Light scattering simulations with the discrete dipole approximation

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The discrete dipole approximation (DDA) is reviewed, discussing both theoretical and numerical aspects. Existing applications and capabilities of the method are shown, as well as its place among other methods of light scattering simulation. Finally, remaining challenges are pointed out.

INTRODUCTION

DDA is a general method to compute scattering and absorption of electromagnetic waves by particles of arbitrary geometry and composition. The Maxwell equations are solved in the frequency domain employing volume discretization. Initially DDA was proposed by Purcell and Pennypacker (PP) [1], who replaced the scatterer by a set of dipoles. These dipoles interact with each other and the incident field, giving rise to a system of linear equations, which is solved to obtain dipole polarizations. All measured scattering quantities can be obtained from these polarizations. This approach was further developed and popularized by Draine and coworkers (see e.g. [2]) and others.

Due to its conceptual simplicity and public availability of efficient computer implementations, DDA has gained popularity in many practical applications. An extensive review of DDA, including both theoretical and computational aspects, was recently performed by Yurkin and Hoekstra [3]. This paper is based on this review but also includes a discussion of the most recent advances and challenges in this field. Due to space limitations, I discuss only those references that were not discussed in the review.

THEORETICAL FORMULATION AND NUMERICAL CONSIDERATIONS

Considering a physical picture of the point dipoles, "the DDA equations" can be derived, one of the equivalent forms of which is the following:

$$\mathbf{P}_i = \overline{\boldsymbol{\alpha}}_i \left(\mathbf{E}_i^{\mathrm{inc}} + \sum_{j \neq i} \overline{\mathbf{G}}_{ij} \mathbf{P}_j \right), \qquad (1)$$

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where $\mathbf{P}_i$ and $\overline{\boldsymbol{\alpha}}_i$ are the polarization vector and polarizability tensor of the i-th dipole , $\mathbf{E}_i^{\text{inc}}$ is the incident field at the center of this dipole, and $\overline{\mathbf{G}}_{ij}$ is the Green's tensor describing the interaction between any two dipoles. Material properties (e.g. any distribution of the refractive index in the scatterer) are fully contained in the values of $\overline{\boldsymbol{\alpha}}_i$. DDA (and Eq. (1) in particular) can be derived from the integral equation for the electric field, which is discretized by dividing the scatterer into small cubical subvolumes. This gives more mathematical insight into the approximation, pointing at ways to improve the method.

The original PP formulation is based on the expressions for $\overline{\boldsymbol{\alpha}}_i$ and $\overline{\mathbf{G}}_{ij}$, obtained in the limit of point (infinitely small) dipoles separated by finite distances. All formulations of DDA thereafter modify expressions for $\overline{\boldsymbol{\alpha}}_i$ and/or $\overline{\mathbf{G}}_{ij}$. Here I mention only a few of them: 1) the lattice dispersion relation (LDR) is the most widely used DDA formulation, which adds corrections to the polarizability of the order of dipole size parameter squared; 2) filtered coupled dipoles (FCD) and the integration of Green's tensor (IGT) are rather recent formulations, which modify expression for $\overline{\mathbf{G}}_{ij}$ based on the sampling theorem and integration of the Green's tensor over the cubical subvolume, respectively.

More generally, DDA belongs to a broad range of method of moments, applied to the volume integral equation for the electric fields, which are actively discussed in the electrical engineering community. Unfortunately, the latter is almost independent from the ELS community, making it hard to compare DDA with similar methods.

The main numerical challenge is the solution of a system of linear equations in Eq. (1), the total number of which is three times the number of dipoles. The important advantage of DDA is that this system can be solved in $O(N \ln N)$ operations, which allows one to consider scatterers described by up to a *billion* dipoles on a modern supercomputer. This surprising speed is due to 1) using an iterative solver, which usually converges after much fewer than N iterations (N_{it}); 2) using FFT to compute the convolution-like matrix-vector product in $O(N \ln N)$ operations. The latter employs the special structure of DDA interaction matrix resulting from translation invariance of $\overline{\mathbf{G}}_{ij}$ and placing dipoles on a regular rectangular lattice. The regular dipole grid is, however, a significant limitation in terms of possible DDA improvements. In particular, dipole sizes and locations cannot be varied individually to better describe particle shape. This limitation is removed by a fast multipole method (FMM), an alternative to FFT acceleration, which potentially has the same order of operations. However, the FMM is not likely to be implemented in any production DDA code in the near future due to its complexity.

The overall time of a DDA simulation is largely determined by N_{it}, which increases with size and refractive index of the scatterer and depends on the choice of iterative solver and DDA formulation. Although it is almost impossible to predict N_{it} *a priori* for a particular scattering problem, existing benchmark studies may help to estimate this quantity and to choose a suitable iterative solver. Moreover, N_{it} only slightly depends on the number of dipoles; hence, refining discretization for a fixed scattering problem implies predictable costs of computer resources.

APPLICATIONS AND COMPARISON WITH OTHER METHODS

Being suitable for scatterers in a wide range of size and refractive index and with any internal structure, DDA has found numerous applications in different fields of science. Originally, the driving application was remote sensing in astrophysics [1,2] (interstellar and interplanetary dust, surfaces of atmosphereless Solar system bodies, etc.) and planetary atmospheres (e.g., mineral aerosols [4] and hydrometeors). Applications involving biological cells (from bacteria to human blood cells [5]) have pushed DDA to supercomputers and size parameters above 100 (for index-matching scatterers).

Another class of applications, requiring supercomputers, involves particles near plane interfaces (e.g. silver nanospheres on a dielectric substrate, covered by a thin liquid layer) and porous layers or rough surfaces (e.g. paper coatings and paint pigments). The complexity of these problems is caused by direct discretizations of the large part of the plane medium. In some cases the latter can be avoided using a different expression for $\overline{\mathbf{G}}_{ij}$, based on the electric field of a point dipole in the presence of the plane interface. However, this has certain drawbacks in terms of fast evaluation of the matrix-vector product and the only code, featuring this improvement, is not publicly available [6].

Probably the most frequent application of DDA nowadays is simulating optical properties of metal nanoparticles [7]. In this field DDA is often considered as a "black box" that is supposed to always produce correct numerical results. However, gold and silver (especially in the IR range) are far from the well-proven range of DDA applicability ($|m-1|<2$). This may cause large simulation times and low accuracy, which should be carefully considered in applications [8]. Moreover, the choice of DDA formulation is more important, since e.g. the FCD may largely outperform the LDR in certain cases.

The reverse of the DDA wide applicability range in terms of scatterer morphology is its very limited ability to employ particle symmetries. Therefore, DDA may be not the best option for axisymmetric homogeneous scatterers, for which surface-based methods, such as extended boundary condition (a.k.a. null-field or T-matrix) or discrete sources methods, are more suitable. However, for very large scatterers (e.g. red blood cells) the latter methods may have poor accuracy or fail completely, leaving DDA as a preferable option [5].

Homogeneous asymmetric scatterers generally require similar computation times for the DDA and surface-based methods for fixed particle orientation. The latter are faster for simulation of orientation-averaged scattering properties. For general inhomogeneous scatterers the finite difference time domain method is the only viable alternative to DDA. The relative performance of these two methods is mostly determined by the refractive index. In particular, DDA is faster for index-matching particles.

The increase of DDA applicability to scatterers much larger than the incident wavelength allowed breaching the gap between "rigorous" and geometrical optics methods [4]. The agreement between the two methods in the intermediate size range is good, although it was shown only for orientation-averaged integral scattering quantities.

CONCLUSION

DDA is the method of choice for many light scattering applications, featuring a solid theoretical base, a large volume of benchmark data, and efficient publicly available computer codes. However, a number of challenges still remain: 1) theoretical improvements of the DDA formulation, especially for large refractive indices; 2) numerical improvements, in particular different iterative solvers and/or preconditioners; 3) implementation of existing ideas in the publicly available codes. The latter ideas include, e.g., weighted discretization and Green's tensor for particles near the plane interface.

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