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WEBSCAT: A web application for the analysis of electromagnetic scattering from small particles

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ABSTRACT

Development of an online web application to simulate and display plane wave scattering from small particles is presented. In particular, the computation of angular variation of the scattering properties (scattering matrix elements, scattering coefficients, single scattering albedo etc.) of particulate matter by using the Mie theory and the *T*-matrix method was incorporated in the application. Comparison of the results generated by using the web application with other reported benchmark results has shown that the web application is accurate and reliable for electromagnetic scattering computations.

1. Introduction

The phenomenon of light scattering is applied for probing the physical (size, shape etc.) and optical (refractive index) characteristics of spherical and nonspherical particles where the particle size ranges from micrometer to nanometer. This technique has a high relevance in diverse fields like atmospheric science, oceanography, astronomy, and engineering sciences with specific applications in remote sensing, light detection and ranging (lidar) systems, environmental monitoring (e.g., visibility and haze problems), measurement of air quality parameters, meteorology, optical diagnostics for industrial aerosol processes and combustion, climate modeling, ocean optics, astrophysical issues such as the exploration and characterization of particulate matter in different planetary atmospheres and most recently nanoscience issues (e.g., characterization of nanoparticles by optical tools) [1–17]. As is known the light scattering efficiency of a particle depends on several parameters. Firstly it depends on the scattering angle, that is, the angle between incident and scattered radiation in the scattering plane. This angular variation of the scattered signal also depends on the physical (size, shape, porosity etc.) as well as optical (refractive index) properties of the scatterer and therefore carries its signature. Inversely it is possible to utilize these signatures or scattering informations to extract the characteristics of the scatterer [18–21]. Thus study of the angular scattering dependency of small particulate matter not only helps for better understanding of radiation transfer through a medium containing the scatterer but is a unique tool to classify or even identify the scattering particle [22].

In recent years, a tremendous amount of progress has been made in the study of electromagnetic scattering by spherical and nonspherical particles [1–4,23–25]. The theory developed

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by Mie in 1908 [26–28] is the most widely used numerical method for the calculation of light scattering properties of homogenous spherical particles with both real and complex indices of refraction [1,11,29–31]. However the complexity involved in the scattering results, for shapes other than spherical, made the Mie theory inadequate to be applied to non-spherical shapes as the scattering properties of nonspherical particles can differ quantitatively and even qualitatively from those of volume- or surface-equivalent spheres [3,4,32,33]. Although, various attempts were made to develop numerical approaches, like using a semi-empirical approach, ray tracing technique, etc. [34,35], particular optical phenomena, such as halos, arcs, pillars and zenith-enhanced backscatter observed for ice crystals using lidar, single scattering with lidar and radar depolarization observed for cirrus clouds etc., could not be described by these techniques. Hence, in the last two decades significant number of efforts were given for the better understanding of the effect of nonsphericity on light scattering, resulting in the development of several new theories, numerical techniques, approximations and simulation techniques for computing the scattered electromagnetic radiation [2–4,23,24,36]. Some of these techniques are the separation of variable method (SVM) [37–39], the finite element method (FEM) [40–42], the finite difference time domain (FDTD) method [43–45], the point matching method (PMM) [46], the discrete dipole approximation (DDA) [47,48], the *T*-matrix method (TMM) [3,4,49–52], the geometrical optics approximation (GOA) [53,54], the Monte Carlo simulation [55–57] etc.

The recent growth in high performance computing systems helped in developing fast, accurate and reliable computer programs or software based on these theories to simulate light scattering problems; quite a few of which are also integrated with graphical user interfaces (GUIs) to make the interaction between a user and the software easier [58–63]. However, sometimes adequate knowledge of the respective programming language, installation techniques, etc., is necessary to run such software. Moreover, sometimes major difficulties like platform dependency, non-availability of suitable compiler [64], etc., also occur. In this context, there is a growing need for user-friendly web based interfaces to enable the researchers to run light scattering computations online.

In this work, we report the development of the extended version of **T**ezpur **U**niversity **SCAT**tering Software (TUSCAT) [63] in the form of a web application **WEB SCAT**tering application (WEBSCAT) to simulate and display plane wave scattering from small particles. As of now, the web application is capable of calculating or analyzing the light scattering properties of particles having spherical, spheroidal and cylindrical shape which is exactly same as that of TUSCAT [63]. For scattering problems involving spherical particles, the web application uses the Mie theory while for problems involving non-spherical particles (spheroid and cylinder), it uses the *T*-matrix method.

2. Description of the web application

Two computer programs TUMiescat.java and TUTscat.java based on the Mie theory and the *T*-matrix approach for light scattering computations were developed for the implementation of these theories in the form of a web application. TUMiescat.java is the java version of the code TUMiescat.c [31] which is based on the computer codes developed by Bohren and Huffman [1] and Ahmed [11]. It is a fast, accurate and reliable computer program capable of performing Mie calculations for single particles as well as a variety of size distributions (gamma, normal and lognormal). Next, variations in the light scattering patterns for nonspherical particles (spheroids and cylinder) with changes in the size, size distribution and refractive index in a volume element were computed using a computer program TUTscat.java. As in the case of TUMiescat.java the particle size distributions considered were gamma, normal and lognormal. These two programs were then integrated with the web application.

The web application uses and involves Java Server Faces (JSF) coupled with Primefaces [65] component suite, which features more than 90 Ajax powered rich set of JSF components, in order to develop a user-friendly web based user interface to enable the researchers to enter the required input parameters for light scattering calculations and observe the results more intuitively. This preliminary version of the application is capable of simulating light scattering properties of spherical, cylindrical and spheroidal particles having gamma, normal and log-normal size distribution. The web application is so designed that the numerical results of the scattering matrix elements and the efficiencies can be saved and downloaded for further analysis. Moreover in order to provide an analytical tool for light scattering experiments from monodisperse particles, a facility for comparing experimental results from some unknown particle with computed data is also incorporated in the web application.

2.1. Input parameters

2.1.1. Theoretical calculation mode

Real part:	real part of the particle refractive index
Imaginary part:	imaginary part of the particle refractive index
Incident wavelength:	incident wavelength in μm
Particle Geometry:	drop down menu to select particle geometry
A/B ratio:	axial ratio (for spheroids)
D/L ratio:	diameter to length ratio (for cylinders)
Accuracy of computation:	accuracy of *T*-matrix computation
Size distribution:	drop-down menu to select size distribution
Radius:	radius (for spherical particles) or volume equivalent particle radius (for non-spherical particles) in μm
Lowest particle radius:	lowest particle radius (or equivalent radius) of the selected size distribution in μm
Highest particle radius:	highest particle radius (or equivalent radius) of the selected size distribution in μm
Alfa:	α for gamma distribution
Sigma:	standard deviation (σ) for normal and lognormal distribution
Modal radius:	modal radius or equivalent radius of the selected size distribution