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LIGHT SCATTERING THEORY AND PROGRAMS: OPEN PROBLEMS AND QUESTIONS

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(Invited paper)

ABSTRACT. Over the years many theories and computational tools have been developed to compute light scattering. In this short review we look at latest developments in the field to determine if there are still open questions and which are the driving forces for current developments.

1. Introduction

Since the first meetings within this series of conferences back in 1996 there had been much progress in the field of light scattering; both advanced theories and efficient computational tools have been developed over the years. Of course also new driving forces have also arisen during the last decade. Today there is much interest in near field microscopy, plasmonics and structural color. Back in 1996 there was much interest in single particles of various shapes whereas nowadays much interest lies in systems of particles and the interplay of a scattering particle with its surrounding medium. In this paper I would like to review the state of light scattering especially theory and simulation particularly to look at open questions and new challenges. In this review I will focus on the T-Matrix methods and DDA related methods because I am most acquainted with these methods.

2. T-Matrix method

A good overview over the T-Matrix method and related methods can be found in the review by Mishchenko at al. [1, 2, 3]. If you have a look at these papers you will find its broad range of application and information on what kind of problems have been solved over the years. In the beginning most papers were restricted to spheroids of moderate aspect ratios whereas you can now find papers on fibres or flat plates that have a large aspect ratios [4]. There are similar advances in the Discrete Sources Method which can also handle flat or elongated particles with a large aspect ratios [5, 6, 7]. Also, the original restriction on rotational symmetric particles has been surpassed and there are papers on scattering by cubes, hexagonal ice crystals and ellipsoids using the T-Matrix approach. Initially the refractive index had to be isotropic. Now, a chiral or biaxially anisotropic refractive index [8] can be treated. However, the problem of a bianisotropic refractive index is yet to be solved as far as I can see. What other kind of problems need to be solved? I did not find a paper on the T-Matrix method with the scattering particle positioned in an nonisotropic medium. So a chiral or anisothropic medium seems to be an open problem. To compute the near field within the circumscribed sphere using the T-Matrix method was considered complicated. The problem was solved recently by Doicu et al. [9] by expanding the field in the near-zone region within the circumscribed sphere in terms of both regular and radiating vector spherical wave functions as suggested by Bringi and Seliga [10]. This will help the T-Matrix method to find more interest in plasmonics. This approach was recently fully investigated by Forestiere [11]. To simulate the near-field scattered by an elongated prolate spheroid they used the Null-Field Method with Discrete Sources [12] and expended the internal field by distributed discrete sources.

3. Discrete Dipole Approximation

A review on the discrete dipole approximation has recently been published by Yurkin and Hoekstra [13]. Using ADDA, Yurkin and Hoekstra [14] simulated scattering by a sphere with size parameter 320 demonstrating the potential of the method. The DDA method has recently been extended to compute the energy loss in Electron Energy Loss Spectroscopy (EELS) [15]. The T-Matrix method has also been extended to compute EELS by Matyssek et. al. [16]. Recently there seems to be much interest in invisible cloaks based on zero backscattering. To investigate this using electromagnetic scattering computations the arbitrary magnetic permeability of the material has to be considered. The Discrete Dipole Approximation (DDA) formalism has been generalized to materials with permeabilities $\mu \neq 1$ by You et al. [17] as well as by Chaumet et al. [18] and by Alcaraz de la Osa et al. [19]. To care for an chiral or anisotropic medium with the DDA approach may be quite complicated.

4. Particles on surfaces

In various kinds of applications there is the problem of a particle positioned on or near a planar surface. Such problems arise in particle surface scanners or in sensor applications. Depending on the size of the scattering particle and its refractive index there is much particle-surface scattering interaction which has to be accounted for in the theory. This can easily be done in the T-Matrix approach and I think there was much progress in this field both in the T-Matrix method [20] and in the discrete sources method (DSM). Both plane wave excitation and evanescent wave excitation can be treated using both methods [21]. Recently a quite complex measurement method has been simulated using both NFM-DS and DSM [22, 23]. This is total internal reflection microscopy (TIRM) where the detected scattered intensity of a particle in an evanescent field is used to measure the height of a particle above a plane interface. Because of scattering interaction with the interface oscillations show up both in the measured and the simulated calibration curves [24]. This result has recently been confirmed independently by Bijamov et al. [25] using the method of auxiliary sources (MAS). DDA has also been developed to exactly take into account particle-surface scattering interaction by Schmehl et al. [26] back in 1997 but only this year did a public domain code became available [27]. To me open problems seems to be multiple layers or optically anisotropic layers.

5. Parallelization

An other current issue is parallelization of exciting programs. Various methods such as Open Multiple-Processing (OpenMP) and Message Passing Interface (MPI) are available. DDSCAT and A-DDA are also available in a parallelized version [13]. Within the T-Matrix methods the NFM-DS has recently been parallelized [8]. With the T-Matrix method the computational demand lies mostly in the need to compute the surface integrals. This can of course been easily done by dividing the surface of the scatterer into different sections and then computing the integral of this sections using a separate parallel thread. Mackowski et al. recently cared for parallelization of a multiple scattering program [28]. A paper on parallizing multiple scattering by coated spheres was published by Boyde et al. [29]. Graphical Processor Units (GPU) can also be used as a parallel processor unit. A suitable parallelization software framework is OpenCL. This framework has recently been applied to program a parallel version of A-DDA [30]. The time consuming matrix vector multiplication of the A-DDA was reimplemented in OpenCL. A speedup of about 5/15 for a $128 \times 128 \times 128$ grid on a consumer type GPU Nvidia GTX 260 compared to a 2.8 GHz AMD Athlon was achived. Parallelization of codes is a wide field and further results are expected in near future.

6. Web GUI for legacy codes

With the ScattPort portal (www.ScattPort.org) we focus on providing access to a collection of computational programs in the field of light scattering. The history and concept of the project and the portal we started is presented by Hellmers and Wriedt [31]. Many light scattering programs and codes have been produced by scientists working at research institutes or universities. Such codes are commonly developed for specific research tasks and as such they lack adequate user guides or graphical user interfaces. Most of the programs are command line based and data input is via input files. Many of the legacy Fortran codes in the ScattPort library are of this category. As this is a common problem in scientific programming different GUI development tools have been developed to provide such programs with a basic in- and output GUI. An example of such a tools is Rappture (Rapid Application Infrastructure) [32]. This has for example been applied to provide a GUI for Zori, a Quantum Monte Carlo program [33]. Javamatic is another early tool that can be used to create a GUI in Java [34, 35]. This may provide some idea what can be done with legany codes in the field of light scattering. Currently there is an large discussion on open access journals. Actually, I think there are much more data that science generates to which we should also consider providing open access.

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