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Numerical solutions of the macroscopic Maxwell equations for scattering by non-spherical particles: A tutorial review

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ABSTRACT

Numerical solution methods for electromagnetic scattering by non-spherical particles comprise a variety of different techniques, which can be traced back to different assumptions and solution strategies applied to the macroscopic Maxwell equations. One can distinguish between time- and frequency-domain methods; further, one can divide numerical techniques into finite-difference methods (which are based on approximating the differential operators), separation-of-variables methods (which are based on expanding the solution in a complete set of functions, thus approximating the fields), and volume integral-equation methods (which are usually solved by discretisation of the target volume and invoking the long-wave approximation in each volume cell). While existing reviews of the topic often tend to have a target audience of program developers and expert users, this tutorial review is intended to accommodate the needs of practitioners as well as novices to the field. The required conciseness is achieved by limiting the presentation to a selection of illustrative methods, and by omitting many technical details that are not essential at a first exposure to the subject. On the other hand, the theoretical basis of numerical methods is explained with little compromises in mathematical rigour; the rationale is that a good grasp of numerical light scattering methods is best achieved by understanding their foundation in Maxwell's theory.

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1. Introduction

Electromagnetic scattering by particles is described by Maxwell's theory of electromagnetism. For spherical particles the scattering problem has been solved over a century ago; this is commonly known as the Lorenz–Mie theory [1]. However, particles in nature often have nonspherical shapes. The optical properties of nonspherical particles usually differ considerably from spherical particles of comparable sizes and chemical composition. For non-spherical particles the electromagnetic scattering problem can only be solved by numerical techniques. The use of such techniques generally places much higher demands on the user than the use of Lorenz–Mie programs. This may have contributed to an overuse of spherical model particles far beyond their narrow range of applicability. This review aims at providing an introduction to the required background knowledge on numerical methods for scattering by nonspherical particles.

Numerical methods for solving Maxwell's equations find numerous applications in physics and engineering, e.g. in atmospheric optics, ocean optics, remote sensing, astronomy, biomedical optics, nano- and near-field optics, process engineering, and combustion diagnostics. Open-source computer codes based on various numerical methods are freely available for general download on the internet [2]. Quite many codes are deceptively easy to use, which could mislead the user into thinking that numerical light scattering codes can be deployed as black-box tools that require little understanding of numerical methods. On the other hand, available reviews and monographs on methods for solving Maxwell's equations are often written for seasoned users. As a consequence, they tend to cover a lot more breadth and depth than practitioners and newcomers need to acquire at their first exposure to the subject.

It is the aim of this paper to fill a gap in the existing literature by providing a brief introduction to numerical solvers of Maxwell's equations that will be tailored to the needs of novices, students, and practitioners who mainly want to become competent users and learn the main features of numerical light scattering methods, but who do not require to fathom all the technical details of numerical methods. Thus this paper mainly pursues pedagogical aims. However, it is not intended to achieve these aims by lowering the standards of mathematical rigour; the central theme is the development of numerical methods from first principles. Instead, the review will maintain a tight focus on a selected number of key methods. The selection is, on one hand, motivated by the pedagogical need of illustrating different key ideas for solving Maxwell's equations. Thus, only one method has been selected to illustrate volume integral equation methods, only one finite difference method, etc. On the other hand, the selection is also guided by the popularity of different numerical methods.

Fig. 1 shows the relative frequency of numerical methods presented at the Electromagnetic and Light Scattering conference series during 1998–2014. The statistics clearly shows that T-matrix methods and the discrete dipole approximation (DDA) tend to be dominant in the electromagnetic scattering community. However, there is no trend indicating that these two methods are entirely displacing other methods. Quite on the contrary, there are continuing efforts to use, develop, and invent alternative methods, each with their own advantages and niches. Among those other methods that will be omitted in the present review are, e.g., the finite element and boundary element method, the method of lines, the method of moments, Fredholm integral equation methods, or the multiple multipole method.

In this review the finite-difference time domain (FDTD) method will be presented as a typical exponent of finite-difference methods. This method also has a great pedagogical value, since it is the most direct method for solving the macroscopic Maxwell equations. The DDA will serve to illustrate volume integral equation methods. The separation of variables method (SVM) will be presented here as a general approach that forms the basis for other approaches, such as the point-matching method and the T-matrix approach. Waterman's extended boundary condition method will be employed to illustrate T-matrix methods. Before proceeding to a discussion of these numerical methods in Section 3, a brief review of Maxwell's equations, boundary conditions, and constitutive relations is

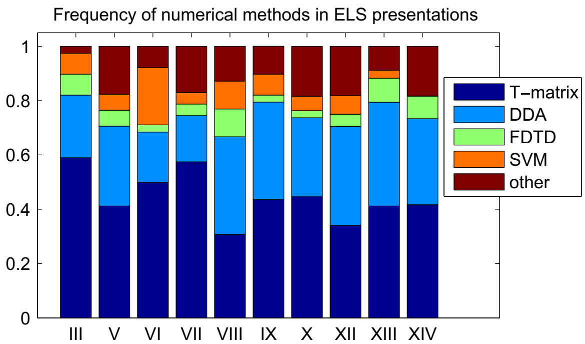

Fig. 1. Relative frequency of numerical methods in papers presented at ELS conferences during 1998–2014. (Data for the fourth and eleventh ELS conference were not available.).