Journal of Quantitative Spectroscopy & Radiative Transfer 174 (2016) 39–55

Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

journal homepage: www.elsevier.com/locate/jqsrt

SMARTIES: User-friendly codes for fast and accurate calculations of light scattering by spheroids

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ARTICLE INFO

Article history:
Received 3 November 2015
Received in revised form
5 January 2016
Accepted 5 January 2016
Available online 20 January 2016

Keywords:
Electromagnetic scattering
Spheroids
T-matrix
Numerical simulations

ABSTRACT

We provide a detailed user guide for SMARTIES, a suite of MATLAB codes for the calculation of the optical properties of oblate and prolate spheroidal particles, with comparable capabilities and ease-of-use as Mie theory for spheres. SMARTIES is a MATLAB implementation of an improved *T*-matrix algorithm for the theoretical modelling of electromagnetic scattering by particles of spheroidal shape. The theory behind the improvements in numerical accuracy and convergence is briefly summarized, with reference to the original publications. Instructions of use, and a detailed description of the code structure, its range of applicability, as well as guidelines for further developments by advanced users are discussed in separate sections of this user guide. The code may be useful to researchers seeking a fast, accurate and reliable tool to simulate the near-field and far-field optical properties of elongated particles, but will also appeal to other developers of light-scattering software seeking a reliable benchmark for non-spherical particles with a challenging aspect ratio and/or refractive index contrast.

1. Introduction

We present a user guide and description of SMARTIES, a numerically stable and highly accurate implementation of the *T*-matrix/Extended Boundary-Condition Method (EBCM) for light-scattering by spheroids, based on our recent work [1–3]. The complete package can be downloaded freely from http://www.victoria.ac.nz/scps/research/research-groups/raman-lab/numerical-tools, see Section 1.4 for licensing information. The name of the program stands for *Spheroids Modelled Accurately with a Robust T-matrix Implementation for Electromagnetic Scattering*, and is also a nod to the well-known colorful candy of oblate shape.

1.1. Description and overview

This package contains a suite of MATLAB codes to simulate the light scattering properties of spheroidal particles, following the general *T*-matrix framework [4]. The scatterer should be homogeneous, and described by a local, isotropic and linear dielectric response (this includes metals, but not perfect conductors). Magnetic, non-linear, and optically active materials are not considered. The surrounding medium is described by a lossless, homogeneous and isotropic dielectric medium extending to infinity.

SMARTIES specifically implements recently developed algorithms for numerically accurate and stable calculations. The general EBCM/*T*-matrix method is described in detail in Ref. [4], while the underlying theory and relevant formulas for our specific improvements are described in Ref. [2], with additional information found in [1,3]. The relevant equations and sections from both Refs. [2,4] are referenced when possible as “inline comments” to the code.

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http://dx.doi.org/10.1016/j.jqsrt.2016.01.005
0022-4073/

The package includes detailed examples and can also be used by a non-specialist with an application-oriented perspective, requiring no specific knowledge of the underlying theory.

The package contains:

- Six ready-to-run example scripts to calculate standard optical properties, namely fixed-orientation and orientation-averaged far-field cross-sections, near fields, *T*-matrix elements, and scattering matrix elements. Examples also cover the simulation of wavelength-dependent spectra of surface-field and far-field properties.
- Two tutorial scripts where such simulations are further detailed with step-by-step instructions, exposing the lower-level calculations of intermediate quantities.
- Additional *high-level* and post-processing functions, which can be used by users to write new scripts tailored to their specific needs.
- A number of *low-level* functions, which are used by the code and might be adapted by advanced users.
- Dielectric functions for a few materials such as gold and silver, implemented via analytic expressions [5,6] or silicon, interpolated from tabulated values.

1.2. Relation to other codes

Standard *T*-matrix/EBCM codes in Fortran have already been developed [7,8], with those by Mishchenko and Travis [9] arguably the most popular. These freely available codes provide a wide range of capabilities (including for example different particle shapes) and have been widely used and tested. The standard EBCM method however suffers from a number of numerical problems and instabilities for large multipole orders, which are necessary for either high precision, large particles, elongated particles, near-field calculations, or any combination of the above. This can result in inaccurate results and in some cases in complete loss of convergence. This unreliable behavior for numerically challenging simulations can make the method difficult to use for non-experts, who may find it hard to "tune" the parameters that ensure accuracy and convergence. It also impedes the theoretical study of the intrinsic convergence properties of the *T*-matrix method, obfuscated by (implementation-dependent) numerical loss of precision [3].

Recently, we have identified the primary causes for numerical instabilities in the special (but important) case of spheroidal particles [1] and proposed a new algorithm to overcome them [2]. Thanks to those improvements, high accuracy and reliable convergence can be obtained over a wider range of parameters, especially towards high aspect-ratio (elongated) particles where the standard EBCM implementation would fail [3]. This document aims to present and discuss a publicly available Matlab implementation of these recent developments. Our package should complement, rather than replace, existing *T*-matrix codes such as those of Mishchenko and Travis [9]. The present code offers a number of advantages:

- Thanks to the improvements in accuracy and convergence, we believe this code will be readily accessible to non-expert users and allow the routine calculation of optical properties of spheroids as easily as with Mie theory for spheres. An example is provided in Section 2.7 as a demonstration.
- We also provide specific routines to compute near fields and surface fields, which will be beneficial to the exploitation of this powerful method in areas such as nanophotonics, optical trapping, plasmonics, etc., where the *T*-matrix/EBCM method has not been widely applied.
- Matlab provides an easy-access, interactive environment to carry out a broad range of numerical simulations, and plot/export the results conveniently.
- The accuracy of the obtained results can be easily estimated for any type of calculation, owing to the well-behaved convergence of the improved algorithm.
- A wider range of parameters can be simulated, especially scatterers with large aspect ratios.

A number of limitations should be also be noted:

- These codes are limited to spheroidal particles, for which we identified and circumvented numerical problems that are very specific to this geometrical shape.
- Matlab is inherently slow compared to compiled languages such as C or Fortran, which may be an issue for intensive calculations (for example the simulation of polydisperse samples, with particles varying in size and shape). We envisage that this implementation could serve as a template for a future port of this new algorithm to a more efficient language.
- The calculation of some derived properties, e.g. the scattering matrix, has not been optimized and could be particularly slow.
- Although the range of parameters that may be simulated with reasonable accuracy has been extended towards larger aspect ratios, the method is still limited to moderate particle sizes; and even small sizes only for particles with a large relative refractive index. In this case, the matrix inversion step is the limiting factor and extended-precision arithmetic as implemented in [9] would be required to overcome it.

1.3. Aims of this manual

This document was written with two types of users in mind:

- Researchers interested in simulating electromagnetic scattering by nonspherical particles for practical applications, and seeking an efficient and (relatively) foolproof program with ease of use comparable to Mie theory.
- Other developers of electromagnetic scattering software interested in benchmarking calculations against a highly accurate reference.

With this dual perspective, we have divided the source code into *low-level* and *high-level* functions, including complete scripts for specific calculations, but also documented how to access intermediate quantities such as the