Capabilities of the ADDA Code for Electromagnetic Simulations

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Abstract—The code ADDA is an open-source implementation of the discrete dipole approximation (DDA), which is a numerically exact method based on the volume-integral formulation of the Maxwell equations in the frequency domain. It can simulate interaction of arbitrary electromagnetic fields with finite scatterers having arbitrary shape and internal structure. ADDA can run both on CPU or GPU, but can also employ a multiprocessor distributed-memory system, parallelizing a single DDA calculation. Moreover, computational complexity of ADDA scales almost linearly with number of discretization voxels (dipoles), which allows one to consider large system sizes and/or fine discretization levels. ADDA is written in C99 and can be used on almost any operating system. It provides a complete control over the scattering configuration, including incident beam, particle morphology and orientation. ADDA can be used to calculate a wide variety of angle-resolved and integral scattering quantities. In addition to far-field scattering by various beams, this includes near fields as well as excitation by a point dipole or a fast electron. Moreover, ADDA can rigorously and efficiently simulate the scattering by particles near a plane homogeneous substrate or placed in a homogeneous absorbing host medium. It also incorporates many DDA improvements aimed at increasing both the accuracy and computational speed. This contribution describes the main features of ADDA and presents several simulation examples.

Keywords—discrete dipole approximation, scattering, near-field, Bessel beams, electron-energy-loss spectroscopy, absorbing host medium, graphical user interface

I. INTRODUCTION

The simulations of interaction of electromagnetic fields with particles and particle systems is an important part of optics and the field of electromagnetism, in general. It has benefited from development of the efficient simulation methods and computer codes, as well as from steady increase of computational power. Among wide range of these methods the most universal are volume-discretization ones, which apply to arbitrary inhomogeneous systems. Such discretization can be applied to differential Maxwell's equations, resulting in finite-difference time-domain (FDTD) [1] and finite-element methods (FEM) [2]. The third approach is based on the frequency-domain Maxwell's equations, reformulated as the volume-integral equation (VIE) [3]. The

VIE is commonly employed for open-domain problems (such as scattering), since the boundary conditions at infinity are automatically satisfied and only the volume of the particles need to be discretized.

The methods based on the VIE also have several other names: the method of moments (more often used for the surface-integral methods) [5], the Green's dyadic formalism or method [6], and the discrete (or coupled) dipole approximation (DDA) [7]. Traditionally, the DDA is limited to non-magnetic materials and step-pulse basis functions. Moreover, this name was initially proposed in connection to a simple physical picture of a scatterer replaced by a set of point dipoles [8]. Still, the DDA is the most often used term in recent literature related to VIE methods. Importantly, there exist several high-quality open-source DDA codes, widely used in various fields of science.

ADDA is an open-source implementation of the DDA, written in C99 [9]. It was publicly released in 2006 [10], and is continuously developed by an international team – https://github.com/adda-team/adda/. In this conference paper we discuss the main features of its current version (v. 1.4.0). To make it self-contained we partly repeat the descriptive information from the manual [11] and previous publications [9], [12]. However, we also offer a preview of the new exciting features (including simulation results), which are planned to be included in the next release.

II. GENERAL DESCRIPTION AND PROBLEM PARAMETERS

The core of ADDA is a well-documented console application with a powerful command line interface. It is designed to be highly portable, thus, can be compiled on almost any platform, including clusters (super-computers). Additionally, ready-to-use executables for Windows are provided. Moreover, ADDA is designed for multiple parallel runs, including scripted execution. We are also developing a cross-platform graphical user interface (GUI) based on Java to facilitate single simulations with ADDA, especially for new users. Its beta version is available at https://github.com/adda-team/adda-gui .

Since ADDA employs volume discretization, it can handle particles of arbitrary shape and composition, with the only limitation of them being non-magnetic. 16 parametric shape models are available as built-in options in ADDA, from the

simplest sphere to a red blood cell, as well as a homogeneous axisymmetric shape given by its contour. Moreover, one can specify arbitrary piecewise-homogeneous model, discretized into rectangular-cuboid voxels (dipoles), by an input file. We also provide visualization tools and converters from common 3D shape formats. ADDA can automatically refine the computational grid (replacing each voxel by n^3 smaller ones) and randomly place spherical inclusions. The user may specify a diagonal tensor for anisotropic complex refractive index.

The scattering problem may include a particle located in vacuum or in a homogeneous host medium. Alternatively, the particle can be placed near a plane homogeneous substrate, which is treated rigorously with only a moderate extra computation effort in comparison with the free-space case [13]. ADDA v. 1.4.0 supports only a non-absorbing host medium, but the absorbing one is already available at a separate branch https://github.com/Sunmosk/adda-complex_freq. A user has full control over the particle orientation (or, equivalently, over the direction of the incident beam). Automatic orientation averaging can also be performed. For the incident beam a user can choose a plane wave, a Gaussian beam, the field of a point dipole, or arbitrary field distribution read from file. Separate branches add support for Bessel beams (https://github.com/stefaniagl/adda) and the field of a fast electron (https://github.com/alkichigin/adda).

Initially, ADDA simulated the far-field scattering properties, including the angle-resolved Mueller and amplitude matrices, integral cross sections (extinction, scattering, and absorption ones), as well as the asymmetry parameter. But now the electric fields inside or near the scatterer can also be simulated. ADDA can calculate decay-rate (emission) enhancements for point emitters (dipoles) near the particle (both radiative and non-radiative parts). Calculation of radiation forces is also supported, both total (sum over a scatterer) and for each dipole; however, the computational efficiency of this calculation is currently poor. Latest additions, based on the abovementioned excitation by a fast electron (in development), is the calculation of the electron-energy-loss and cathodoluminescence probabilities. This works even in the case of the dense or absorbing host medium, which implies Cherenkov radiation of the electron.

One of the development goals of ADDA has always been its robustness. First, over the years it has been tested against many other methods and codes. Second, each new release is automatically tested against the previous one. Third, ADDA is a truly open-source project with an issue tracker and continuous availability of the latest source code, which can be used for pre-release testing. That is why ADDA is highly trusted by the community, which is supported by about 400 journal papers containing simulations performed with this code.

III. COMPUTATIONAL COMPLEXITY AND EFFICIENCY

Another major development goal of ADDA is computational efficiency (since it originated in the Computational Science Lab of University of Amsterdam). The main computational bottleneck is the system of $3N$ linear equations, where N is the total number of voxels (dipoles). This system is solved by an iterative method from the Krylov-subspace family. Importantly, the regular spacing of dipoles allows the use of the FFT-convolution method to compute matrix-vector products. Thus, both the simulation time and

required memory are approximately *linear in N*. This holds when the number of iterations $N_{iter} \ll N$ (true in most applications) and even in the presence of substrate. In contrast to many other simulation methods, N_{iter} in the DDA stays almost constant when the grid is refined without changing any other problem parameters. Moreover, if the whole scattering system is smaller than or comparable to the wavelength, N_{iter} is mostly determined by the refractive index and, thus, can be estimated a priori [14]. Additional performance boost can be obtained by a judicious choice of the initial guess for the iterative solver. In the case of large optically soft particles, the promising option for such guess is the use of Wentzel-Kramers-Brillouin approximation (implemented in ADDA for the default incident direction).

Another distinctive feature of ADDA is the MPI-based parallel execution of a *single* simulation using the distributed-memory computer cluster. This allows one to employ more than 1 billion dipoles for discretization, which is useful for particles much larger than the wavelength and/or having a lot of small details, and also when higher accuracy is required. However, ADDA can also efficiently work in a sequential mode (without parallelization), as well as running on a multi-core processor with shared memory. Finally, ADDA also supports GPU acceleration (using a single GPU) based on OpenCL.

Apart from the classical DDA formulation (interaction of point dipoles) ADDA includes two modern ones, specifically the filtered coupled dipoles [15] and the integration of Green's tensor [16]. In some cases, they lead to drastic improvement in terms of N_{iter} and accuracy. For example, these formulations enable simulations for non-absorbing high-index particles with moderate sizes. Moreover, apart from standard cubical dipoles (voxels) ADDA can employ rectangular cuboid ones [16]. This is helpful for highly prolate or oblate particles, leading to drastic performance boost when their smallest dimension is much smaller than the wavelength. Those modern formulations bridge the gap between the original physically-inspired DDA and other VIE-based methods.

IV. SIMULATION ACCURACY

The word "approximation" in the DDA should be regarded as a historical artifact, since in reality this is a "numerically exact" method. More specifically, the DDA can reach any accuracy if sufficient computational resources are available [10]. However, these resources are not necessarily practically achievable, and *a priori* estimate of the simulation accuracy for a particular problem or the required discretization level is not easily available. The only general recommendation is to ensure the dipole size d to be at least 10 times smaller than both the wavelength inside the particle and any of its characteristic dimensions (the latter is the main constraint for nanoparticles). Additional guidelines are discussed in the benchmark papers, such as [17] and others mentioned in [11].

In principle, ADDA is easy to run out of the box for any specific problem, especially using the GUI. However, such simplistic approach is not optimal if a series of simulations is planned. Instead, it is worthwhile to invest additional efforts in an accuracy study for a few representative cases. This may consist of comparing the DDA results against other methods (if the latter are available) or of simulations with varying values of d around the default one proposed above. Fortunately, for sufficiently small d the error of any computed

quantity behaves as linear + quadratic with d [10]. This can be employed to estimate the optimal d (for reaching a desired accuracy) and, more importantly, to improve the accuracy using the Richardson extrapolation [18]. In some cases, the latter may lead to 10-times accuracy improvement with minor increase of computational cost. While this behavior looks fascinating, it is somewhat expected from the low order of basis functions, employed in the discretization of the VIE.

V. SIMULATION EXAMPLES

Since there are a lot of published simulation results obtained with ADDA, we present only examples for the new features. The first example is the simulation in the absorbing host medium (Fig. 1). We selected the simplest sphere to enable the validation with the Lorenz-Mie theory [19] and somewhat excessive discretization to have perfect agreement.
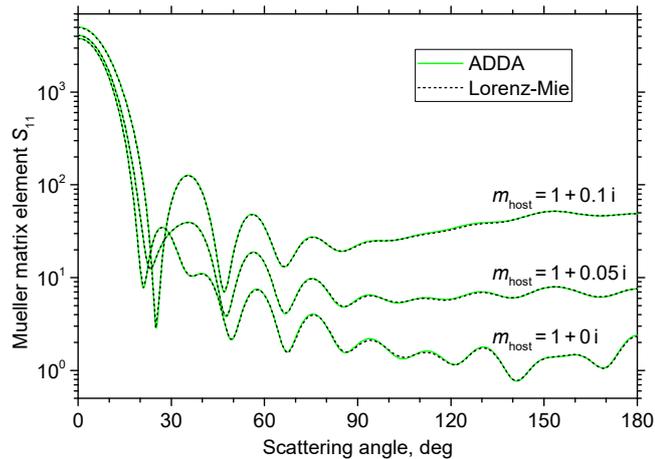
Fig. 1. Angle-resolved light-scattering intensity (in the logarithmic scale) for a spherical particle ($x = 10$, $m = 1.5 + 0.1i$) in an absorbing host medium with complex refractive index m_{host} illuminated by a plane wave. Discretization: 30 dipoles per the wavelength, corresponding to 48 dipoles across the sphere diameter.

The second example is the interaction of a fast electron with a silver sphere (Fig. 2). Again, the results are validated with the Lorenz-Mie theory [21], but we additionally used the Richardson extrapolation for a range of discretization levels in ADDA, resulting in the improved accuracy and internal error estimate (consistent with respect to the reference). Importantly, this is performed by a single run of a Python script, specially designed for such simulations.
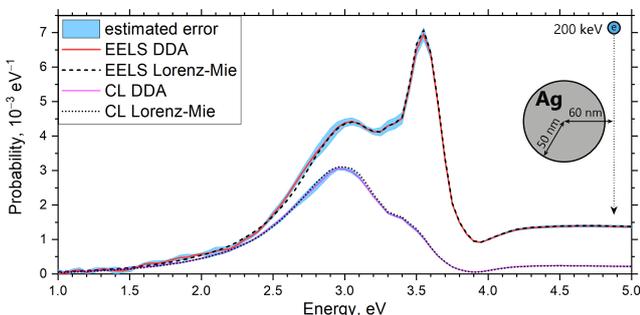
Fig. 2. Electron-energy-loss (EELS) and cathodoluminescence (CL) spectra for a silver sphere in vacuum, the parameters of the problem are in the inset. Spectra are simulated in ADDA with Richardson extrapolation for cubical grids of 64, 54, 45, 38, 32, 27, 23, 19, and 16 dipoles per diameter. Silver refractive-index spectrum is taken from [22].

The last example is the scattering of a Bessel beam by wavelength-sized particles (Fig. 3). We considered several

shapes; the results for a sphere were validated by the generalized Lorenz-Mie theory (GLMT) [20]. We show the scattering intensity in two planes, perpendicular and parallel to the incident polarization. There is some discrepancy around the backscattering direction due to moderate discretization, which can be removed by refining discretization (data not shown).
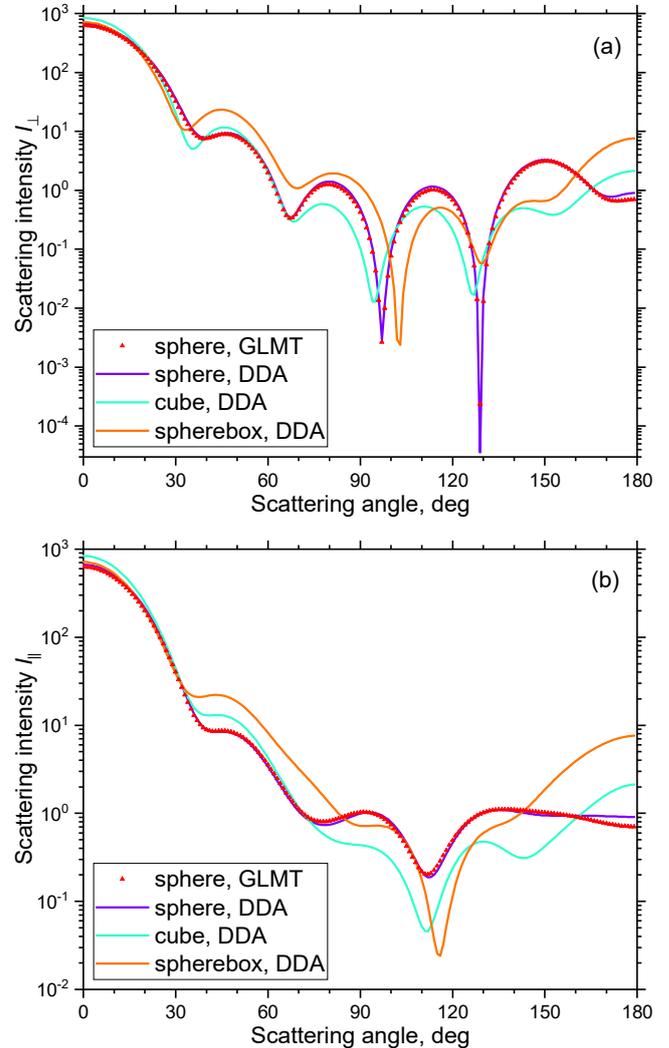
Fig. 3. DDA simulations of on-axis scattering intensities (a) $I_\perp$ and (b) $I_\parallel$ (in the logarithmic scale) of zero-order CS (circular symmetric intensity) Bessel beam with half-cone angle $\alpha_0 = 15°$ by various particles with the volume-equivalent radius equal to the wavelength. Refractive index of the sphere and cube is $m = 1.33$; for the "spherebox" they are $m_1 = 1.33$ and $m_2 = 1.55$ – for the outer cube and inner sphere, respectively. In ADDA we used 15 dipoles per the wavelength.

The examples of this section illustrate that the corresponding ADDA features are ready for general use, although they are not yet incorporated in the official release.

VI. CONCLUSION

ADDA is a mature code applicable to a wide range of problems of interaction of electromagnetic waves (fields) with arbitrary inhomogeneous particles. Its main distinctive features are parallel execution (based on MPI or OpenCL) and high computational efficiency, making it especially suitable for very large problems and massive parameter sweeps. In addition to classical scattering and near-field simulations, a number of new features are available for testing. The latter includes simulation of electron-energy-loss spectroscopy and

accounting for absorbing host medium, as well as built-in implementation of excitation by arbitrary Bessel beams. Further development plans are described in the issue tracker https://github.com/adda-team/adda/issues. They include simulation of radiative heat transfer as well as extension to multi-layered substrates and periodic boundary conditions. We invite all researchers to provide feedback and to consider contributing to ADDA.

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