Fast Discrete Dipole Approximation for Particles on Surface

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We present a modification of the discrete dipole approximation (DDA) to simulate light scattering by particles of arbitrary shape and composition located above the plane homogeneous substrate. The modification retains the 3D-FFT acceleration scheme of the free-space DDA and hence its computational complexity. The modification is implemented in the recent version of the open-source ADDA code, available for anyone to use. The test simulations, compared with the T-matrix method, confirm the correctness of the implementation.

INTRODUCTION

The DDA is a general method to simulate light scattering by arbitrary shaped particles [1]. It is mostly applied to finite particles in a homogeneous medium (e.g. vacuum). However, there are a multitude of applications, where a particle is located near a plane surface. The extension of the DDA to such problems is possible [2,3] but the resulting dipole-dipole interaction (Green's tensor) lacks the translational symmetry, which breaks standard 3D-FFT acceleration of the matrix–vector products used in the DDA. As a result, existing DDA implementation either do not use FFT at all [3] or use only 2D-FFT due to the remaining translational symmetry parallel to the surface [2]. The computational complexity of the method is then $O(N^2)$ or $O(N^{4/3}\log N)$ respectively, where N is the number of dipoles used to discretize a particle. A 3D-FFT acceleration for such cases, with complexity $O(N\log N)$, was presented for a similar volume-integral equation method [4], but has never been used in the DDA.

DDA FORMULATION, IMPLEMENTATION, AND TEST SIMULATIONS

In principle, generalizing the DDA to particles on surface boils down to complementing the free-space Green's tensor with the "reflected" part. When the dipoles are placed on a regular grid, the matrix-vector product of the free-space part is transformed into a discrete convolution, which can be computed through 3D-FFT. The reflected part has the same translational symmetry parallel to the surface (xy-plane), but depends on the sum of z-coordinates of probe point and source [4]. Thus, the sum over z is now a discrete correlation, which still can be computed through the FFT. Moreover, we rearranged the computations so that they can be carried together with the free-space part based on the same zero-padded polarization vector. The only difference is that an extra inverse Fourier transform (along the z-axis) is required, followed by element-wise product with Fourier transform of the reflection matrix. The extra computational time is only a fraction of that for the free-space matrix-vector product.

The above ideas were implemented in the open-source code ADDA. In particular, the "surface mode" is included in the recently released version 1.3b4, available online [5]. Moreover, they are fully integrated with other parts of ADDA, including employed parallelization technologies (MPI and OpenCL).

To test the implementation we considered a silver sphere (radius 50 nm, refractive index 0.25 + 3.14i) placed on glass substrate (refractive index 1.5), illuminated by plane wave from below propagating at 60° relative to the surface normal (evanescent illumination). Wavelength is 488 nm, and ADDA v.1.3b4 was used with two levels of discretization (64 and 128 dipoles per sphere diameter). We compared the perpendicular and parallel scattering intensities ($S_{11} - S_{12}$ and $S_{11} + S_{12}$ respectively) in the main scattering plane with the reference T-matrix results, provided by Vladimir Schmidt using NFM-DS 1.1 [6]. The relative errors of the DDA were less than 5% and 2.5% for two discretization levels.

CONCLUSION

We developed a reliable, fast, open-source, and easy-to-use tool to simulate interaction of electromagnetic fields with particles of arbitrary shape and composition located on or near a semi-infinite plane substrate. In particular, only the particle itself needs to be discretized and the simulation time is not principally larger than that when no substrate is present. We believe this tool may find many applications in different fields, ranging, for example, from nanostructures on substrate to surface roughness on large dust particles.

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