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Classification of Software for the Simulation of Light Scattering and Realization within an Internet Information Portal

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Abstract: Light scattering studies are done by researchers of various scientific areas. As the calculation of the scattering behavior by small particles is rather complex, corresponding programs usually can be used for specific problems only and therefore a multitude of programs have been developed over the years. To enable researchers to find the best fitting one for their scattering problem a categorization scheme for such software is presented here. This scheme is used within an actual project to set up a new internet information portal on the topic of light scattering. The approach for the integration of the scheme as well as the implementation of a corresponding search tool is described in this article.

Keywords: Light scattering, internet information portal, software, categorization scheme, search interface
Categories: H.3.1, H.3.3, H.3.4, H.3.5

1 Introduction

Investigation of light scattering by small particles is a method to characterize particle properties like size, shape or refractive index. For this usually scattering diagrams (distribution of the light intensity depending on the scattering angle) or the spectral characteristics (intensity depending on the wavelength of the light) are analyzed. These investigations are of interest for various scientific branches and industrial processes. Examples are the detection of smallest particles like fibers or dust in environmental engineering, the investigation of the influence of natural airborne particles like Sahara dust on the radiative transfer within in the atmosphere or cosmic dust in astronomy [Mishchenko 02].

The calculation respectively simulation of light scattering is needed for several reasons. For example it enables to make predictions about the optical behavior of particles before experimental studies. By conducting light scattering simulation experimental setups can be planned and designed. It is also possible to design the appearance of new products based on the optical properties of the particles used for the surface. Light scattering calculations are also needed to solve the so called 'inverse scattering' problem. In this case the aim is to determine particle properties from measured scattering diagrams by comparing the measured data with sets of calculated results for different given particle properties. As the properties are known for the calculated ones, the diagram that is most similar to the measured one gives the wanted information.

2 Basics of light scattering theories

The way how to calculate light scattering depends on the particle size in relation to the wavelength of the incident light. In principle there are three size areas which are treated differently.

Light scattering by particles that are very small compared to the wavelength (about molecular size, $2\pi r/\lambda << 1$, with r as the radius of a sphere circumscribing the particle) is described by the so called ‘Rayleigh-scattering’. One example for this is the ‘blue sky’. If the particles are much bigger then the wavelength ($2\pi r/\lambda >> 1$) then ‘geometrical optics’ are applied. In this size area light propagation is described in terms of ‘rays’. These two size areas are easy to treat mathematically in several cases, as exact analytical solutions exist for diverse particle shapes.

In between there is the area which often is referred to as ‘Mie (size) regime’ [Mie 08] (see also 2.2.1). A number of particles that currently are investigated can be found here: airborne particles like dust, asbestos fibres, sand, soot, snow and ice crystals as well as colour pigments or biological particles like cells, spores, pollen, etc.

Unfortunately there is no specific analytical solution to calculate light scattering by particles within the Mie regime. This can be done only numerically. As a result there exist several methods to do so. These different methods additionally are implemented differently into computer programs. As a result there is no general software that can be used for all kind of calculations but a wide spectrum of different computer programs with specific advantages and disadvantages. Often a program can be applied only for a special purpose. If some other problem has to be investigated one might be forced to use a different program.

2.1 Approaches to calculate light scattering within the Mie regime

To solve the scattering problem one has to find solutions in the frame of Maxwell’s equations which describe the propagation of electric and magnetic fields and their interaction with matter. Taking into account properties of the studied materials and media there are four different mathematical approaches which are characterized by the following keywords: ‘initial value analysis’, ‘boundary value analysis’, ‘volume integral analysis’ and ‘surface integral analysis’ [Kahnert 03].

In a next step these mathematical approaches have to be transferred into numerical algorithms which are then used in corresponding computer programs [Wriedt 98]. These two steps lead to restrictions, for example it might be required to transfer an infinite integral within the mathematical description of the scattering method into a finite series for the computer program.

That means: if one wants to calculate light scattering for a given scattering problem, firstly the best fitting mathematical ansatz has to be chosen. This choice is already important, as not every scattering problem can be handled by all four approaches. Based on the four mathematical approaches a number of different so called light scattering methods were developed over the years. The way how a mathematical ansatz is applied within the scattering method also has influence on the range of applicability of the program. Finally such a method has to be integrated into a computer program. Again, the way how this is done (e.g. which numerical standard routines are used) has influence on the program characteristics. In [Fig. 1] the process is outlined.

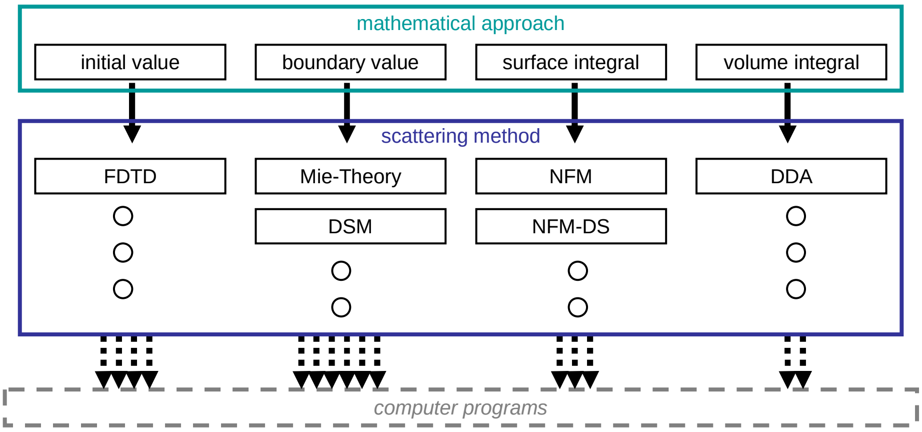

Figure 1: connection between mathematical approaches, light scattering methods and computer programs.

2.2 Examples for different light scattering methods and their specific advantages and disadvantages

Next, the most popular light scattering methods are described together with their specific advantages and disadvantages [Mishchenko 00], [Wriedt 09].

The outlined methods can be classified in the following way: the analysis of differential equations (initial value, boundary value) is done within Mie-Theory (MIE), Separation of Variables (SVM), Finite Element Method (FEM), Finite Difference Time Domain (FDTD) and Point Matching Method (PMM) as well as its modifications Generalized Multipole Technique (GMT) and Discrete Sources Method (DSM). A volume integral method is the Discrete Dipole Approximation (DDA). The Nullfield Method (NFM) uses a surface integral solution.

2.2.1 Mie Theory

The theory by Gustav Mie (MIE) was the first to describe light scattering by small particles. The incident and scattered electro-magnetic fields are described by spherical vector wave functions using the boundary conditions on the particle surface. With the method very fast calculations are possible, but from theory these are restricted to spherical particles and multilayer spherical particles respectively.

2.2.2 Separation of Variables

With the Separation of Variables Method (SVM) light scattering by single particles can be calculated. The particles can be prolate as well as oblate (e.g. spheroids). However, the SVM is only applicable for not too big particles.

2.2.3 Finite Element Method

In the frame of the Finite Element Method (FEM) the particle and some part of the surrounding area are examined. This volume is divided into single, small elements. The advantage of this method is that the particle can be arbitrarily shaped. The biggest disadvantage is that for increasing particle sizes the overall volume that has to be divided increases. As a result the number of calculation steps and therefore the calculation time as well as the memory requirements increase disproportionately.

2.2.4 Finite Difference Time Domain

The basics of the Finite Difference Time Domain (FDTD) are similar to those of the FEM. Again the particle as well as the surrounding volume is divided, here using an aligned discretization of space and time. For the single volume elements the values for the next time step are calculated taking into account the values from the actual and last time step. Because of this the number of equations that have to be solved is less than within the FEM.

2.2.5 Point Matching Method / Generalized Multipole Technique

In the frame of the Point Matching Method (PMM) the known incident field and the unknown scattered field are matched point wise taking into account the boundary conditions at the particle’s surface. An advanced variant of the PMM is the Generalized Multipole Technique (GMT) which uses several origin points for the field expansions and generalized point matching for the solution process. By this it is possible to calculate light scattering by more complicated particle shapes.

2.2.6 Discrete Dipole Approximation

Within the Discrete Dipole Approximation (DDA) the particle volume is divided into small polarizable volume elements. Every single dipole is excited by the incident field as well as the interaction of all the other dipoles within the particle volume. This leads to a system of linear equations which number is equal to those of the volume elements. The solution for the scattered field is gained by superposition of the fields by the single dipoles. The DDA is one of the most popular methods to calculate light scattering. It can be applied to any particle shapes, but the computational efforts and the calculation times are high.

2.2.7 T-Matrix Method / Nullfield Method

Strictly speaking the T-Matrix Method (TMM) does not describe an explicit scattering method, but a special kind of formulation of the scattering problem. In the frame of the TMM all information about the scattering process is stored within a single matrix, the T-matrix. This matrix can be stored and used for further calculations, which decreases the needed calculation time extremely. The T-matrix usually is calculated by using the Nullfield-Method (NFM). For this reason the expressions TMM and NFM are often used synonymously.

2.3 Comparison of different scattering theories in regard to different particle shapes

The following table [Tab. 1] presents a comparison between the described light scattering theories. Shown are the underlying mathematical approaches as well as the particle shapes that can be handled by the methods.

	Mie Theory	Separation of Variables	Finite Elements	Finite Difference Time Domain	Point Matching	Generalized Multipole	Discrete Dipole Approximation	T-Matrix / Nullfield Method
Boundary value	**X**				**X**	**X**		
Initial value		**X**	**X**	**X**				
Volume integral							**X**	
Surface integral								**X**
Spherical particle	**X**	**X**	**X**	**X**	**X**	**X**	**X**	**X**
Non-spherical particle		**(X)**	**X**	**X**	**X**	**X**	**X**	**(X)**
Extreme aspect ratio			**X**	**X**	**X**	**X**	**X**	**(X)**
Using symmetry					**X**	**X**	**(X)**	**X**
Any shape			**X**	**X**			**X**	**(X)**
Volume discretization			**X**	**X**			**X**	
Surface discretization					**X**	**X**		**X**

Table 1: Comparison of different light scattering methods. 'X' denotes suitable, '(X)' implies limited applicability or functionality. In this case e.g. it can depend on the particular implementation into a computer program whether the attribute is valid or not.

3 Selection criteria for the application of software

The relations shown in [Tab. 1] could be used now to categorize computer programs for the calculation of light scattering. But the result would be a quite academic scheme that requires a profound knowledge about light scattering, e.g. for the decision whether a program can be used for a specific particle shape. As the investigation of light scattering is used as a kind of tool in various scientific areas and the corresponding researchers usually do not want to bother about the details, using only this approach might be of less use for them.

Therefore additionally another way will be suggested here. What is needed is a categorization scheme that takes into account the 'non-experts' demands. These demands will not necessarily be restricted to aspects connected with light scattering, e.g. also the usability can be a relevant factor or the possibilities to adjust the program to specific problems.

Usually the (type of the) particle will be in the center of attention. The following [Fig. 2] demonstrates a decision process in regard to the particle shape.

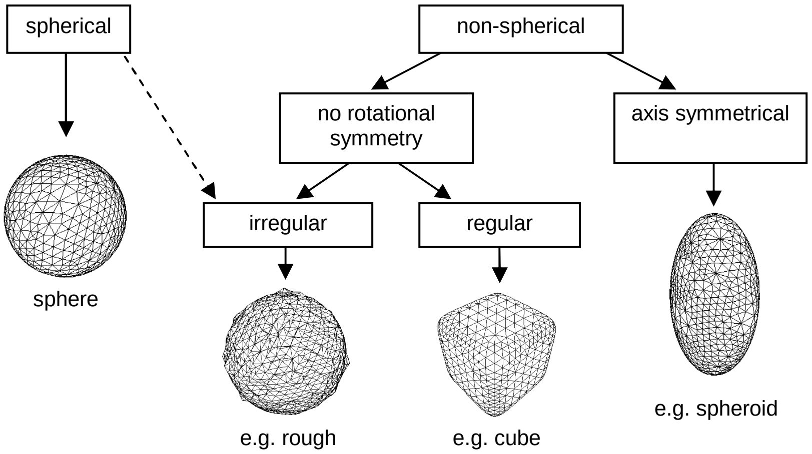

Figure 2: Scheme for the classification of some particle shapes

As mentioned above, also other aspects might be of interest for a useful categorization scheme to help potential users finding an appropriate program. For particles not only the shape is relevant, but also refractive index and composition. For the scattering problem as a whole also the nature of the incident light and the medium surrounding the particle have to be considered. Additionally demands on the program itself can be important, regarding to the supported computer platform, ease to use, availability, price, etc.

One can define four key factors for a light scattering program: parameters regarding to the particle, parameters of the scattering problem, specific demands on the software and general demands on the software. These key factors can be divided further:

- Particle shape: geometry, aspect ratio, symmetry.
- Particle composition: homogeneous, inhomogeneous.

- Refractive index of the particle: real, complex, anisotropic, etc.
- Description of the particle within the program: simple geometries (e.g. rotational symmetric) usually can be described analytically by a formula. In this case there will be a set of parameters to describe the shape, varying the parameters will change the shape. If the particle shape is complex (e.g. no symmetry and rough) it will be necessary to transfer the particle shape to a three-dimensional model that can be imported by the program. In this case the file format for the shape model is relevant.
- Nature of the incident light: plane wave, Gaussian beam.
- Nature of the medium surrounding the particle: absorbing, non-absorbing, anisotropic, etc.
- Calculation results: with most programs the scattering diagram (intensity depending on the scattering angle) is calculated. Some programs additionally enable to calculate other parameters like e.g. the Mueller-Matrix which contains information about the polarization.
- Expandability of the program: information whether a program can be used for advanced scattering problems. The use of such a flexible program is especially useful when already calculated results can be used again for a more complicated setup, e.g. when simulation results for single particles can be used to calculate the scattering behavior of a cluster of particles.
- Underlying light scattering theory: this can be of interest for comparative calculations. To check the validity of simulation results usually one (exemplarily) calculates the same light scattering problem additionally with another program based on a different method. If both results are identical the obtained result is considered to be correct.
- Availability, software license: free to edit, free to use, commercial, operating system, etc.
- Programming language: this is useful information if the program is free to edit and modifications are necessary or wanted.
- Usability of the program: source code or binary.

The following [Fig. 3] shows single attributes, arranged in order to the four main key factors and the corresponding subdivision list.

By using a categorization scheme as outlined in [Fig. 3] it is possible to set up an internet tool to help potential users finding the best fitting software for their purposes. In the following chapter a corresponding strategy and the technical realization are described.

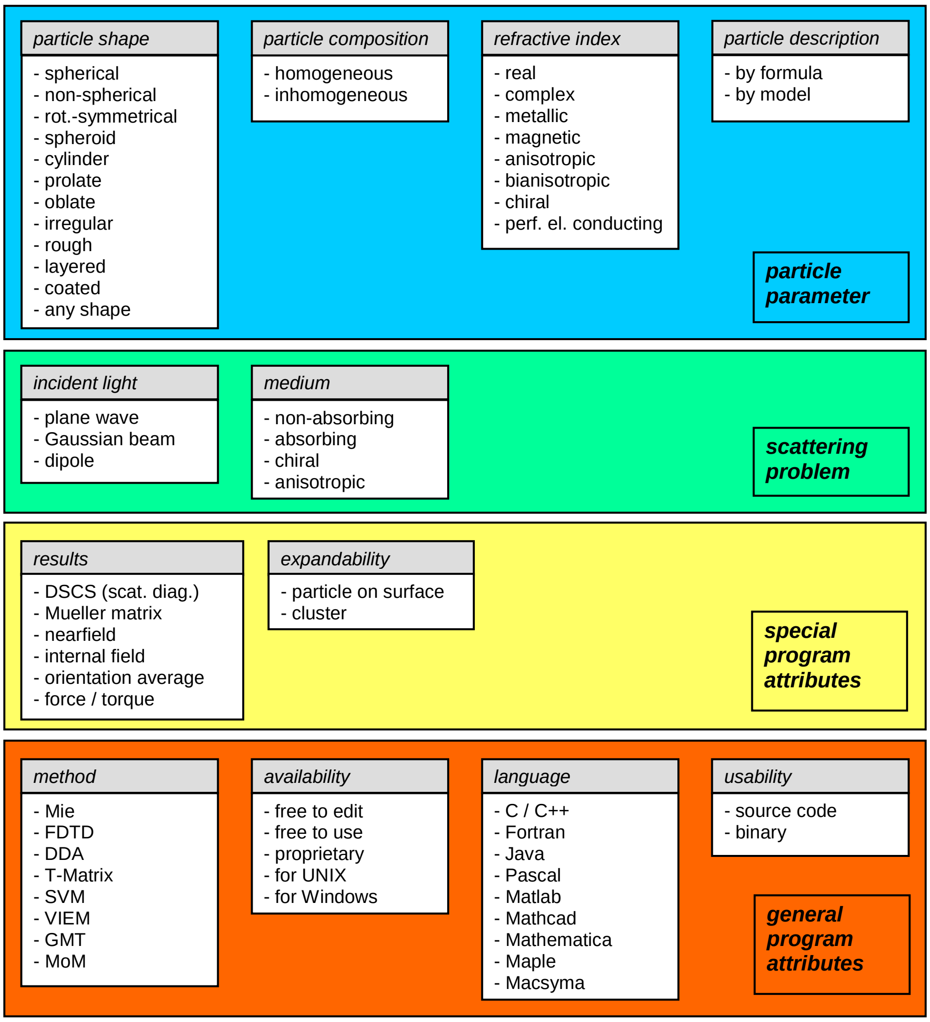

Figure 3: categorization scheme for light scattering software. It consists of four key factors, divided into 12 subdivisions together with the corresponding attributes.

4 Realization in a internet search tool

In a project funded by the German Research Foundation DFG a new internet information portal on the topic of light scattering is currently under development [Wriedt 08], [Hellmers 09], [ScattPort 09]. An essential element of this new portal is an extensive list of programs for the calculation of light scattering. The structure of the list follows the pattern of the predecessor internet pages [LESP 02] to offer recurring users a familiar sight. But as the number of programs over the years got more than 200 it is difficult now to keep track of them. For this reason a search tool is under development to help the portal users finding the software they are interested in. In this case the realization was done as follows:

- Every program has an own description page within the internet portal.
- The attributes described in [Fig. 3] are related to a special set of metadata. In this case it is necessary to relate every attribute to a single, distinct catchword.

  A detailed list of the metadata used for the light scattering information portal can be found in the appendix at the end of this paper.
- For every program the corresponding metadata keywords are assigned (in the 'header' section of the corresponding single internet page with the description).
- On the server hosting the internet pages an advanced local search engine is installed. This local search engine collects the information about all sites containing program descriptions (metadata and full text).
- The corresponding search index can be accessed via an internet search interface (see also [Fig. 4]). A search query leads to a list with results (web pages with program descriptions) generated by the search engine.

In this case the search engine *htdig* [htdig 10] is used. It offers the following advantages:

- *htdig* indexes the (not visible) metadata as well as the (visible) full text. Additionally there is an option to weight the ratio of the information by a 'meta description factor'. By this, metadata can be assigned a higher relevance for queries. But as also the full text is indexed a kind of 'fuzzy' search can be done by the user. This provides a good flexibility – as described in the following section about the search interface.
- It is possible to configure *htdig* in such a way that a search term that is found as whole word gets a much higher relevance than if it is found as part of a word. An example: there is an attribute 'homogeneous'. A simple search would match the whole word, but also the attribute 'inhomogeneous', which has the opposite meaning. One workaround would be to give the attribute 'inhomogeneous' a specific meta information that is unmistakable. Using *htdig* it is not necessary as it can discriminate between both words.
- One can create a list of synonyms to relate specific terms to each other. If one of these terms then is used for a search query, *htdig* will also search for the related term. An example: 'T-matrix' and 'Nullfield Method' (see also the chapter about different light scattering methods).

The corresponding internet search interface consists of two parts – see [Fig. 4]. Firstly there is a HTML 'text' input field. Here a user can insert any words for queries. The search engine will look for matches within the full text as well as the metadata. By this a kind of 'fuzzy' search can be done, as a user can insert any terms that are of interest for him.

Secondly there are grouped HTML 'checkbox' fields. The terms (only visible in the source code of the web page) behind the field names (visible for the user) are the metadata terms. Using these ‘checkbox’ fields one can start a ‘strict’ search just for the metadata and therefore for the corresponding program attributes.

A detailed list of metadata terms in relation to the categorization scheme presented in [Fig. 3] can be found in the appendix of this paper.

ScattPort Software Search

This search allows you to search the list of light scattering programs to find the best fitting

Match: All Format: Long Sort by: Score

Search:

(I) particle properties

particle shape	**particle composition**	**refractive index**	**particle model**
☐ spherical	☐ homogenous	☐ real	☐ by formula
☐ non spherical	☐ inhomogenous	☐ complex	☐ by model
☐ rot. sym.		☐ metallic	
☐ prolate		☐ magnetic	
☐ oblate		☐ anisotropic	
☐ irregular		☐ bianisotropic	
☐ any shape		☐ chiral	

Figure 4: Part of a screenshot of the actual search interface of the light scattering internet information portal.

The best search strategy for a user now is to begin by marking all ‘checkbox’ fields with program attributes that are of interest. If the search query delivers no results one should reduce the number of marked fields, starting with the least important attributes. This should be done step by step until the search was successful.

The ‘text’ field offers some additional flexibility for the refinement of the search query.

5 Summary

The calculation of light scattering by small particles is of interest for various research fields. Unfortunately within the Mie regime calculations can be done only numerically and the corresponding mathematical theories are quite complex. This is a significant drawback especially for researchers who are no specialists on the topic and who just need to use corresponding calculations for their current research problems. For them a tool to find the most suitable software for their specific problems would be helpful.

In this article approaches to categorize light scattering software are described. The approach favored here takes into account not only mathematical and particle related attributes, but also more general information about the software, like availability and usability. Therefore it is convenient especially for non expert users.

This categorization scheme can be used in a next step to set up a corresponding internet search tool for software. For this the program attributes are related to metadata which is stored in HTML web pages describing the programs. A local search engine then indexes the information. Users can find programs suitable for their scattering problems by using an internet search form. This search offers a strict search for program attributes as well as a fuzzy full text search. By this a high flexibility for the user is gained.

A corresponding system is currently set up at the University of Bremen within a project funded by the German Research Foundation DFG.

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Appendix

Used metadata, see also [Fig. 3].
Additionally a categorization of five exemplarily chosen programs is presented.

program **attribute**	NFM-DS T-Matrix	DDSCAT	LightLab Far Field Mie	
particle shape				particle parameter
spherical			**X**	
nonspherical	**X**	**X**		
rot_sym				
spheroid				
cylinder				
prolate				
oblate				
irregular				
rough				
layered	**X**			
coated	**X**			
any_shape	**X**	**X**		
part. composition				
homogeneous				
inhomogeneous	**X**	**X**		
refractive index				
real_ref_ind				
complex_ref_ind	**X**	**X**	**X**	
metallic_ref_ind				
magnetic_ref_ind				
anisotropic_ref_ind	**X**	**X**		
bianiso_ref_ind				
chiral_ref_ind	**X**			
perf_el_cond	**X**			
particle model				
formula_particle	**X**			
model_particle				
incident light				scattering
plane_wave		**X**	**X**	

gaussian_beam	**X**			
dipole				
medium				
non_absorbing	**X**	**X**	**X**	
absorbing				
chiral				
aniso_medium				
results				special program attr.
dscs	**X**	**X**	**X**	
mueller_matrix	**X**			
nearfield				
internal_field				
orient_avg	**X**	**X**		
torque				
expandability				
particle_on_surface	**X**			
cluster	**X**			
method				general program attributes
mie			**X**	
fdtd				
dda		**X**		
tmatrix	**X**			
svm				
viem				
gmt				
mom				
availability				
edit_free	**X**	**X**		
use_free				
proprietary			**X**	
unix				
windows			**X**	
language				
c_language				
fortran	**X**	**X**		
java				
pascal				
matlab				
mathcad				
mathematica				

maple				
macsyma				
usability				
sourcecode	**X**	**X**		
binary			**X**	