, such as the CCG method, converge in $O(\gamma K^2)$ scalar multiplications, where γ is some constant that is, in general, of the order of K . However, as was observed recently for $\tilde{\mathbf{A}}$ matrices defined by the DDA, γ is of the order of 10–20 ($2K^2$ multiplications per iteration, with 5–10 iterations resulting in excellent convergence in many cases).² Because K is large in the DDA application, such rapid convergence is both surprising and welcome. It was also observed that the first guess using a fourth-order Born expansion,^{2,8,15} although close to the final solution in terms of the fractional error, does not substantially improve subsequent convergence of the CCG iteration scheme.

This rapid convergence possibly arises from the symmetry of $\tilde{\mathbf{A}}$. Consider this further by expressing Eq. (1) in a more explicit form:

$$\sum_{k=1}^N \mathbf{A}_{jk} \mathbf{P}_k = \mathbf{E}_{\text{inc},j} \quad (j = 1, \dots, N), \quad (4)$$

where $\mathbf{P}_j$, $j = 1, \dots, N$ are three-dimensional vectors of dipole moments, $\mathbf{E}_{\text{inc},j}$ is the electric field at position j due to the incident plane wave, and $\mathbf{A}_{jk}$ are 3×3 matrices defined as

$$\mathbf{A}_{jk} = \frac{\exp(ikr_{jk})}{r_{jk}} \left[k^2 (\hat{\mathbf{r}}_{jk} \hat{\mathbf{r}}_{jk} - \mathbf{I}_3) + \frac{(ikr_{jk} - 1)}{r_{jk}^2} (3\hat{\mathbf{r}}_{jk} \hat{\mathbf{r}}_{jk} - \mathbf{I}_3) \right] \quad (j \neq k) \quad (5)$$

and

$$\mathbf{A}_{jj} = \alpha_j^{-1}, \quad (6)$$

where the wave number $k = 2\pi/\lambda$, $r_{jk} = |\mathbf{r}_j - \mathbf{r}_k|$, $\hat{\mathbf{r}}_{jk} = (\mathbf{r}_j - \mathbf{r}_k)/r_{jk}$ is a unit vector in the direction between the k th and j th dipoles, α_j is the polarizability tensor of the j th dipole, and $\mathbf{I}_3$ is a three-dimensional, diagonal unit matrix. Tensor $\hat{\mathbf{r}}\hat{\mathbf{r}}$ is a dyadic product³⁵ of two unit vectors and can be represented as a 3×3 matrix with components $(\hat{x}\hat{x}, \hat{x}\hat{y}, \hat{x}\hat{z}, \hat{y}\hat{x}, \hat{y}\hat{y}, \hat{y}\hat{z}, \hat{z}\hat{x}, \hat{z}\hat{y}, \hat{z}\hat{z})$. The definition of $\tilde{\mathbf{A}}$ is the same as that of Draine,² because $\mathbf{r} \times (\mathbf{r} \times \mathbf{P}) = (\mathbf{r}\mathbf{r} - r^2\mathbf{I}_3) \cdot \mathbf{P}$. The relationship between α_j and the dielectric tensor, including radiative reaction corrections, is discussed by Draine.² In this paper we assume that the polarizability is isotropic for all dipole positions and that the particle is homogeneous, i.e. $\alpha_j = \alpha_0 \mathbf{I}_3$ for all j . These assumptions are more limiting than need be but do provide some simplification, as we describe below. Equation (5) is a function of the distance and the direction between the dipoles j and k . Thus, for the particle presented in Fig. 1, there are many pairs of dipoles that are separated by the same distance and are oriented

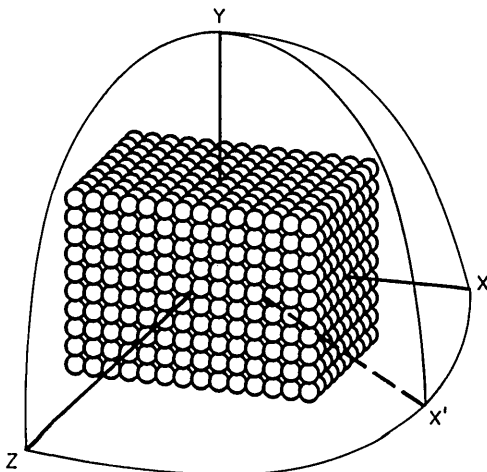


Fig. 1. Discrete-dipole array for a cube composed of 1400 dipoles.

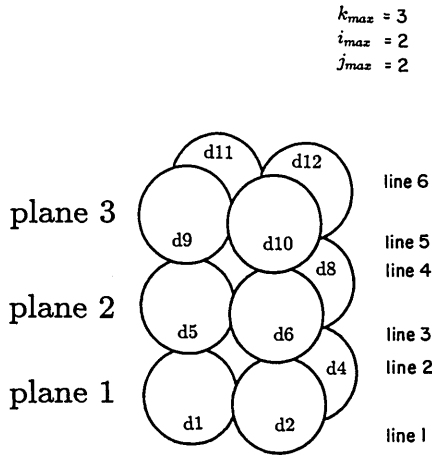


Fig. 2. Idealized array of discrete-dipole structure composed of 12 atoms.

with respect to one another along the same direction. In addition, tensor $\hat{\mathbf{f}}\hat{\mathbf{f}}$ is invariant under the $\hat{\mathbf{f}} \rightarrow -\hat{\mathbf{f}}$ transformation, and so is the distance r_{ij} . Therefore we can write

$$\mathbf{A}(\mathbf{r}_j, \mathbf{r}_k) = \mathbf{A}(\mathbf{r}_k, \mathbf{r}_j) = \mathbf{A}(\mathbf{r}_j - \mathbf{r}_k) \quad (j, k = 1, \dots, N, j \neq k), \quad (7)$$

where $\mathbf{A}(\mathbf{r}_j, \mathbf{r}_k) \equiv \mathbf{A}_{jk}$. As we now show, Eq. (7) bears a strong resemblance to the definition of a symmetric Toeplitz matrix.

BLOCK-TOEPLITZ MATRICES

A $(K+1) \times (K+1)$ symmetric Toeplitz matrix^{31,33} $\tilde{\mathbf{A}} = [a_{jk}]$ has $K+1$ independent elements, defined by $a_{jk} = a_{|j-k|}$ for $j, k = 1, \dots, K$ such that

$$\tilde{\mathbf{A}} = \begin{bmatrix} a_0 & a_1^T & \dots & a_K^T \\ a_1 & a_0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & a_1^T \\ a_K & \dots & a_1 & a_0 \end{bmatrix}, \quad (8)$$

where T indicates (matrix) transpose, the elements on each

diagonal are equal, and $a_0 = a_0^T$. If the a_j 's are themselves matrices, then $\tilde{\mathbf{A}}$ is said to exhibit block-symmetric-Toeplitz structure.

It will now be shown that the DDA matrix has a special form of block-symmetric-Toeplitz structure for particles that are homogeneous rectangular solids. Such particles can in general be approximated by arrays of identical dipoles at lattice positions (i, j, k) , where $i = 1, \dots, i_{\max}$, $j = 1, \dots, j_{\max}$, $k = 1, \dots, k_{\max}$, and $N = i_{\max}j_{\max}k_{\max}$. Consider the simple case of a three-dimensional particle composed of 12 dipoles as in Fig. 2 (with $i_{\max} = 2$, $j_{\max} = 2$, $k_{\max} = 3$). For the sake of discussion, let the dipoles be identified as d1, d2, ..., d12. Let us denote the group of four dipoles lying in one plane as $[p1]$ (dipoles d1, ..., d4), as $[p2]$ for dipoles d5, ..., d8, and $[p3]$ for dipoles d9, ..., d12. Let us denote the group of two dipoles lying in one line as $[l1]$ for dipoles d1 and d2, $[l2]$ for dipoles d3 and d4, $[l3]$ for dipoles d5 and d6, $[l4]$ for dipoles d7 and d8, $[l5]$ for dipoles d9 and d10, and $[l6]$ for dipoles d11 and d12. Each dipole interacts with the other dipoles in the array, with the strength of the interaction depending on the distance and the direction. The position of each dipole can be described by three integers (p, q, r) , which are components of the $\mathbf{r}$ vector: $\mathbf{r} = p\hat{e}_1 + q\hat{e}_2 + r\hat{e}_3$, where $\hat{e}_1, \hat{e}_2$, and $\hat{e}_3$ are unit vectors in three perpendicular directions. The matrix in Table 1 is a schematic representation of terms that describe the interactions among the 12 dipoles used for this example; each element a_{jk} is a 3×3 matrix given by Eqs. (5) and (6). There are nine plane submatrices (blocks) to consider, and these are emphasized by the lines in the table. For example, the upper left-hand block represents the interactions between the $[p1][p1]$ groups of dipoles. The block structure of the dipole interaction can then be expressed as

$$\tilde{\mathbf{A}} = \begin{bmatrix} [p1:p1] & [p1:p2] & [p1:p3] \\ [p2:p1] & [p2:p2] & [p2:p3] \\ [p3:p1] & [p3:p2] & [p3:p3] \end{bmatrix}, \quad (9)$$

where the nine blocks $[p1:p1]$, $[p1:p2]$, $[p1:p3]$, $[p2:p1]$, $[p2:p2]$, $[p2:p3]$, $[p3:p1]$, $[p3:p2]$, and $[p3:p3]$ represent those bordered by the lines in the matrix of Table 1. Matrix $\tilde{\mathbf{A}}$ has BT structure, and all nine of the blocks are themselves BT. For example, $[p1:p1]$ subblock has the structure

$$[p1:p1] = \begin{bmatrix} [l1:l1] & [l1:l2] \\ [l2:l1] & [l2:l2] \end{bmatrix}, \quad (10)$$

Table 1. Matrix of Interaction Forces a_{jk} among Twelve Dipoles^a

	d1	d2	d3	d4	d5	d6	d7	d8	d9	d10	d11	d12
d1	a_{000}	a_{010}	a_{100}	a_{110}	a_{001}	a_{011}	a_{101}	a_{111}	a_{002}	a_{012}	a_{102}	a_{112}
d2	a_{010}	a_{000}	a_{110}	a_{100}	a_{011}	a_{001}	a_{111}	a_{101}	a_{012}	a_{002}	a_{112}	a_{102}
d3	a_{100}	a_{110}	a_{000}	a_{010}	a_{101}	a_{111}	a_{001}	a_{011}	a_{102}	a_{112}	a_{002}	a_{012}
d4	a_{110}	a_{100}	a_{010}	a_{000}	a_{111}	a_{101}	a_{011}	a_{001}	a_{112}	a_{102}	a_{012}	a_{002}
d5	a_{001}	a_{011}	a_{101}	a_{111}	a_{000}	a_{010}	a_{100}	a_{110}	a_{001}	a_{011}	a_{101}	a_{111}
d6	a_{011}	a_{001}	a_{111}	a_{101}	a_{010}	a_{000}	a_{110}	a_{100}	a_{011}	a_{001}	a_{111}	a_{101}
d7	a_{101}	a_{111}	a_{001}	a_{011}	a_{100}	a_{110}	a_{000}	a_{010}	a_{101}	a_{111}	a_{001}	a_{011}
d8	a_{111}	a_{101}	a_{011}	a_{001}	a_{110}	a_{100}	a_{010}	a_{000}	a_{111}	a_{101}	a_{011}	a_{001}
d9	a_{002}	a_{012}	a_{102}	a_{112}	a_{001}	a_{011}	a_{101}	a_{111}	a_{000}	a_{010}	a_{100}	a_{110}
d10	a_{012}	a_{002}	a_{112}	a_{102}	a_{011}	a_{001}	a_{111}	a_{101}	a_{010}	a_{000}	a_{110}	a_{100}
d11	a_{102}	a_{112}	a_{002}	a_{012}	a_{101}	a_{111}	a_{001}	a_{011}	a_{100}	a_{110}	a_{000}	a_{010}
d12	a_{112}	a_{102}	a_{012}	a_{002}	a_{111}	a_{101}	a_{011}	a_{001}	a_{110}	a_{100}	a_{010}	a_{000}

^a A bar over an index indicates negative value.

where $[l1:l1]$, $[l1:l2]$, $[l2:l1]$, and $[l2:l2]$ are 2×2 line subblocks. The blocks $[l1:l1]$ and $[l2:l2]$ are also equivalent and are BT since the interactions among the dipoles in a line depend only on the distance and not on the direction of the dipoles. Interaction between dipoles from two different planes is thus described by $[p_m:p_n]$, where $m, n = 1, 2, 3$ and $m \neq n$. The invariance to the $\mathbf{r} \rightarrow -\mathbf{r}$ transformation gives $a_{p,q,r} = a_{-p,-q,-r}$. Thus the matrix $[p_m:p_n]$ is the transposed $[p_n:p_m]$, and the interaction matrix is BT and block symmetric. Each of the block matrices is of BT structure itself. The resulting plane-plane interactions, and within each plane the line-line interactions, and within each line the dipole-dipole interactions, lead to the embedded BT structure; the notation³³ TTT is appropriate to indicate such a three-level matrix. More specifically, this structure might be denoted $T_{sb}\{T_b[G_s]\}$ block-symmetric-Toeplitz, with blocks that are themselves BT (but not symmetric), with subblocks that are themselves BT (but not symmetric), and with 3×3 subblocks that are symmetric (but not Toeplitz).

ALGORITHM AND ITS IMPLEMENTATION

We now exploit the properties of the BT matrix in order to solve Eq. (1) in fewer than $O(K^3)$ operations and with less than $O(K^2)$ storage. If we assume that each block has the dimension $p \times p$ and that there are n blocks, then $K = pn$ (in the present application, n is the number of planes and $p/3$ is the number of dipoles in one plane).

It is clear from Eq. (8) that, for the block-symmetric BT matrix, the first block column is sufficient to store the whole matrix; thus the required storage is p^2n , which is smaller than K^2 by a factor n . Friedlander *et al.*³² and Gohberg and Heinig³⁴ have shown that the inverse of the Toeplitz matrix can be stored in $2p^2n$ storage. This result is nontrivial because the inverse of the Toeplitz matrix is non-Toeplitz, so the special structure of Eq. (8) disappears. The particular algorithm that we present below takes advantage of the BT structure with general (i.e., non-Toeplitz) subblocks (TG structure). Unfortunately, it seems that there are no algorithms currently in existence that would allow us to capitalize further on the TTT structure of the DDA matrices.³³ Thus the algorithm is of order p^3n^2 , which can be orders of magnitude better than for direct solvers, which are $O(p^3n^3)$.

The following algorithm³²⁻³⁴ is used to solve Eq. (1) and find $\tilde{\mathbf{A}}^{-1}$. Let $\tilde{\mathbf{A}}$ be a BT matrix of order $(n+1)p$ defined by Eq. (8). Let us denote by $A_k = [A_{k,k}, A_{k,k-1}, \dots, A_{k,0}]$ and by $B_{k,k}, B_{k,k-1}, \dots, B_{k,0}$ the last and the first block row of (unknown) $\tilde{\mathbf{A}}^{-1}$, respectively. We define the $p \times p$ matrix polynomials $A_k(z) = \sum_{i=0}^k A_{k,i}z^i$ and $B_k(z) = \sum_{i=0}^k B_{k,i}z^i$. These polynomials satisfy the recurrence relations

$$A_k(z) - X_k B_k(z) = A_{k-1}, \quad (11)$$

$$B_k(z) - Y_k A_k(z) = z B_{k-1}(z), \quad (12)$$

where the $p \times p$ matrices X_k and Y_k are given by

$$X_k = -A_{k-1} \begin{bmatrix} \mathbf{a}_1 \\ \vdots \\ \mathbf{a}_k \end{bmatrix}, \quad Y_k = -B_{k-1} \begin{bmatrix} \mathbf{a}_k^T \\ \vdots \\ \mathbf{a}_1^T \end{bmatrix}. \quad (13)$$

With an arbitrary matrix polynomial $A_k(z) = \sum_{i=0}^n A_{k,i}z^i$ let us associate matrices

$$\mathcal{L}_k[A(z)] = \begin{bmatrix} \mathbf{a}_0 & 0 & \dots & 0 \\ \mathbf{a}_1 & \mathbf{a}_0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ \mathbf{a}_k & \dots & \mathbf{a}_1 & \mathbf{a}_0 \end{bmatrix} \quad (14)$$

and

$$\mathcal{L}_k^T[A(z)] = \begin{bmatrix} \mathbf{a}_0 & \mathbf{a}_1 & \dots & \mathbf{a}_k \\ 0 & \mathbf{a}_0 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \mathbf{a}_1 \\ 0 & \dots & 0 & \mathbf{a}_0 \end{bmatrix} \quad (15)$$

for any $k \leq n$. The Gohberg-Semencul-Heinig algorithm (for the block-symmetric case) for the inverse of $\tilde{\mathbf{A}}$ is

$$\tilde{\mathbf{A}}^{-1} = \mathcal{L}^T[A_k^T(z)] \mathcal{L}_k[M_k^{-1}A_k(z)] - \mathcal{L}_k^T[zB_k^T(z)] \mathcal{L}_k[zN_k^{-1}B_k(z)], \quad (16)$$

where $M_k = A_{k,0}$ and $N_k = B_{k,k}$. The essence of the algorithm is that the full inverse of $\tilde{\mathbf{A}}^{-1}$ can be constructed from the two block columns, and the algorithm exploits (recursively) the special structure of BT matrices.

RESULTS

We begin this section with a short discussion of the DDA results for spheres. Let the scattering properties be described by the scattering matrix f_{ml} defined by Draine.²

Figure 3 presents $|f|^2$ (proportional to the differential cross section) for a dipole array of $N = 304$ (Figs. 3a-3c) and $N = 2176$ (Figs. 3d-3f). The size parameter $x = 3.1518$ and the refractive index $n = 1.089 + i0.18$ correspond to an ice sphere of radius $a_{\text{eq}} = 5.42 \mu\text{m}$ and $\lambda = 10.8 \mu\text{m}$, respectively.

Crosses (perpendicular electric field) and squares (parallel electric field) in Figs. 3b and 3d are derived from Mie's solution for spheres.³⁷ Crosses and squares in Figs. 3c and 3f represent relative (percentage) error:

$$E = 100 \left| \frac{|f|_{\text{DDA}}^2}{|f|_{\text{Mie}}^2} - 1 \right|. \quad (17)$$

Notice that the scales in Figs. 3c and 3d are different. The three sets of dashed and solid curves in Fig. 3a apply to three different angles of incidence of radiation. For the ideal sphere these three curves exactly overlap. The array used to represent the sphere in the DDA is not, however, rotationally symmetric, so the results for the three different incidence directions are not degenerate³⁸; this is particularly evident in the case of $N = 304$ dipoles. Draine² has presented a validity criterion from which one would estimate that $N = 304$ dipoles should give overall scattering results accurate to approximately 8.5% for this problem. While the total scattering and extinction cross sections conform to this error estimate, and forward scattering is quite close to the exact results for spheres, it is seen that large fractional errors occur for the differential scattering cross sections at scattering angles $\theta > 65^\circ$; the error is more than 60% for backscattering ($\theta = 180^\circ$). The main point of this discussion is that one needs quite large values of N to provide sufficient lattice

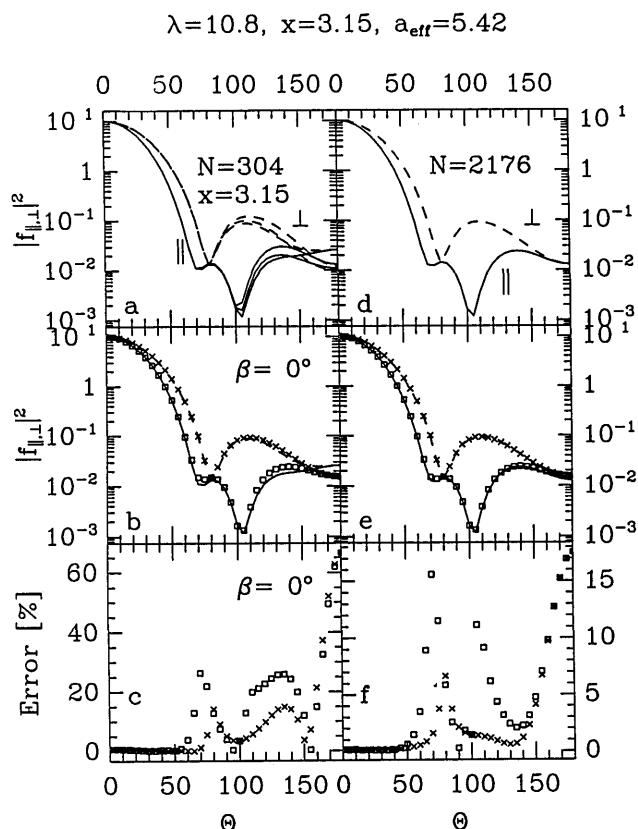


Fig. 3. Comparison of differential cross section for sphere with refractive index $n = 1.089 + 0.18i$ and size parameter $x = 2\pi a_{\text{eq}}/\lambda = 3.15$. Solid and dashed curves (in a, b, d, and e) are the DDA results obtained with the CCG method using $N = 304$ and $N = 2176$ dipoles. Radiation is incident along the x' axis (in the xz plane) and polarized along the y axis. a, b, d, e, Differential cross sections for scattering in the $x'y$ plane. The solid (dashed) curves are for the scattered electric field parallel (perpendicular) to the scattering plane. a, Results for three different incidence directions. b, e, Results for light incident along the x axis; crosses (triangles) show exact results for a sphere for electric field parallel (perpendicular) to the scattering plane. c, f, Percentage error (see text) resulting from the finite number of dipoles.

resolution to get reliable results in sidescatter and backscatter.

The algorithm described in this paper provides a practical way to solve the DDA scattering problem for large values of N , and we proceed now to present some results for cubes and parallelepipeds. The Gohberg-Semencul-Heinig algorithm has been implemented in a FORTRAN package³³ available from NETLIB.³⁹ Figure 1 shows a lattice of $N = 1400 = 14 \times 10 \times 10$ dipoles. For incident radiation propagating in the positive x direction and linearly polarized in the y direction, two scattering planes are considered: the xy and xz planes. In both cases two linear polarizations are considered: parallel and perpendicular to the scattering plane. We consider a sequence of rectangular targets, consisting of $(4 + 2M) \times 4 \times 4$ dipoles, for $M = 0, 1, \dots, 9$. The elongation is in the x direction, and we hold the refractive index n and $2\pi a_{\text{eq}}/\lambda = 3.158$ constant as we vary M . Figure 4 shows CPU time [on a Titan/Ardent computer, with a Linpack benchmark rating of 6×10^6 floating point operations per second (Mflops); the Linpack benchmark is available from NETLIB³⁹] for three different methods: CCG,² Linpack

direct solver,^{40,41} and the BT algorithm. Notice that the Linpack solver is slow (N^3 dependence), whereas the CCG and Toeplitz methods are comparable, with CPU time $\propto N^2$, and much faster than Linpack for large N . For an arbitrary matrix, the CCG method should be slower than Linpack because the former is iterative. However, the CCG method converges rapidly in our case, which probably indicates that the CCG method is able to exploit the hidden block symmetry of the problem. We have also run larger problems, and the results are presented in Table 2. Already for $N = 512$ the Linpack solver is the slowest of the three methods. For $N = 1000$ we were unable to store the 3000×3000 complex matrix required for the Linpack solver. Although results in Table 2 indicate that the BT results are slower than those for CCG, it is worth stressing that the BT is a direct method; thus, in principle, for each new incident direction/polarization, the original $\tilde{A}^{-1}$ can be used to obtain the solution $\tilde{P} = \tilde{A}^{-1}\tilde{E}_{\text{inc}}$ in only K^2 operations (whereas each subsequent CCG calculation requires γK^2 operations, with $\gamma \approx 10$ –20). This is an important point for orientational averages: For example, it was observed by Singham and Salzman¹³ that

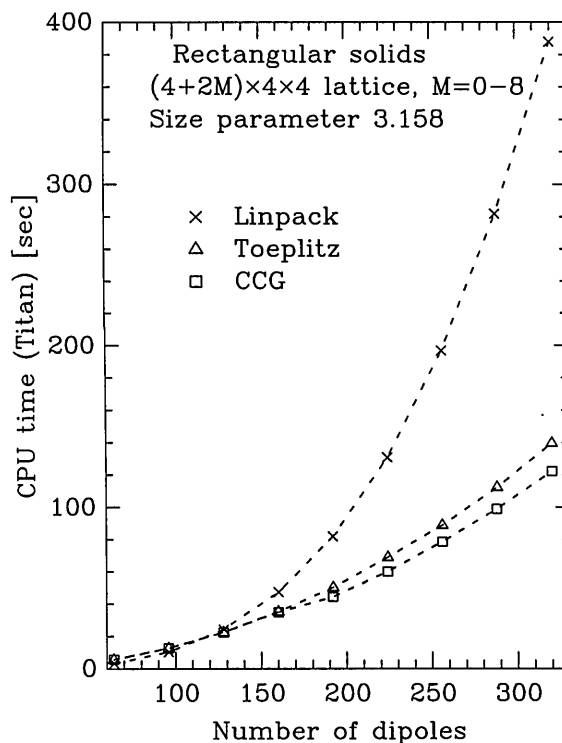


Fig. 4. CPU time (on a Titan/Ardent workstation) as a function of dipole number for three methods: CCG, direct matrix solver (Linpack), and the BT solver.

Table 2. Comparison of Direct (Linpack), BT, and CCG Methods^a

Cube	Dipoles	CCG	Linpack	Toeplitz
$4 \times 4 \times 4$	64	5.7	3.3	5.6
$6 \times 6 \times 6$	216	62.7	115.5	113.6
$8 \times 8 \times 8$	512	350.5	1584.3	1051.8
$10 \times 10 \times 10$	1000	1329.3	—	6254.2

^a Titan/Ardent CPU time is given in seconds.

the number of orientations required for proper averaging depends on the size parameter and varied, in their case, between 3000 and 15,000. We should mention that the current implementation of the Toeplitz package³³ does not store the factored matrix $\tilde{A}^{-1}$, but this is a (remediable) deficiency of the particular implementation and not that of the algorithm.

Figure 5 shows results for a cube represented by a $10 \times 10 \times 10$ dipole array, and Fig. 6 shows results for a rectangular prism represented by a $14 \times 10 \times 10$ array; both are for the same physical wavelength and volume as for all previous cases: i.e., $\lambda = 10.8 \mu\text{m}$ and effective radius $a_{\text{eff}} = 5.42 \mu\text{m}$. Figures 5a–5c and 6a–6c are for the $x'y$ scattering plane, and the angle between the incident light direction (x') and the coordinate axis x is $\beta = 30^\circ$. (The particle is fixed in the xyz -coordinate system.) Figures 5d–5f and 6d–6f are for the xz scattering plane. Comparison with the Mie solutions (for a sphere of the same volume as the cube) is given in Figs. 5b and 5e and 6b and 6e. The linear polarization P is presented in Figs. 5c and 5f and 6c and 6f. For both the cube and the rectangular solid, shown in Figs. 5 and 6, respectively, the forward scattering (and therefore extinction) is shown to be well represented by the equivalent sphere assumption. However, the sidescatter and the backscatter cross sections

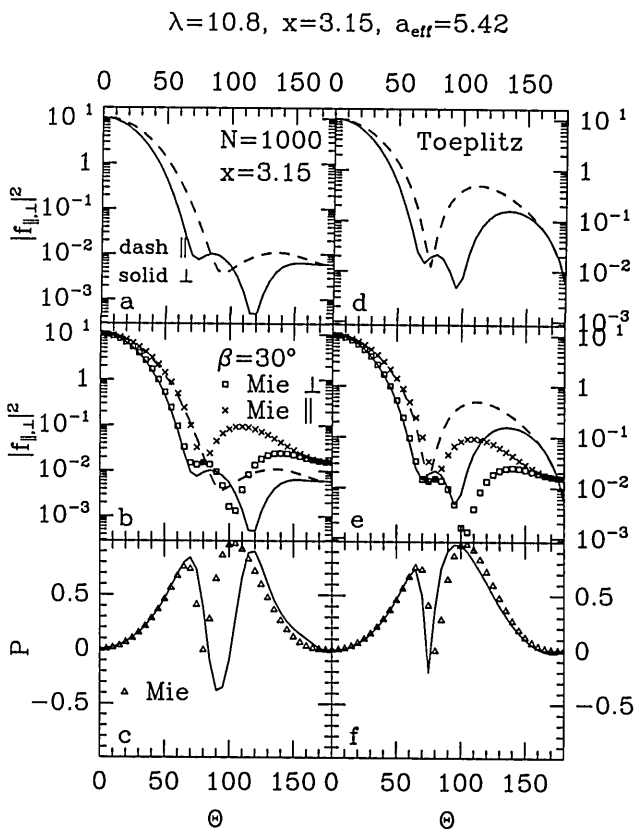


Fig. 5. Differential cross section for cube for size parameter $x = 3.15$ and refractive index $n = 1.089 + 0.18i$. Solid and dashed curves are obtained by using the BT method and the DDA approximation with $N = 1000$ dipoles. Light is incident along the x' axis in the xz plane, at an angle $\beta = 30^\circ$ from the x axis; a–c, the $x'y$ scattering plane; d–f, $x'z$ scattering plane. Triangles are exact results for a sphere of equal volume.

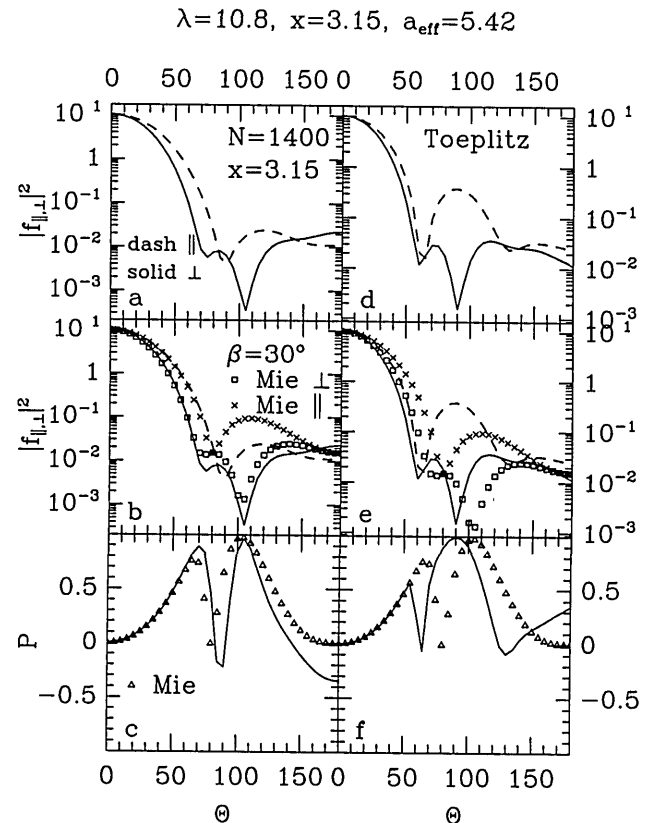


Fig. 6. Same as Fig. 5 but for a 1.4:1:1 rectangular solid, elongated in the x direction. Solid and dashed curves are obtained by using the BT method and the DDA approximation with $N = 1400$ dipoles.

are considerably different, and significant depolarization in backscatter is present (Figs. 6a and 6d).

CONCLUSIONS

We have reported on a study that deals with the application of the DDA to the problem of scattering of electromagnetic radiation by rectangular-shaped particles. We show that the characteristic matrix equation in the DDA approximation is governed by a symmetric BT matrix, and we exploit the properties of such matrices in the solution of the DDA equation. As a practical test we solved a system of 1400 dipoles that corresponds to direct inversion of a 8400×8400 real matrix. A number of algorithms have been developed over the past decade^{31,32} that make use of the properties of BT matrices, but application of such algorithms to the solution of scattering problems has been lacking. This paper therefore provides one example of how BT matrix properties facilitate the solution of the problem of electromagnetic scattering on nonspherical particles.

Particular advantages of the Toeplitz algorithms used in this study are that (1) here the requirements for storage of the DDA matrix on a computer are significantly reduced compared with the more general case, (2) the full inverse of the DDA matrix can be constructed from just two block columns of the matrix, and (3) the CPU time requirements for large N are comparable with those for the CCG method (which does not provide $\tilde{A}^{-1}$) and far less than for direct

solvers. These numerical savings are especially relevant to the DDA and to the problem of orientational averaging.

Scattering of radiation by homogeneous rectangular solids (including cubes and needles as special cases) is likely to be of some interest.^{1,17,42} However, extension to more-general shape particles is important but may turn out to be difficult. If the particle is a rectangular solid but is inhomogeneous (so that not all dipoles have the same polarizability), then the matrix retains the *TTT* structure except for the 3×3 blocks along the diagonal, these being the only elements of the DDA matrix that depend on the dipole polarizability. Many recent papers^{32,43} deal with Toeplitz embedding of an arbitrary matrix. Being close to Toeplitz drastically reduces the computational effort involved in matrix inversion. It is clear that deviations from a rectangular solid (e.g., a hexagonal prism) lead to non-Toeplitz structure, but the resulting DDA matrix may, in some sense, be close to Toeplitz. Another possibility is to introduce fictitious dipoles of zero polarizability to extend the shape to a rectangular solid in the hope that the resulting algorithm is fast even though the number of dipoles being treated increases.

The FORTRAN code DDSCAT used in this study is available from the authors on request.

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