Application of fast-Fourier-transform techniques to the discrete-dipole approximation

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We show how fast-Fourier-transform methods can be used to accelerate computations of scattering and absorption by particles of arbitrary shape using the discrete-dipole approximation.

The discrete-dipole approximation (DDA) is a flexible technique for calculating scattering and absorption by an arbitrary object.[1,2] The target is approximated by an array of N-point dipoles at positions $\mathbf{r}_i$, with polarizabilities α_i. Scattering and absorption by this dipole array are then calculated to high accuracy.

The polarization $\mathbf{P}_i = \alpha_i \cdot \mathbf{E}(\mathbf{r}_i)$ of each dipole responds to the total electric field at its position; $\mathbf{E}(\mathbf{r}_i)$ is the sum of an incident wave,

$$\mathbf{E}_{\mathrm{inc},i} = \mathbf{E}_0 \exp(i\mathbf{k}\cdot\mathbf{r}_i - i\omega t), \tag{1}$$

and a contribution from all the other dipoles,

$$\mathbf{E}_{\mathrm{self},i} = -\sum_{j\neq i} \mathbf{A}_{ij}\cdot\mathbf{P}_j. \tag{2}$$

Thus

$$(\alpha_i)^{-1}\mathbf{P}_i + \sum_{j\neq i}\mathbf{A}_{ij}\cdot\mathbf{P}_j = \mathbf{E}_{\mathrm{inc},i}. \tag{3}$$

Since $\mathbf{E}_{\mathrm{inc},i}$ and $\mathbf{P}_i$ are three-dimensional vectors, the matrix $\mathbf{A}$ can be thought of as a symmetric $N \times N$ array of 3×3 blocks. The fundamental DDA equation (3) can be derived from a simple discretization of an integral equation formulation of the continuum scattering problem[3,4]; the resulting prescription for the polarizabilities α_i differs slightly {in terms $O[(kd)^2]$, where d is the dipole spacing} from the prescription used here (Clausius–Mossotti relation with radiative-reaction corrections).[2]

The conjugate-gradient (CG) algorithm may be used to solve Eq. (3) by iteration.[2,5] In brief, beginning from an initial guess $\mathbf{P}_j^{(0)}$, the CG method generates a sequence $\mathbf{P}_j^{(n)}$ $(n = 1, 2, \ldots)$ that converges monotonically to the exact solution for $n = 3N$ and may yield an excellent approximation in far fewer than $3N$ iterations. The CG method does not require the actual components of $\mathbf{A}$ but only matrix–vector products of the form $\mathbf{A}\cdot\mathbf{X}$ and $\mathbf{A}^\dagger\cdot\mathbf{X}$, where † signifies the Hermitian conjugate. The fast-Fourier transform (FFT) can be used to evaluate these products if the dipoles are located on a cubic lattice: $\mathbf{i} \equiv (i_x, i_y, i_z)$, $\mathbf{r}_i \equiv (i_x d, i_y d, i_z d) + \mathbf{r}_0$, where $i_x \in \{1, 2, \ldots, N_x\}$, $i_y \in \{1, 2, \ldots, N_y\}$, etc.; $N_L \equiv N_x N_y N_z$ is the number of lattice sites in a rectangular volume containing the N occupied sites. Explicitly,[2]

$$\mathbf{A}_{ij}\cdot\mathbf{P}_j = \frac{\exp(ikr_{ij})}{r_{ij}^3}\left\{k^2\mathbf{r}_{ij}\times(\mathbf{r}_{ij}\times\mathbf{P}_j) + \frac{(1-ikr_{ij})}{r_{ij}^2} \times [r_{ij}^2\mathbf{P}_j - 3\mathbf{r}_{ij}(\mathbf{r}_{ij}\cdot\mathbf{P}_j)]\right\} \quad (\mathbf{j}\neq\mathbf{i}). \tag{4}$$

Since this equation depends on $\mathbf{r}_i$ and $\mathbf{r}_j$ through their difference $\mathbf{r}_{ij} \equiv \mathbf{r}_i - \mathbf{r}_j$, $\mathbf{A}_{ij}$ depends only on the difference of its indices. We define

$$\mathbf{A}_{ij} \equiv \begin{cases}\mathbf{A}'_{i-j} & \text{if } \mathbf{i}\neq\mathbf{j} \\ 0 & \text{if } \mathbf{i}=\mathbf{j}\end{cases}. \tag{5}$$

Let the lattice be doubled in each dimension, e.g., $i_x \in \{1, 2, \ldots, 2N_x\}$, and regard $\mathbf{A}'_i$ and $\mathbf{X}_i$ as periodic in each dimension, e.g., $\mathbf{X}_{(i_x,i_y,i_z)} = \mathbf{X}_{(i_x\pm 2N_x,i_y,i_z)}$. Set $\mathbf{X}_i = 0$ if $N_x < i_x \leq 2N_x$, $N_y < i_y \leq 2N_y$, or $N_z < i_z \leq 2N_z$. Then, for example, the product $\mathbf{Y}_i \equiv (\mathbf{A}\cdot\mathbf{X})_i$ is

$$\mathbf{Y}_i = \sum_{j_x=0}^{2N_x}\sum_{j_y=0}^{2N_y}\sum_{j_z=0}^{2N_z}\mathbf{A}'_{i-j}\cdot\mathbf{X}_j \equiv {\sum_j}' \mathbf{A}'_{i-j}\cdot\mathbf{X}_j. \tag{6}$$

Because Eq. (6) is a convolution, it can be evaluated by Fourier transforms[5]: $\hat{\mathbf{Y}}_n = \hat{\mathbf{A}}'_n \cdot \hat{\mathbf{X}}_n$. Here $\hat{\mathbf{Y}}$, $\hat{\mathbf{A}}'$, and $\hat{\mathbf{X}}$ are the discrete Fourier transforms of $\mathbf{Y}$, $\mathbf{A}'$, and $\mathbf{X}$, e.g.,

$$\mathbf{Y}_n \equiv {\sum_i}' \mathbf{Y}_i \exp\left[i\left(\frac{n_x i_x}{2N_x} + \frac{n_y i_y}{2N_y} + \frac{n_z i_z}{2N_z}\right)\right]. \tag{7}$$

$\mathbf{Y}$ can then be computed from the inverse of Eq. (7).

Evaluating $\hat{\mathbf{A}}'_n \cdot \hat{\mathbf{X}}_n$ for all $\mathbf{n}$ involves $O(N_L)$ operations, and, if N_x, N_y, and N_z are highly factorizable, the Fourier transforms require $O(N_L \ln N_L)$ operations with the FFT algorithm[5]; thus $\mathbf{A}\cdot\mathbf{X}$ can be evaluated in $O(N_L \ln N_L)$ rather than $O(N^2)$ operations. If N_x, N_y, and N_z are primes, the CPU time scales as $O(N_x^2 N_y N_z) + O(N_x N_y^2 N_z) + O(N_x N_y N_z^2) \sim O(N_L^{4/3})$.

Table 1. Number of Iterations Required for a Cube

Target Properties				Size Parameter $x = 2\pi a/\lambda$					
m	$\lvert m-1\rvert$	$\lvert\epsilon-1\rvert$	N	1	2	3	5	7	10
$1 + 0.1i$	0.10	0.20	512	2	3	4	5	6	7
$1.1 + 0i$	0.10	0.21	512	3	4	5	7	8	11
$1.33 + 0.01i$	0.33	0.77	512	6	9	10	16	29	62
$1 + i$	1.00	1.00	512	7	8	11	22	30	42
$1 + i$	1.00	1.00	4096	7	8	11	22	31	45
$2 + 0i$	1.00	3.00	512	18	34	54	125	270	626
$3 + 4i$	4.47	25.30	4096	73	69	81	148	222	336

Note the following points: (1) Use of the FFT is not limited to homogeneous solids, since the $\mathbf{A}_{ij}$ do not depend on the potentially position-dependent polarizabilities α_i. (2) The method is not limited to brick-shaped solids: an arbitrary shape can be represented by zeroing the polarizations at lattice sites that lie outside its boundary before evaluating $\hat{\mathbf{P}}$. (3) Evaluation of $\mathbf{A} \cdot \mathbf{X}$ by FFT's is formally exact and is probably less sensitive to round-off errors than direct evaluation because it requires fewer operations per lattice site. (4) Since $\mathbf{A}$ is symmetric, the product $\mathbf{A}^\dagger \cdot \mathbf{X}$ required by the CG algorithm can be obtained directly from $\mathbf{A}^\dagger \cdot \mathbf{X} = (\mathbf{A} \cdot \mathbf{X}^*)^*$.

Many applications of the CG and FFT algorithms to electromagnetic scattering problems have appeared in the engineering literature during the past five years (see Ref. 6 for a review). Most of this research concerns scattering from conducting bodies, such as antennas and radar targets. The CG–FFT method appears to be unknown to optical physicists and astrophysicists working with the DDA, however (had we not first reinvented this method, it would not have occurred to us to look for these earlier studies), hence the present Letter.

Our FORTRAN implementation requires storage for a total of $\approx 51N_L$ complex numbers. Each scalar element of $\mathbf{A}'_{\mathbf{i}}$ is either symmetric or antisymmetric under a change of sign in any component of $\mathbf{i}$, and each 3×3 block is internally symmetric. Because $\hat{\mathbf{A}}'$ inherits these symmetries, it can be represented by $6(N_x + 1)(N_y + 1)(N_z + 1)$ complex numbers. Since $\hat{\mathbf{A}}'$ does not change between CG iterations and is independent of the direction of $\mathbf{k}$ and of the polarization of $\mathbf{E}_{\text{inc}}$, it is computed only once for each k. In order to obtain the total scattering and absorption cross sections averaged over orientation, it is necessary to solve Eq. (3) for two polarizations at each of several directions for $\mathbf{k}$.[2]

The accuracy to which an estimate $\mathbf{P}_i^{(n)}$ is a solution of Eq. (3) may be measured by the fractional error err$^{(n)}$, the rms residual in Eq. (3) per occupied site divided by $|\mathbf{E}_0|$. Table 1 shows the number of iterations n necessary to achieve err$^{(n)} < 10^{-3}$, for cubical targets with different refractive indices m and for different values of the scattering parameter $x \equiv ka$, where $a \equiv (3V/4\pi)^{1/3}$ is determined by the target volume V. In all cases we took $\mathbf{P}_i^{(0)} = 0$ for the starting point. Evidently, n is an increasing function of both $|\epsilon - 1|$ and x. However, n does not appear to depend significantly on N.

Figure 1 shows, for a cubical target, the CPU time per iteration as a function of N. Times are shown for Sun 4/65 and IBM 6000/320 computers and for two FFT routines (from Brenner[7] and Temperton[8]). The CPU time per iteration increases approximately as $N \ln N$. Brenner's FFT routine works for any N but is especially efficient when N_x, N_y, N_z are powers of two. Temperton's routine requires that N_x, N_y, N_z be products of 2, 3, and 5, so the target must be embedded in a lattice with this property.

Figure 1, together with Table 1, can be used to estimate the CPU time required to obtain a DDA solution for one incident direction and polarization state. Once the solution $\mathbf{P}_i$ is obtained, an additional $O(N)$ operations are required to compute the scattering in any particular direction; if many scattering angles are required, the CPU time consumed by the scattering calculations may be appreciable. The scattering amplitude for any particular scattering direction (see Eq. 3.12 of Ref. 2) is simply a Fourier transform of the $\mathbf{P}_i$ and hence in principle could be obtained by interpolation on the (previously computed) $\hat{\mathbf{P}}_i$.

We have compared the exact solution for scattering by a sphere with DDA results using different values of N. The scattering matrix element S_{11} for unpolarized light[9] is shown for a refractive index $m = 1.33 + 0.01i$ and a scattering parameter $x = 5$, 10, and 15 in Figs. 2, 3, and 4, respectively. Also shown is the relative error in S_{11} as a function of the scattering angle θ; note that the relative error is rather uniformly distributed over θ. In Fig. 5 we show results for $m = 3 + 4i$ and $x = 5$. In Figs. 2–5 we also give, for each N, the fractional errors in the efficiency factors for extinction (Q_{ext}), scattering (Q_{sca}), and absorption (Q_{abs}) and the rms value of the

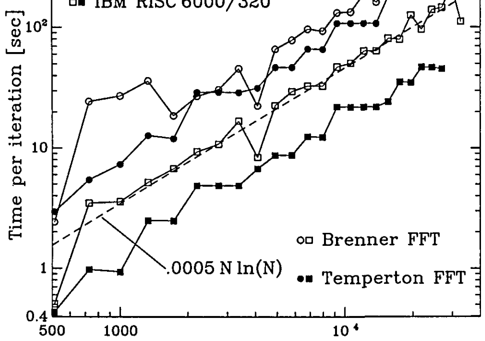

Fig. 1. CPU time per iteration for cubes represented by different numbers of dipoles for two different computers and two different FFT routines.

relative error in S_{11} (averaged over scattering directions). In Fig. 3 we also show the computed S_{11} for radiation incident normal to one of the faces of a cube represented by 125,000 dipoles. The overall scattering pattern evidently deviates appreciably from the solution for a sphere.

For $m = 1.33 + 0.01i$ (with $|\epsilon - 1| \approx 0.77$) accuracies of ~5% in $Q_{\rm ext}$, $Q_{\rm abs}$, and $Q_{\rm sca}$ are achieved, for $x = 10$, with $N \approx 3 \times 10^4$ dipoles; similar accuracies are achieved for $S_{11}(\theta)$ with $N \approx 7 \times 10^4$. By comparison of Figs. 2 and 5 we see that the number of dipoles required to achieve a specified accuracy scales approximately as $|m|^3x^3$, as suggested by Draine.[2] Figures 2–5 also support the suggestion[2] that, for fixed m and x, the errors scale approximately as $N^{-1/3}$. These results show that the DDA, together with the CG–FFT algorithm, makes possible accurate calculations of scattering and absorption by dielectric targets with size parameters x as large as 15 or greater.

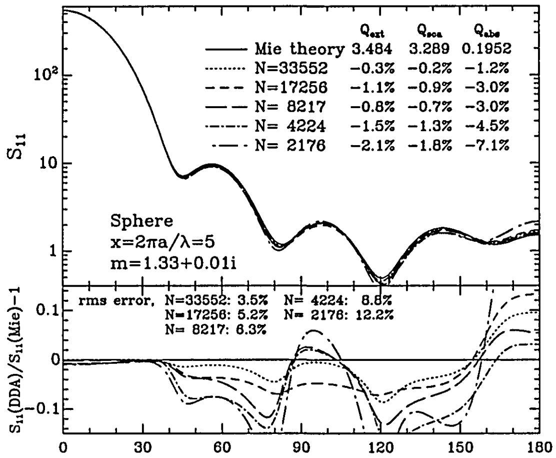

Fig. 2. Scattering by a sphere with refractive index $m = 1.33 + 0.01i$ for $x = ka = 5$. Exact results for S_{11} are compared with S_{11} results computed using the DDA with different numbers of dipoles N.

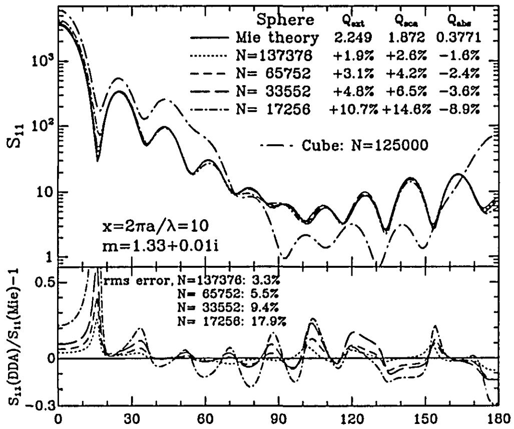

Fig. 3. Same as Fig. 2 but for $x = 10$ and also showing S_{11} for scattering by a cube of equal volume.

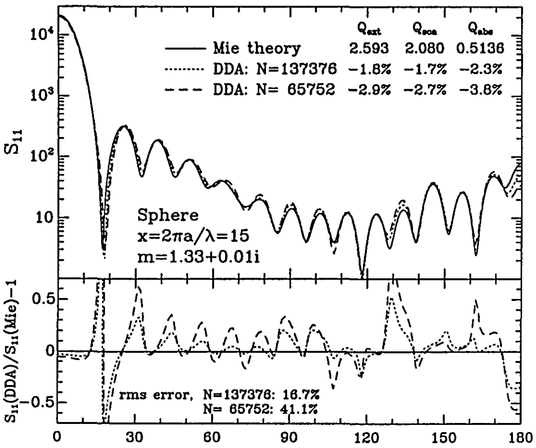

Fig. 4. Same as Fig. 2 but for $x = 15$.

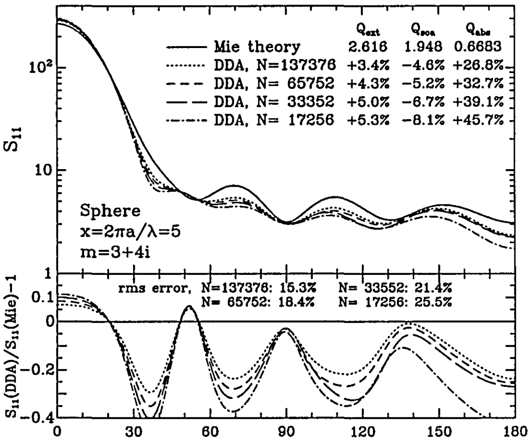

Fig. 5. Same as Fig. 2 but for $m = 3 + 4i$.

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