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New approaches for a light scattering Internet information portal and categorization schemes for light scattering software

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ABSTRACT

Light scattering is important in a number of scientific fields and thus the efficient collation and exchange of this information becomes essential. The Internet allows information to be easily shared but the required content may be distributed over a number of web pages and thus may be difficult to locate using standard search engines.

In this paper the current state of the development of a new light scattering Internet information portal is described. The upcoming technical realization for the web pages as well as the benefits for the users is outlined. One of the key features of the portal will be the comprehensive list of light scattering programs. For this also approaches to categorize light scattering software are investigated. This can help to develop search tools enabling scientists to find the best fitting program to their scattering problem.

1. Introduction

Light scattering is a subject of interest for different research fields such as physics, geophysics, astronomy, meteorology, biology, particle characterization, and nanooptics. Due to the wide range of applicability, an effective exchange of information is of high importance for the scientific light scattering community. In addition to the traditional approach via publications in journals and books, the Internet has proved itself to be an easy to use and an especially rapid platform for information exchange.

In a current project funded by the German Research Foundation, DFG, a new Internet information portal for the light scattering community is under development. This new portal will be based on the existing Internet pages 'List of Electromagnetic Scattering Programs' [1], offering a list of mostly open source programs, news such as conference announcements, and information about latest books. The comprehensive list of computer programs to calculate light scattering will be expanded with tools to help users to find fitting software to their scattering problems. For this purpose suitable categorization schemes for such programs are investigated.

The main difference to the existing web page will be the concept to involve users into the publishing process by enabling them to provide own content directly to the web page. In this way users will no longer be just 'passive consumers' of a given information offer but active participants. While the paper by Wriedt and Hellmers [2] describes the general motivation and structure of such an information portal, this article goes more into the details and presents the current position of the project.

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First, the technical background and the current development of the new web pages are described. Then approaches for light scattering software categorization schemes are discussed.

2. Realization of the new web page

One main objective of this new information portal is to involve the members of the science community as active contributors into the process of keeping the information up to date. Therefore, a content management system (CMS) is used. The main attribute of a CMS is that it separates the content from the presentation on the Internet pages. For example, the design of the web pages can be changed or expanded easily without influencing the current content. A CMS also simplifies adding new information. It is possible to provide users with their own accounts so they can create and edit their own articles and use the page independently from the developers and providers, respectively. For this no profound knowledge of HTML is necessary as a CMS offers an easy to understand interface usually consisting of a text-editor and an upload tool for images.

The current development for the light scattering information portal is based on the free Joomla [3] CMS which is published under GNU General Public License. This CMS by default offers multiple options such as a search interface, the generation of lists of latest news and most popular topics or a printer-friendly layout for articles. It can be expanded by more useful extensions such as a discussion board or a page access counter. Another advantage is a 'front-end' user interface for registered editors. This keeps the process of publishing for such registered users simple, see Fig. 1.

A user enters the information portal start-/homepage where an interface allows to log in as registered user. After that the pages of the information portal are shown in the same way as for unregistered users but with the accessible topics marked by a special symbol. For example, all articles the user has contributed are marked by an 'edit' button. Additionally there is access to an additional, personal menu that enables the addition of new content. By clicking 'submit' (for a new article) or 'edit' (for an existing article) an easy to use text-editor is opened and a new article can be added or an existing article can be updated. The whole process is intuitive and no special HTML knowledge is necessary.

The CMS allows different kinds of privileges to be granted for contributors using this kind of 'front-end'. Usually a freshly created article will not become available online immediately, but after a check by a supervisor. Like the administrator on a server or an operating system the supervisor has higher privileges on the system and can check the added or updated text first to decide whether it shall be published or not, see also Fig. 2.

As there are a large number of administration options which cannot be integrated into a 'front-end' interface, a supervisor will use a special 'back-end' interface that is designed to handle more complex settings. The 'back-end' menu of the Joomla CMS is also highly intuitive and can be quickly and easily learnt. This 'back-end' is available online via a web browser, meaning that tasks and privileges of a supervisor can be given to several people residing all over the world. Supervisors also administrate user accounts and provide access to the system. As it is necessary to prevent spam or product placement material entering the portal, only bona fide researchers will have the right to contribute content.

3. Computer programs and categorization schemes for light scattering software

Another focus of the current project is on the revision of the list of computer programs to simulate light scattering on the existing Internet pages 'List of Electromagnetic Scattering Programs' [1]. This list will be revised and updated. Additionally approaches to classify the software are studied. A resulting classification or categorization scheme can be used to program an Internet tool to help users to find suitable programs for solving their specific scattering problems.

3.1. Top-down approach

The basic problem has a scatterer or a particle of known properties illuminated by light of a defined wavelength. The incident light can by described by electro-magnetic waves and therefore satisfies Maxwell's equations. Considering the particle's properties plus additional mathematical assumptions allows the set of equations to be solved.

There are different approaches to the solution of this mathematically ill-posed problem (see, e.g. Wriedt and Comberg [5] or Mishchenko et al. [6]). In principle the solutions can be divided into four categories (see, e.g. Kahnert [7]):

- direct solution using a boundary value approach,
- direct solution using an initial value approach,
- using a volume integral approach,
- using a surface integral approach (Green's theorem).

In most light scattering programs one of these four approaches is used. Therefore it is possible to categorize light scattering programs according to the theory and algorithm they are based on.

Now, all these theories have significant advantages or disadvantages that affect different program attributes that might be of interest for a user. For example, a Mie code is suitable only for spherical particles but on the other hand is very fast

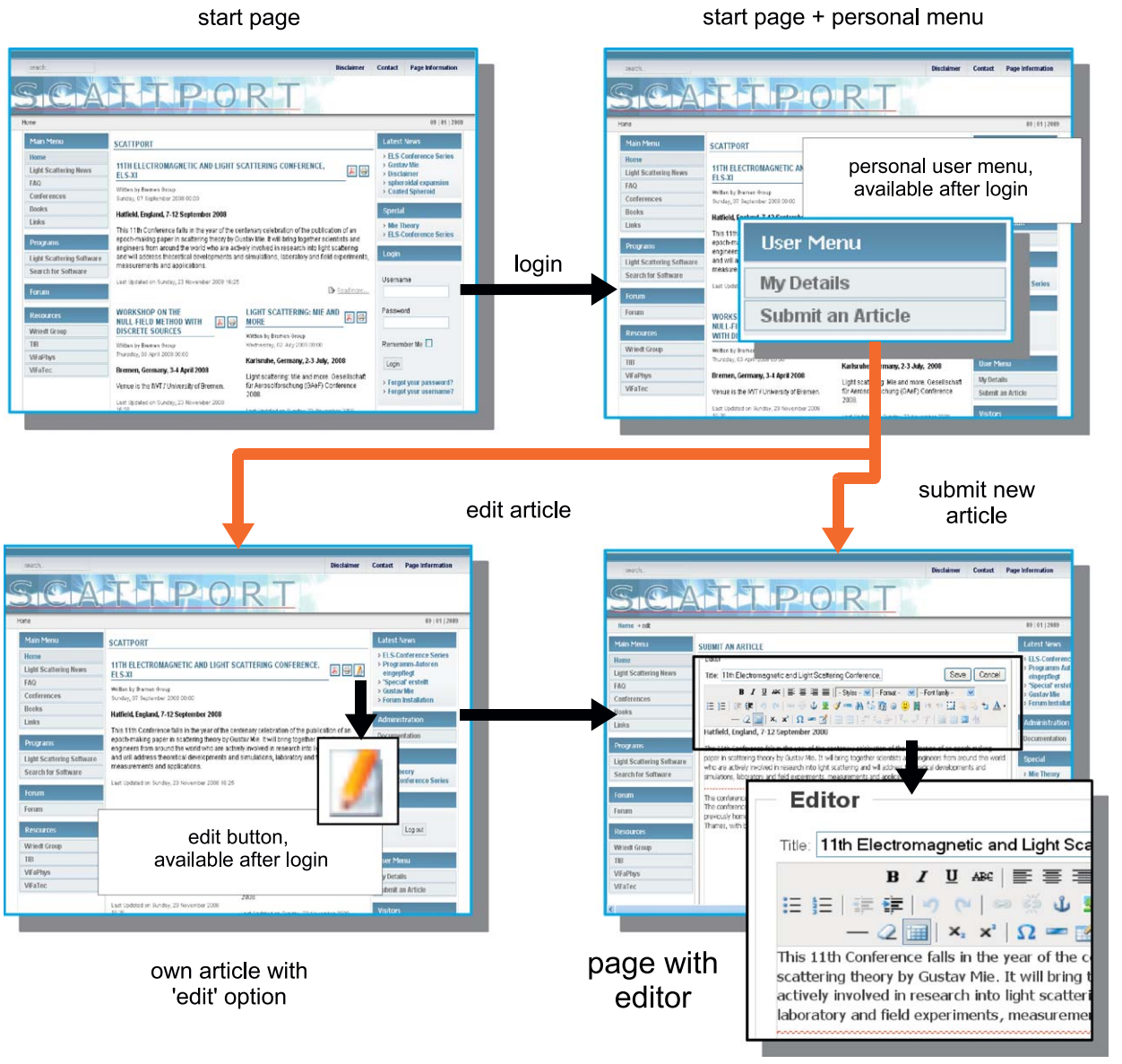

Fig. 1. Sketch of the publishing process for a portal user. On the homepage a login menu can be accessed. After the login the user has access to a menu that enables submission of new articles. Additionally all user-submitted articles are marked with an 'edit' button. Both 'submit' and 'edit' open an easy to use text-editor to create or change content.

while the discrete dipole approximation (DDA) can be used for irregular particle shapes but is slow compared to a Mie program. Table 1 demonstrates some correlations between scattering theories and resulting program attributes.

This is a highly theoretical approach to categorize light scattering software. Choosing a suitable program for solving a given scattering problem requires a great amount of experience and knowledge of the specific advantages and disadvantages of the underlying scattering theories.

3.2. Bottom-up approach

In practice it seems to be more reasonable to argue from a 'bottom-up' approach: a user usually wants to calculate light scattering for a defined scattering problem. In most cases it will be the particle that is the centre of attention. So the first question will be whether a program can calculate light scattering by the particle of interest or not. The algorithm and theory behind the software is then secondary. So from a user's point of view a categorization scheme for light scattering software should be orientated in regard to the particle characteristics such as size, shape (spherical, non-spherical, symmetrical, irregular, etc.) and refractive index, followed by considerations due to the other parameters of the scattering

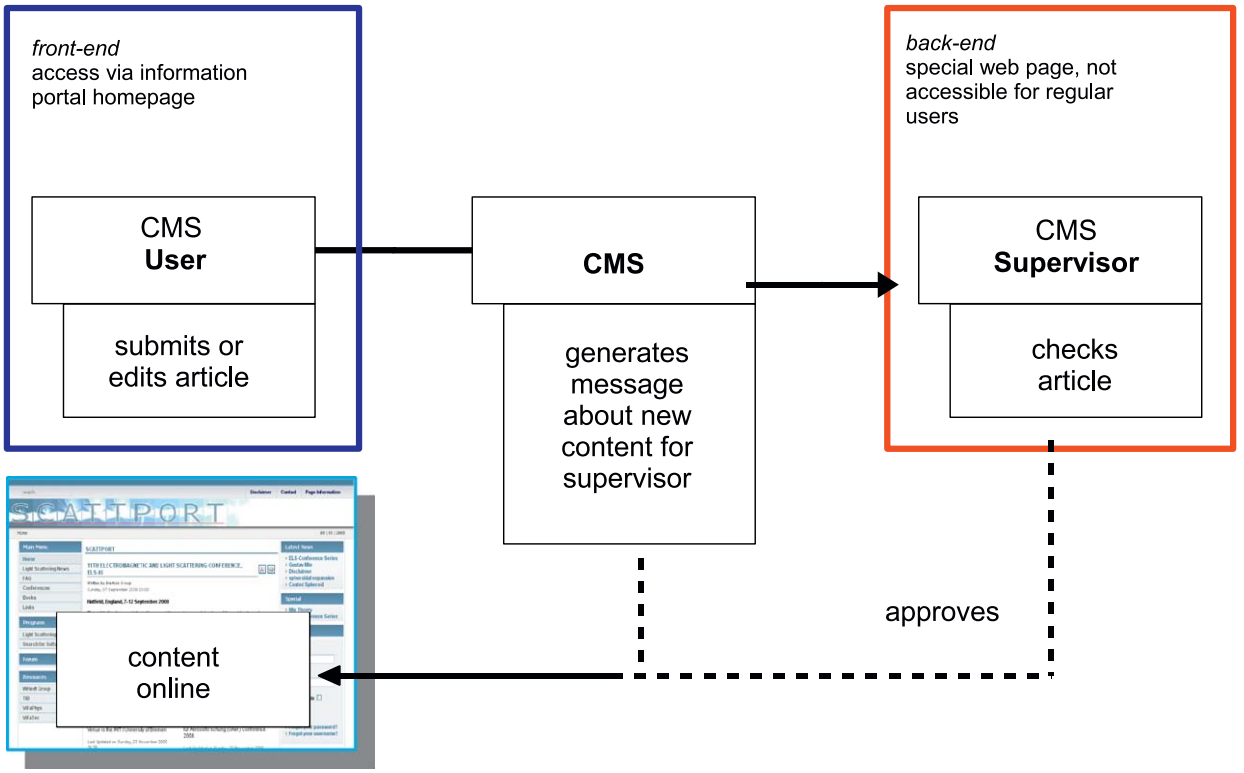

Fig. 2. Sketch of the publishing process within the system. After a user created (or changed) content the new article is not available online automatically. Before publishing a supervisor/system administrator has to check it. Any time a supervisor logs into the system a message about pending articles is displayed. When the supervisor decides to approve the article, it is published online.

Table 1
Connection between different light scattering methods (vertical) and four basic mathematical approaches (horizontal, upper block).

	Mie	SVM	NFM	GMT	DDA	FDTD	BEM	FEM
Boundary value	+	+		+				+
Initial value						+		
Volume integral					+			
Surface integral			+					
Spherical particle	+	+	+	+	+	+	+	+
Non-spherical particle		(+)	+	+	+	+	+	+
High aspect ratio		(+)	(+)	+	(+)	+	+	(+)
Considering symmetry			+	+				
Any particle shape			(+)	(+)	+	+	+	+
Volume discretization					+	+		+
Surface discretization			+	+			+	

Here Mie = Mie theory, SVM = separation of variables method, NFM = nullfield method, GMT = generalized multi-pole technique, DDA = discrete dipole approximation, FDTD = finite different time domain, BEM = boundary equation method, FEM = finite element method. Additionally it is shown what kind of particle shapes are appropriate to the model (horizontal, lower block). '+' denotes suitable, '(+)' implies limited applicability or functionality, e.g. it can depend on the particular implementation into a computer program whether the attribute is valid or not. This table is for demonstration, and no claim for completeness is made.

problem such as the type of incident light (plane wave or Gaussian beam) and media (non-absorbing, absorbing, etc.). Also one has to take into account what results have to be calculated (farfield, nearfield, Mueller matrix elements, etc.) and whether further computational investigations (e.g. orientation averaged scattering) have to be carried out or not. Additionally program attributes such as 'software is free to use' or 'the code can be edited and modified' might be of interest.

All these details lead to a kind of checklist that should be followed to get to the fitting program—see Fig. 3. Based on such a process then the software could be categorized and structured—see Table 2.

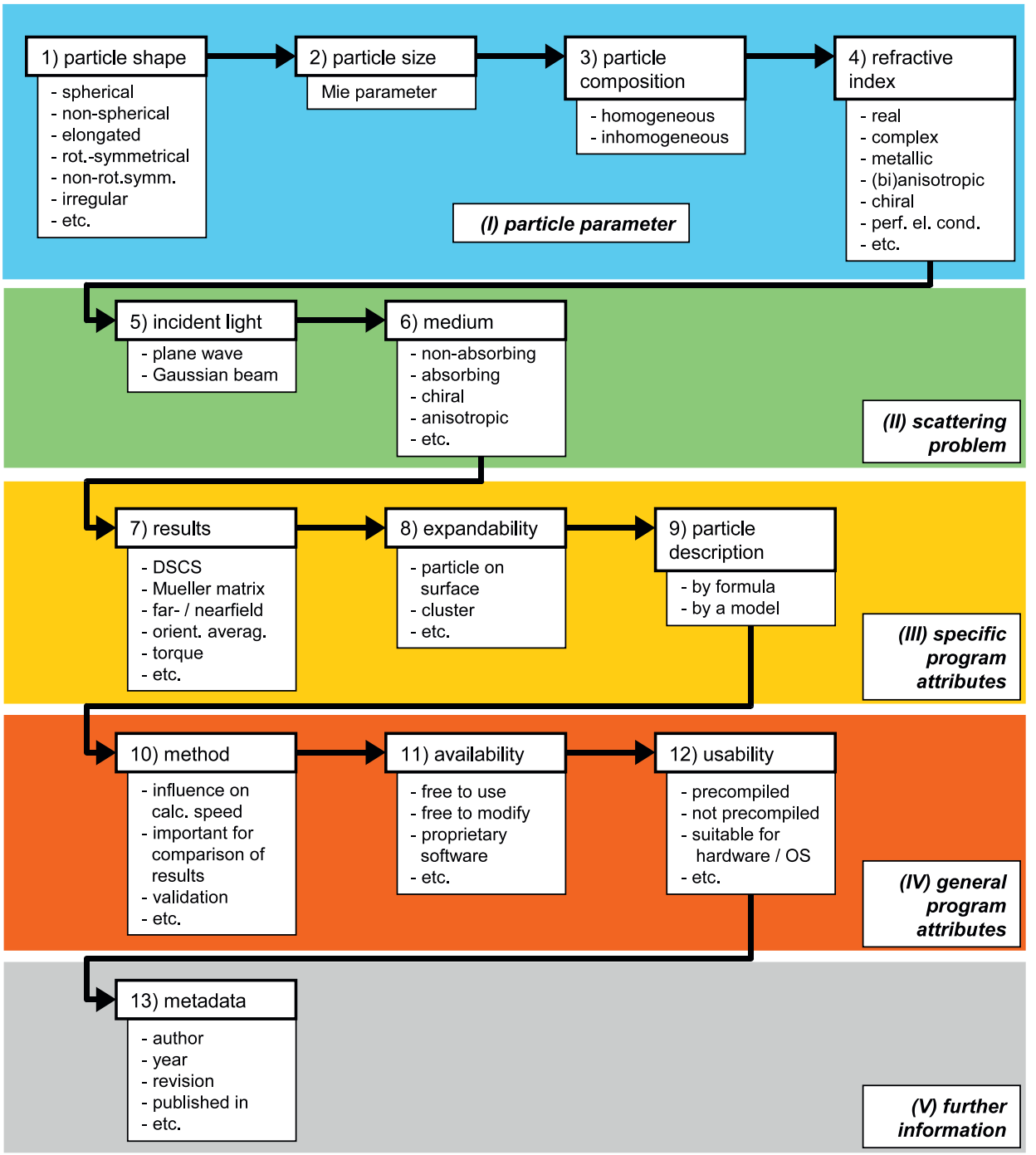

Fig. 3. Example of an overview of elements contributing to the process of finding a suitable light scattering program from the user's point of view.

4. Outlook

A light scattering Internet information portal based on the CMS described above is currently under development and will be online soon. The light scattering community will be invited for tests, content and further suggestions. By means of this feedback it is planned to improve the portal further step by step. One idea, for example, is to add a forum-module to the information page which would allow an easy and direct discussion between several scientists without much delay.

Table 2
Attribute scheme for selected light scattering programs as a result of the checklist shown in Fig. 3.

	NFM-DS TMATRIX	*DDSCAT*	*DSM*	*MMP*	*Microwave Studio*	
spherical	+	+	+	+	+	(I)
rotational-symmetry	+	+	+	+	+	
non-rot-symmetry	+	+		+	+	
concave shape	(+)	+	+	+	+	
any shape	(+)	+		+	+	
high aspect ratio	(+)	(+)	+	+	+	
inclusions	+	+	(+)	+	+	
anisotropy	+	+			+	
perf. elec. conducting.	+		+	+	+	
metallic ref. index	+	(+)	+	(+)	+	
plane wave	+	+	+	+	+	(II)
Gaussian beam	+					
particle on surface	+		+			(III)
cluster	+	+		(+)	+	
particle by formula	+	+	+			
particle by model	+	+		+	+	
scattering method	NFM-DS	DDA	GMT	GMT	FIT/FDTD	(IV)
discrete surface	+		+	+		
discrete volume		+			+	
free to use	+	+		+		
free to edit	+	+		+		
proprietary					+	
author	Doicu Wriedt	Draine Flatau	Eremin	Hafner	CST Inc.	(V)

The development of a detailed categorization scheme for light scattering software is necessary in order to implement an Internet search tool that can enable users of the information portal to find suitable computer programs for their scattering problems. The corresponding technical development of a capable search engine would be the next logical step.

5. Summary and conclusion

A new Internet information portal for the light scattering community is now under development. Compared to other existing offers an interactive approach will allow users to become active members who can contribute own content to the portal. At this point any ideas and suggestions by the light scattering community for such an information portal are welcome.

Also needed is a capable categorization scheme for light scattering software. A 'bottom-up' approach that focuses on the user's need (in regard to the scattering problem) rather than on light scattering theories in particular is suggested.

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