Development of a software package for the analysis of electromagnetic scattering from small particles

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An integrated software package incorporated with a graphical user interface (GUI) was developed for modeling electromagnetic scattering from virtual small particles and also yield characteristic properties of real particles from experimental data. Its interactive features enable the user to observe the changes in output scattering properties in real time. In addition to its ease of use, it has high computational accuracy, efficiency, reliability and adaptability.

INTRODUCTION

The light scattering behavior of isolated spherical and nonspherical particles (ice particles, aerosols and hydrosols) where the particle size ranges from micrometer to nanometer is a subject of intensive research in the fields of remote sensing, climatology, radiative transfer, environmental science, astrophysics etc. The intensity of light scattered by a particle (or ensemble of particles) is a function of the angle between the incident and scattered radiation, size (and dispersion of sizes) of particles, shape (and dispersion of shapes) of particles, optical properties of particles (refractive index, permittivity, absorption), particle orientation, incident wavelength, polarization of the incident wave, density, structure of aggregates (fluffy, fractal, dense, etc.), and quality of particle surfaces (roughness, buffing, etc.). It is very important to study the angular scattering dependency of small particulate matter as such results contain information by which the particle may often be classified or even identified and helps for better understanding of radiation transfer through a medium containing the scatterer. Various theoretical approaches which involve computational techniques are used to explain experimentally observed light scattering patterns due to particulate matter. Some of these techniques are Mie theory, separation of variables (SVM) method, Ray optics or geometrical optics approximation, Waterman's T-matrix method, finite difference time domain (FDTD) method, discrete dipole approximation (DDA) etc. [1, 2]. Usually the solutions of these light scattering theories are very complex, hard to visualize and sometimes it becomes difficult to extract the physical characteristics of the scattering system from these solutions. However the recent rapid growth in the high performance computing systems, helped in developing efficient and accurate computer programs to simulate light scattering problems. Integration of such high performance computer programs with an interactive Graphical User Interface (GUI) makes the interaction between a user and a computer program very easy and helps the researchers to observe the results in near real time and verify their own techniques [3].

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In this contribution, an efficient and reliable software package named TUSCAT is developed on java platform and presented to simulate and display the plane wave scattering from small particles. The package uses and involves a user friendly GUI in order to enable the users to enter the required input parameters for light scattering calculations and observe the results more intuitively. The numerical results of the scattering matrix elements and the efficiencies can also be saved in a user defined data file. The computational programs behind TUSCAT are based on Mie theory for spherical particles and T-matrix theory for nonspherical particles (cylindrical and spheroids). Moreover, another very important facility for comparing experimental results from some unknown particle with theoretical results was also incorporated in the software so as to provide an analytical tool for light scattering experiments from monodisperse and polydisperse particles.

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aprile 2	act rai annon	Highest Partical Radius	Scattering efficiency(Qsca)
Vise Distribution	# Size		2.517932
Size Distribution	Radius	Increamant Step	Absorption efficiency(Qsca)
Monodisperee 💌		Number Of Particles	0.167101
	Incident Wave Length		Circula Crutterian Alberta (alberta)
	-	Incident Wavelength	0.937766
Refractive index(Particle)			
Real Part	If Size Parameter	Sigma	Assymmetry Parameter (g))
1.75	12	H-11D-D-1	0.697337
maginary Part		Modul Parates	Radiation Pressure(Opr)
0.002			0.929186
Refractive index(Medium)			Dackson Marine Difference (Obach)
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1.00	Lowest Partical Radius	Lowest Partical Radius	
maninary Dart			
	Highest Partical Radius	Highest Partical Radius	
	Increamant Step	Increamant Step	
	Number Of Particles	Number Of Particles	
	Incident Wavelength	Incident Wavelength	Experimental Data Analysis
			Upload Experimental Data
Calculate	Sigma	Sigma	Plot Experimental Graph
Show Plotted Graph	Modal Radius	Modal Radius	Overplot Theoretical Graph

DESCRIPTION OF THE GRAPHICAL USER INTERFACE (GUI)

Figure 1. Screenshot of the GUI of the developed software package.

TUSCAT incorporates a user friendly GUI programmed in java (JDK 1.5). Fig. 1 shows a screenshot of the control panel of the GUI when calculations were done for a spherical particle of size parameter 12.0 and refractive index 1.75+i0.002. The medium refractive index was taken to be 1.0+i0.0. At the top of the window, a menu bar is used to save the calculated scattering matrix elements and the efficiencies and give initial information of the software. On the left hand side of the GUI, drop down menus are used to select the shape of the particles and size distribution of the particles. Complex refractive index of the particle and the medium can be given at the appropriate boxes below these dropdown menus. The theoretical calculations are initiated when the 'Calculate' button is pressed and similarly when 'Show plotted graph' button is pressed the software generated plots for different scattering matrix elements are shown as shown in Fig. 2. At the middle of the GUI four rectangular panels are provided to allow the user for entering the input parameters for the desired size distribution. It is worth mentioning that only one of these rectangular panels is activated against the respective selection of the required size distribution in the size distribution drop down menu. On the right hand side of the GUI, the calculated values of extinction, scattering, absorption and backscattering efficiencies, single scattering albedo, asymmetry parameter and radiation pressure are displayed in their respective panels. At the bottom right of the GUI, the most important part of TUSCAT i.e. panel for experimental data analysis is placed. This facility can be used to compare the plots for the experimental data from an unknown scattering particle with the superimposed plots for theoretical data generated by varying the input parameters, to find the characteristic properties of that particle.

For nonspherical particles, the input boxes are slightly modified in the control panel and the plots for the scattering matrix elements are displayed in a similar plotting window.



Figure 2. Screenshot of the plotting window.



Figure 3. Normalized graphs of (a) $P_1/4\pi$, (b) $P_2/4\pi$, (c) $P_3/4\pi$ and (d) $P_4/4\pi$ as a function of scattering angle for Water haze H (as described by D. Deirmendjian [4]).

RESULTS AND DISCUSSION

TUSCAT was tested several times to optimize its performance and accuracy. The results for scattering efficiencies, radiation pressure, single scattering albedo, asymmetry parameter and the scattering matrix elements for different input parameters agree qualitatively well with the available computer programs and sources in the literature. For checking the accuracy of our program we used it to give the normalized values of $P_1(\theta)/4\pi$, $P_2(\theta)/4\pi$, $P_3(\theta)/4\pi$ and $P_4(\theta)/4\pi$ and compare the results with the normalized benchmark results (Table T.29) of D. Deirmendjian [4] for an ensemble of gamma distributed particles (Water haze H) having refractive index 1.322+*i*0.00001, total number of particles 100 cm⁻³, modal radius 0.1 µm, alpha 2, gamma 1 at 1.19 µm incident wavelength. It was observed that graphs for both the results tally within acceptable limits of deviation as shown in Fig. 3 (a)-(d) ensuring the efficiency and reliability of TUSCAT.

CONCLUSION

An interactive software package, TUSCAT was developed as an analytical tool for modeling light scattering properties of small particles and for the analysis of the experimental results from some unknown scatterer. The GUI associated with the software enables the user to visualize the effect of changing input parameters on the resulting scattering patterns in near real time. Works are in progress to improve the software package for the calculation of light scattering properties of other nonspherical shapes like Chebyshev particles, star shaped etc.

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REFERENCES

- [1] M.I. Mishchenko, J.W. Hovenier, and L.D. Travis. *Light Scattering by Nonspherical Particles: Theory, Measurements, and Applications.* San Diego, California: Academic Press (2000).
- [2] N.V. Voshchinnikov, V.B. Il'in, Th. Henning, B. Michel, and V.G. Farafonov. Extinction and Polarization of Radiation by Absorbing Spheroids: Shape/Size Effects and Some Benchmarks. JQSRT 65 (2000).
- [3] D. Ko. Kasper and C. Kimani. Toussaint Jr. A simple GUI for modeling the optical properties of single metal nanoparticles. JQSRT **110** (2009).
- [4] D. Deirmendjian. *Electromagnetic Scattering on Spherical Polydispersions*. Elsevier, New York (1969).