Capabilities of ADDA code for nanophotonics

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Capabilities of ADDA code for nanophotonics

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Abstract. The open-source code ADDA is based on the discrete dipole approximation (DDA) – a numerically exact method derived from the frequency-domain volume-integral Maxwell equation. It can simulate interaction of electromagnetic fields (scattering and absorption) with finite 3D objects of arbitrary shape and composition. Besides standard sequential execution on CPU or GPU, ADDA can run on a multiprocessor distributed-memory system, parallelizing a single DDA calculation. This together with almost linear scaling of computational complexity with number of dipoles (discretization voxels) allows large system sizes and/or fine discretization levels. ADDA is written in C99 and is highly portable. It provides full control over the scattering geometry (particle morphology and orientation, incident beam) and allows one to calculate a wide variety of integral and angle-resolved quantities, including those related to point-dipole excitation. Moreover, ADDA can rigorously and efficiently account for plane homogeneous substrate near the particle, and employ rectangular-cuboid voxels. It also incorporates a range of state-of-the-art DDA improvements, increasing both the accuracy and computational speed of the method. At the conference we will describe the main features of current version of ADDA with special emphasis on nanoparticles and present several simulation examples.

1. Introduction

The rapid development of nano optics and related fields have unfolded not only through theory and experiment, but also through simulations of interaction of electromagnetic fields with particles and particle systems. The latter benefited both from Moore law and from development of the various efficient simulation methods and computer codes. Among large variety of these methods the volume-discretization ones are the most versatile, since they potentially apply to arbitrary inhomogeneous systems. This discretization can be applied to differential Maxwell's equations in time or frequency domain, leading to broad classes of finite-difference time-domain (FDTD) [1] and finite-element methods (FEM) [2], respectively. The third approach is based on the volume-integral equation (VIE) reformulation of the frequency-domain Maxwell's equations [3]. While a fair performance comparison of those classes of methods is a complicated and rare endeavor [4], VIE is commonly used for open-domain problems (e.g., scattering) since it automatically satisfies the boundary conditions at infinity and require one to discretize only the volume of the particles itself. Moreover, the landscape of VIE methods is not yet dominated by commercial software packages.

Apart from straightforward naming by VIE itself, those methods bear a number of other names: method of moments (much more commonly reserved for surface-integral methods) [5], Green's dyadic method/formalism [6], and discrete (or coupled) dipole approximation (DDA) [7]. The latter is not

necessarily the most popular name, but is the most specific in defining this class of methods, although the DDA is traditionally limited to step-pulse basis functions and non-magnetic materials. Moreover, this name was initially proposed in a light-scattering community through a simple physical analogy of replacing the scatterer by a set of point dipoles [8]. The inherent openness of this community led to appearance of several high-quality open-source DDA codes, which later found use in various fields of science.

ADDA is a C99 implementation of the DDA [9], which was first publicly released in 2006 [10], and is now developed by an international team – https://github.com/adda-team/adda/. In this extended abstract we describe the main features of its current version with special emphasis on potential applications to nanoparticles. Further details can be found in the extensive manual [11] and online wiki pages.

2. General description and problem parameters

ADDA is a console application with powerful command line interface and internal help system. It is easy to compile on almost any platform, including super-computers (clusters). Alternatively, ready-to-use executables for Windows are available. Input/output files and directories are designed to facilitate multiple parallel runs and scripted combination with other tools. The whole software package is well documented and easy to try.

Being based on volume discretization, ADDA can handle non-magnetic particles of arbitrary shape and composition. The built-in options include 16 parametric shape models from a sphere to a red blood cell and a homogeneous axisymmetric shape specified by an arbitrary plane contour. Arbitrary piecewise-homogeneous rectangular-cuboid voxel (dipole) model can be read from file; converters from common 3D shape formats and visualization tools are available. ADDA incorporates basic grid refinement (replacing each dipole by n^3 smaller ones) and automatic random placement of spherical inclusions. Anisotropic complex dielectric permittivity (or refractive index) is supported, if specified by a diagonal tensor.

The specified particle may be placed in vacuum, in non-absorbing homogeneous host medium, or near a plane homogeneous substrate. Fortunately, the rigorous treatment of the latter incurs only a moderate slowing-down of computations in comparison with free-space case [12], and we plan to make it almost negligible by the time of the conference. Orientation of the particle and/or direction of the incident beam can be varied; automatic orientation averaging is also possible. Incident beam can be a plane wave, a Gaussian beam, emission of a point dipole, or arbitrary one read from file. At the conference we will present built-in implementation of the Bessel beams.

Initially, ADDA focused on far-field scattering properties, such as angle-resolved amplitude and Mueller matrices, integral cross sections (scattering, absorption, and extinction), and asymmetry parameter. But now it can also calculate electric fields inside and near the particle, as well as emission (decay-rate) enhancements for point emitters near the particle (radiative and non-radiative parts). Radiation forces can also be calculated, both total and for each single dipole, although this calculation is currently inefficient.

Development of ADDA was always performed with robustness in mind. It was heavily tested by comparison with other methods and codes. New releases are tested against the previous ones by automatic testing suites. Moreover, ADDA features full-blend open development process, including issue tracker and availability of the current source, which allows pre-release testing. As a result, ADDA is trusted by the community, resulting in more than 300 journal papers incorporating ADDA simulations.

3. Computational complexity and efficiency

Since ADDA originated in the Computational Science Lab of University of Amsterdam, it was developed around computational efficiency. The computational bottleneck is the large linear system of size $3N$, where N is the number of dipoles. It is solved by Krylov-subspace iterative methods, where the matrix-vector product is computed using FFT-convolution method, based on the regular spacing of

dipoles. Thus, the simulation time and memory requirements are almost *linear in N* (even in the presence of substrate), assuming that number of iterations $N_{\mathrm{iter}} \ll N$ (which is almost always true). Also, N_{iter} is almost constant when the grid is refined for a given system and can be a priori estimated in some cases, especially if the system is smaller than or comparable to the wavelength. In that case N_{iter} is mostly determined by the refractive index [13].

Distinctive feature of ADDA is the ability to run a *single* DDA simulation in parallel on a cluster using MPI. Computational grid of 1 billion dipoles and even larger can be used. This allows one to simulate particles much larger than the wavelength and/or to use very fine discretization, when the system includes a lot of small details or higher accuracy is required. Simple sequential execution is also possible (and efficient), as well as running on a multi-core processor. Moreover, ADDA can effectively employ modern GPUs (one at a time) using OpenCL.

ADDA includes two modern DDA formulations, namely filtered coupled dipoles [14] and integration of Green's tensor [15]. They may grossly outperform standard formulations (interaction of point dipoles) both in terms of N_{iter} and accuracy. For instance, they allow efficient simulations of optical properties of high-index non-absorbing particles of moderate sizes – relevant for all-dielectric photonics. Another important capability is the use of rectangular cuboid dipoles [15], which a prerequisite for efficient simulation of highly oblate and prolate particles, especially when the smallest dimension is much smaller than the wavelength. This is exactly the case for realistic 2.5D systems and finite-width metasurfaces. Moreover, the whole formulation is stable when taking the limit of zero dipole width, which is supported both by theoretical analysis and numerical simulations. We plan to enable simulations with infinitely-thin dipoles by the time of the conference.

4. Simulation accuracy

Despite “approximation” in its name the DDA is a “numerically exact” method, i.e. it can reach any required accuracy given sufficient computational resources [10]. However, it is hard to estimate *a priori* the accuracy of DDA simulation for a particular problem or the required discretization level to reach satisfactory accuracy. The general recommendation is to make dipole size d smaller (at least 10 times) than the wavelength and any characteristic dimension of the particle; the latter is typically more important for nanoparticles. Some other guidelines can be found in benchmark papers, see [16] and others discussed in [11].

Although ADDA is easy to run for any specific problem, such black-box approach may not be the best choice, especially if one plans a series of simulations for similar particles. In this case we recommend to perform accuracy study for a few representative examples. Either compare DDA results with other methods (if available), or at least perform simulations with different d, both smaller and larger than proposed above. When d is sufficiently small the convergence of any computed quantity is linear + quadratic with d [10], which can be used not only to estimate the optimal d, but also to improve the accuracy by Richardson extrapolation [17]. The latter may in some cases improve the accuracy by 10 times or more at negligible extra computational cost – pure magic! Still, it is an expected consequence of the low order of basis functions used for VIE discretization.

5. Conclusion

ADDA is a mature parallelized code applicable to a wide variety of problems of interaction of electromagnetic fields with arbitrary shaped inhomogeneous particles. Its main features are parallel execution and computational efficiency, making it ideal for very large problems and massive parameter sweeps. ADDA has large development plans, described in the online issue tracker. It includes accounting of multi-layered substrates, simulation of electron energy losses and radiative heat transfer, extension to complex frequency, periodic boundary conditions, and non-local dielectric permittivity. We invite all researchers to provide feedback and to consider contributing to ADDA.

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References

[1] Taflove A and Hagness S C 2005 *Advances in Computational Electrodynamics: the Finite-Difference Time-Domain Method* (Boston: Artech House)
[2] Monk P 2003 *Finite Element Methods for Maxwell's Equations* (New York: Oxford University Press)
[3] Yurkin M A and Mishchenko M I 2018 Volume integral equation for electromagnetic scattering: Rigorous derivation and analysis for a set of multilayered particles with piecewise-smooth boundaries in a passive host medium *Phys. Rev. A* **97** 043824
[4] Liu C, Bi L, Panetta R L, Yang P and Yurkin M A 2012 Comparison between the pseudo-spectral time domain method and the discrete dipole approximation for light scattering simulations *Opt. Express* **20** 16763–76
[5] Lakhtakia A 1992 Strong and weak forms of the method of moments and the coupled dipole method for scattering of time-harmonic electromagnetic fields *Int. J. Mod. Phys. C* **3** 583–603
[6] Girard C, Dujardin E, Baffou G and Quidant R 2008 Shaping and manipulation of light fields with bottom-up plasmonic structures *New J. Phys.* **10** 105016
[7] Yurkin M A and Hoekstra A G 2007 The discrete dipole approximation: an overview and recent developments *J. Quant. Spectrosc. Radiat. Transfer* **106** 558–89
[8] Purcell E M and Pennypacker C R 1973 Scattering and adsorption of light by nonspherical dielectric grains *Astrophys. J.* **186** 705–14
[9] Yurkin M A and Hoekstra A G 2011 The discrete-dipole-approximation code ADDA: capabilities and known limitations *J. Quant. Spectrosc. Radiat. Transfer* **112** 2234–47
[10] Yurkin M A, Maltsev V P and Hoekstra A G 2006 Convergence of the discrete dipole approximation. I. Theoretical analysis *J. Opt. Soc. Am. A* **23** 2578–91
[11] Yurkin M A and Hoekstra A G 2019 User manual for the discrete dipole approximation code ADDA 1.4.0, https://github.com/adda-team/adda/raw/v1.4.0/doc/manual.pdf
[12] Yurkin M A and Huntemann M 2015 Rigorous and fast discrete dipole approximation for particles near a plane interface *J. Phys. Chem. C* **119** 29088–94
[13] Yurkin M A 2016 Performance of iterative solvers in the discrete dipole approximation *2016 URSI International Symposium on Electromagnetic Theory (EMTS)* (Espoo, Finland: IEEE Press) pp 488–91
[14] Yurkin M A, Min M and Hoekstra A G 2010 Application of the discrete dipole approximation to very large refractive indices: Filtered coupled dipoles revived *Phys. Rev. E* **82** 036703
[15] Smunev D A, Chaumet P C and Yurkin M A 2015 Rectangular dipoles in the discrete dipole approximation *J. Quant. Spectrosc. Radiat. Transfer* **156** 67–79
[16] Yurkin M A, de Kanter D and Hoekstra A G 2010 Accuracy of the discrete dipole approximation for simulation of optical properties of gold nanoparticles *J. Nanophoton.* **4** 041585
[17] Yurkin M A, Maltsev V P and Hoekstra A G 2006 Convergence of the discrete dipole approximation. II. An extrapolation technique to increase the accuracy *J. Opt. Soc. Am. A* **23** 2592–601