

Fast near field calculations in the discrete dipole approximation for regular rectilinear grids (submitted)

Piotr J. Flatau

*University of California San Diego, Scripps Institution of Oceanography,
La Jolla, CA, 92093
pflatau@ucsd.edu*

B. T. Draine

*Princeton University Observatory, Princeton,
New Jersey 08544-1001*

Abstract: A near-field calculation of light electric field intensity inside and in the vicinity of a scattering particle is discussed in the discrete dipole approximation. A fast algorithm is presented for gridded data. This algorithm is based on one matrix times vector multiplication performed with the three dimensional fast Fourier transform. Implementation details are provided for the DDSCAT code. It is shown that for moderate and large light scattering near field calculations the computer time required is drastically reduced.

© 2011 Optical Society of America

OCIS codes: (290.0290) Scattering.

References and links

1. Barber P. W. and S. C. Hill "Light scattering by particles: computational methods," (1990), World Scientific Publishing, Singapore, ISBN:9971-50-813-3.
 2. D'Agostino S., P.P. Pompa, R. Chiuri, R. Phaneuf, D. G. Britti, R. Rinaldi, R. Cingolani and F. Della Sala, "Enhanced fluorescence by metal nanospheres on metal substrates," (2009) Optics Letters **34**, 2381.
 3. Draine B. T., and P. J. Flatau, "Discrete dipole approximation for scattering calculations," (1994) J. Opt. Soc. Am. A **11**, 1491–1499.
 4. Draine B. T. and P. J. Flatau, "Discrete-dipole approximation for periodic targets: theory and tests," (2008) J. Opt. Soc. Am. A **25**, 2693–2703.
 5. Draine B.T. and J. J. Goodman, "Beyond Clausius-Mossotti: Wave Propagation on a Polarizable Point Lattice and the Discrete Dipole Approximation," (1993) Astrophys. J. **16**, 1198–1200.
 6. Goodman, J. J., B. T. Draine, and P. J. Flatau, "Application of FFT Techniques to the Discrete Dipole Approximation" (1991), Optics Letters **16**, 1198–1200.
 7. Gutkowitz-Krusin, D., and B. T. Draine, "Propagation of Electromagnetic Waves on a Rectangular Lattice of Polarizable Points" (2004), arXiv:astro-ph/0403082.
 8. Hoekstra, A. J. Rahola, and P. Sloot, "Accuracy of internal fields in volume integral equation simulations of light scattering," (1998), Applied Optics **37**, 8482–8497.
 9. Karamehmedovic M., R. Schuh, V. Schmidt, T. Wriedt, C. Matyssek, W. Hergert, A. Stalmashonak, G. Seifert and O. Stranik, "Comparison of numerical methods in near-field computation for metallic nanoparticles," (2011), Optics Express **19**, 8939.
 10. Xu H. "Electromagnetic energy flow near nanoparticles.I: single spheres," (2004), Journal of Quantitative Spectroscopy and Radiative Transfer **87**, 53–67.
-

1. Methods

1.1. Introduction

Consider a light scattering problem. Given a target of arbitrary geometry we seek to calculate the electromagnetic field outside and inside the target boundary [8, 10, 1, 9]. Exact solutions to Maxwell's equations are known only for special geometries such as spheres, spheroids, or infinite cylinders, so approximate methods are in general required. The discrete dipole approximation (DDA) is one such method. The basic theory of the DDA has been presented elsewhere [3]. Conceptually, the DDA consists of approximating the target of interest by an array of polarizable points. Once the polarizability tensors α_j are specified, Maxwell's equations can be solved accurately for the dipole array. For a monochromatic incident plane wave

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

the polarizations of the dipoles in the target will oscillate coherently. Each dipole i will be affected by the incident wave plus the electric field at location i due to all the other point dipoles

$$\mathbf{E}_i = \mathbf{E}_{\text{inc},i} - \sum_{j \neq i} \tilde{\mathbf{A}}_{ij} \mathbf{P}_j \quad (2)$$

(see [3] for $\tilde{\mathbf{A}}_{ij}$). The vector of polarizations $\mathbf{P}_j$ must satisfy the system of equations

$$\mathbf{P}_i = \alpha_i \left[\mathbf{E}_{\text{inc}}(\mathbf{r}_i) - \sum_{j \neq i} \tilde{\mathbf{A}}_{ij} \mathbf{P}_j \right] , \quad (3)$$

or, defining $\mathbf{A}_{ij} \equiv \tilde{\mathbf{A}}_{ij} + \alpha_i^{-1} \delta_{ij}$,

$$\mathbf{E}_{\text{inc},i} = \sum_{j \in \text{target}} \mathbf{A}_{ij} \mathbf{P}_j . \quad (4)$$

For N dipoles, (3) is a system of $3N$ linear equations where the polarizability tensors α_j are obtained from lattice dispersion relation theory [5, 3, 7]. The matrix $\tilde{\mathbf{A}}$ depends on target geometry, refractive index, and the ratio of interdipole separation to wavelength. After $\tilde{\mathbf{A}}$ has been calculated, equations (4) can be solved for $\mathbf{P}_j$ using iterative techniques when $N \gg 1$.

1.2. Method 1

To calculate the electromagnetic field outside and inside the target boundary one can proceed as follows. Once the polarizations are obtained from (4) the electric field can be calculated from

$$\mathbf{E}_i = \mathbf{E}_{\text{inc},i} - \sum_{j \in \text{target}} \tilde{\mathbf{A}}_{ij} \mathbf{P}_j , \quad (5)$$

where $\mathbf{P}_j$ are now known dipole polarizations. The interaction matrix $\mathbf{A}$ is spatially invariant and depends only on the distance between dipoles. For the special case of near field calculation at the dipole locations inside the target, instead of performing sums in (5) one can immediately obtain the electric field $\mathbf{E} = \mathbf{E}_{\text{inc}} + \mathbf{E}_{\text{scat}}$ as

$$\mathbf{E}_i(\text{at dipole sites}) = \alpha_i^{-1} \mathbf{P}_i , \quad (6)$$

where the 3×3 tensor α_i depends only on the local refractive index. In many applications one is often interested in the near field outside the target. This can be evaluated directly from (5); this method was implemented in program `ddfield` in version 7 of DDSCAT [4]. However, if the number of locations N_{loc} is large this method of direct summation, with complexity $O(3N_{\text{target}} \times 3N_{\text{loc}})$, is computationally very slow.

1.3. Method 2

Using an existing DDA code such as DDSCAT it is possible to solve the near field problem by extending the target shape with pseudo-vacuum sites such that refractive index is set close to 1 for the vacuum sites and solving scattering problem (3) directly. In such case

$$n_i = \begin{cases} n_{\text{target}} & \text{original target sites} \\ n_{\text{vacuum}} \approx 1 & \text{for the pseudo-vacuum sites} \end{cases} \quad (7)$$

This gives

$$\mathbf{P}_i(\text{extended target}) = \begin{cases} \mathbf{P}_{\text{target}} & \text{original target sites} \\ \mathbf{P}_{\text{vacuum}} & \text{pseudo-vacuum sites} \end{cases} \quad (8)$$

In such case the near field at grid sites is obtained directly from (6). The problem with such an approach is that the iterative procedure is carried out for an extended target and that (in the current DDSCAT implementation) the refractive index of pseudo-vacuum sites can not be set exactly to 1 as $\alpha_i^{-1} \rightarrow \infty$ in such a case. Because this algorithm employs fast-Fourier transform (FFT) techniques [6] to speed the matrix-vector multiplications, the complexity of the algorithm is $O[3N_{\text{target+vacuum}} \times M \log(3N_{\text{target+vacuum}})]$, where M is number of conjugate gradient iterations. This can be much faster than method 1, but is burdened by the need to include the pseudo-vacuum sites in the iterative solution of (4).

A requirement of the original DDA calculation is that the grid spacing d be small enough that the structure in both $\mathbf{E}$ and the target be well-resolved (the usual criterion is $|m|k_0d < 0.5$, where m is the refractive index), and therefore this grid is well-suited for sampling the near-field.

2. Method 3 - main results

It is possible to calculate the near-field sums in Eq. 5 by using just one matrix times vector operation. To calculate the electric field at user-selected grid one first runs the DDA calculation for the target shape with N_{target} dipole sites which obtains the polarizations vector $\mathbf{P}_{\text{target}}$. Then, using the original lattice on which the dipoles are located, we define a rectangular volume within which we wish to compute $\mathbf{E}$. The matrix times vector calculation in Eq. (5) is performed, giving the solution

$$\mathbf{E} = \mathbf{E}_{\text{inc}} + \mathbf{E}_{\text{scat}} = \begin{cases} \alpha_j^{-1} \mathbf{P}_j & \text{original target sites } j \\ \mathbf{E}_{\text{inc},i} + \sum_{j \in \text{target}} \mathbf{A}_{ij} \mathbf{P}_j & \text{vacuum sites } i \end{cases}. \quad (9)$$

The algorithmic complexity is $O[3N_{\text{target+sites}} \times \log(3N_{\text{target+sites}})]$. This method exploits the fact that calculation of (5) can be performed efficiently using FFTs [6] provided the near-field sites are located on the regular rectangular grid including the original target.

3. Implementation and results

We now discuss implementation of Method 3 in DDSCAT, taking advantage of efficient matrix-vector calculation using FFTs. In addition, the matrix $\hat{\mathbf{A}}$ is not explicitly stored. We perform two calculations using DDSCAT. First we solve for the polarization $\mathbf{P}_j$ at the original target dipole sites. The second calculation extends the original target shape with the vacuum sites with $\mathbf{P}_i = 0$ at which the electric fields are to be calculated. This gives the following extended polarization vector

$$\mathbf{P}_i(\text{extended target}) = \begin{cases} \mathbf{P}_{\text{target}} & \text{original target sites} \\ 0 & \text{vacuum sites} \end{cases} \quad (10)$$

This extended box-like shape forms a rectilinear grid with the total number of dipoles N_{ext} . The grid contains all of the original sites and extended vacuum sites.

For a sphere with diameter $D = 40d$ the results are presented in Fig. 1. The total internal and near field electric field intensity is shown in a rectangular volume of size $1.5D \times 1.5D \times 1.5D$ ($60 \times 60 \times 60$ lattice sites) centered on the sphere. The refractive index is $(0.96, 1.01)$ and size parameter $x = 5$. For this highly absorptive case the intensity of the total electric field is small inside the sphere. On an Intel Core i3 CPU running at 3.2GHz with 6Gbytes of memory this method is approximately 10^3 faster in comparison to Method 1.

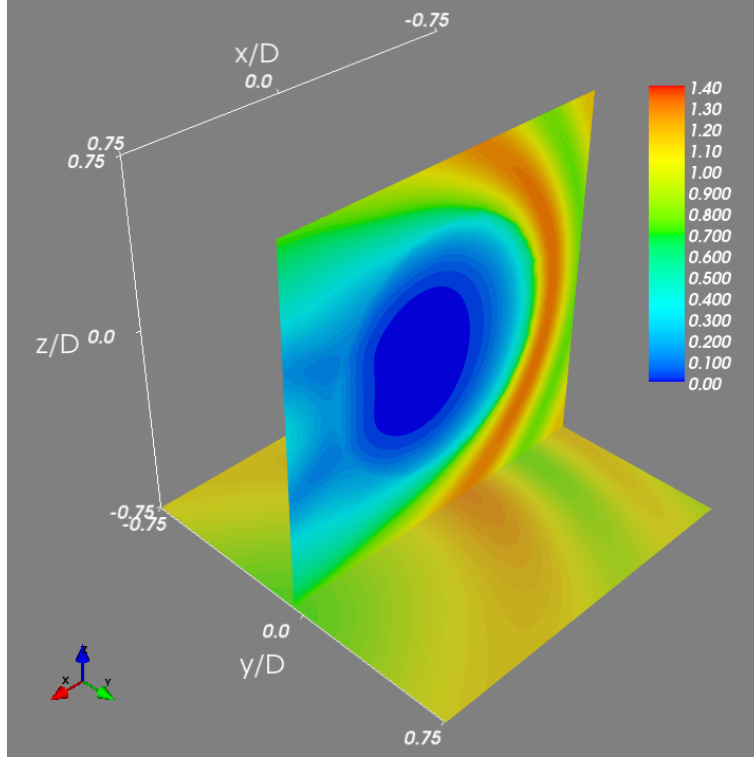


Fig. 1. Normalized electric field intensity $|\mathbf{E}|/|\mathbf{E}_0|$ inside and in the proximity of a sphere calculated for a grid of $60 \times 60 \times 60$ dipoles, on a plane passing through the center of the sphere. The sphere is modeled by 33552 dipoles on a grid with $d = D/40$. The refractive index is set to $(0.96, 1.01)$ and the size parameter $x = k_0 D/2 = 5$. For this highly absorptive case the intensity of the total electric field is very small inside the sphere. The incoming light is linearly polarized with $\mathbf{E}_{\text{inc}} \parallel \hat{\mathbf{y}}$, and propagating in the $+\hat{\mathbf{x}}$ direction.

4. Summary

A new method for calculation of the near field in the Discrete Dipole Approximation is presented. It exploits the fact that calculation of sums in Eq. (5) can be performed fast for sites defined on a regular rectangular grid which includes the original target. The method is 3 orders of magnitude faster in comparison to existing implementations even for moderate amount of dipoles such as $40 \times 40 \times 40$ dipole grid. The method is implemented in version 7.2 of the public-domain code DDSCAT.

5. Acknowledgement

BTD was supported in part by NSF grant AST-1008570.