SPECCHIO: a spectrum database for remote sensing applications

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Abstract

Representative and comprehensive information on the spectral properties of natural and artificial materials on the Earth's surface is highly relevant in aircraft or satellite remote sensing, such as geological mapping, vegetation analysis, or water quality estimation. For this reason, the spectrum database SPECCHIO (Spectral Input/Output) has been developed, offering ready access to spectral campaign data, modelled data, and existing spectral libraries. Web-based and command line interfaces allow for the input of spectral data of heterogeneous formats and descriptions, as well as interactive queries, previews, and downloads. ASCII and ENVI spectral library data formats are currently supported. SPECCHIO is used as a reference database for the retrieval of geophysical and biophysical parameters from remotely sensed data, accounting for the frequent lack of surface spectra. The database is also used for the general management of spectral data, including detailed ancillary data.

Keywords: reference spectrum database, imaging spectroscopy, WWW, inversion problems

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1 Introduction

Spectral measurements from natural and artificial surfaces are a prerequisite for Earth surface and atmospheric remote sensing from nadir-looking airborne or spaceborne optical sensors. Thus, collecting and distributing these data forms the basis for many remote sensing applications, such as geological mapping (Clark, 1990), vegetation analysis (Li et al., 2001), and oceanography (Barnard et al., 1999). Particularly in imaging spectroscopy, a reference spectral collection can improve the characterization and classification of the image by providing endmember spectra (Roberts et al., 1998). As an example, the classification of mineral samples by direct measurements of the spectral properties is facilitated by external reference data (Hunt, 1977).

In the majority of existing spectral data collections, information is distributed across physical files (Joint Committee on Atomic and Molecular Physics Data Exchange (JCAMP-DX) (McDonald and Wilks, 1988), United States Geological Survey (USGS) ASCII (Clark et al., 1993)). Except for the simplicity of storage, this approach has serious drawbacks, such as limited scalability and low-performance query of data, low flexibility of the descriptive data (meta data) structure, and direct dependence on file formats. In connection with the USGS spectral collection (Clark et al., 1993), these deficiencies have been partially removed by the SPECPR analysis tool (Clark, 1993) which allows spectral feature analyses as well as meta data queries based on regular expressions.

In this work, the spectrum database SPECCHIO (Spectral Input/Output) has been designed and implemented. It represents a large and easily accessible spectrum data source and is designed to overcome the limitations of file-based solutions. SPECCHIO consists of three major components, namely web and command line based user interfaces, an underlying relational database management system (DBMS), and a well-defined data model. The design of these components was guided by expected application requirements from scientists with a focus on imaging spectroscopy. Typical queries to a spectrum database may read:

- Give me all the spectra of calcite!
- Are there any hemispherical spectra available from summer wheat?
- Who measured barley reflectance spectra in 1997, and what was the overall set-up?
- Find all the grass reflectance spectra measured at sensor viewing angle 45 degrees!
- Show me all the bare soil radiance spectra measured during the 'Barrax' campaign!

SPECCHIO is designed to manage heterogeneous data from different sources, taking into account the high diversity of applications for spectral data in imaging spectroscopy. User-generated queries for common properties of spectral data yield result sets with detailed information on each matching spectrum, that can be downloaded to the user's local system. Input interfaces allow users to feed single as well as multiple spectra and associated meta data into the database within a single transaction. The consistency of all input data and requirements on the completeness of data documentation are enforced by conditional rules.

SPECCHIO serves as a spectrum reference database for geophysical and biophysical retrieval algorithms based on remotely sensed data. It can replace the direct measurement of spectra on the spot of interest, data which are seldom available outside a full-scale measurement campaign. For example, for atmospheric correction of airborne or spaceborne spectral images, spectra from the database can substitute in-situ ground target measurements, required as radiative transfer input. In addition, SPECCHIO is currently employed to manage large bi-directional reflectance spectrum datasets from field campaigns with a multitude of independent measurement parameters.

We consider SPECCHIO a first step towards a complete spectral data collection providing all kinds of interactions that may be required in imaging spectroscopy research. Spectral data from different sources, such as field campaigns, modelling algorithms, and existing spectral libraries, have been entered into the database and are now available online to the user.

2 Concept

The scientific requirements for SPECCHIO in the field of imaging spectroscopy defined a set of design principles, which are as follows in order of priority:

1. Logical relations and consistency
   Relations are established between spectral attributes, allowing the query for common attributes of spectra. Each spectrum dataset is fully described, complying with prescribed consistency standards. In doing so, semantic redundancy in the database is reduced and data quality preserved.

2. Intuitive interfaces
   Easy data access and handling are a primary goal. Web and command line interfaces shall be best-suited to allow for users database interaction without a priori knowledge. Entering new data may require user instruction, which is entirely given online.

3. Flexibility to changes in science context
   Meta data describe the aspect of reality in which a spectrum is measured. Attributes are labels for meta data. The set of attributes in the database has to provide a sound basis for unambiguous spectrum description. New attributes can be added easily, if required.

4. Independence of file format
   High variety and frequent change of spectral data formats call for maximum flexibility of data input and output. Accordingly, the given I/O interfaces have to be extensible with respect to new spectrum data formats.

5. Scalability
   The amount of spectral data in SPECCHIO shall be limited only by disk size and access to the database. A separation of file and database server guarantees maximum upscaling flexibility.

The development process of the SPECCHIO database followed the rapid prototyping approach using an iterative software life cycle (Leach, 2000). A sequence of requirement, design, implementation, validation, and release phases accompanied by frequent changes in specifications of the individual parts resulted in the current version of the code.

The basic structure of SPECCHIO, defined by the abovementioned principles, is shown in Fig. 1. Typical forms of data sources, and examples of application areas for retrieved data are given. Web and command line interfaces provide maximum access and input/output flexibility. Due to physical separation of database and spectral files, only meta data are stored in the database itself, uniquely linked to the actual spectral data on a file server.

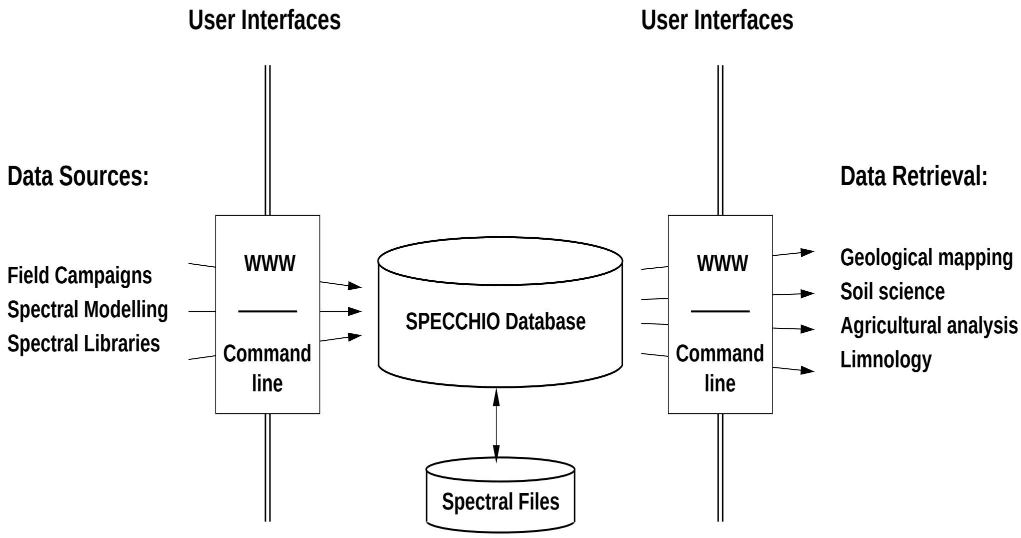

Figure 1: Basic layout of SPECCHIO.

3 Implementation

Design principles as given in the previous section gave rise to a concept that prescribed the software implementation process. Data model, data formats, and technology as used in the SPECCHIO application are described in the following sections.

3.1 Data Model

Data models formally describe the way in which information in databases is organized. A common representation for a data model is an entity-relationship diagram (Date, 1995). In this work, entity properties are referred to as attributes with associated meta data content. A complete set of attributes of one entity is called an instance of that entity.

Fig. 2 shows the data model of SPECCHIO. Spectral information is systematically divided up into seven thematic entities, each of which covers a different aspect of the spectrum description. The entity SPECTRUM contains attributes expected to be most variable between individual spectra, the other entities encompass attributes that are usually common to spectral ensembles. Each instance in the SPECTRUM entity is related to exactly one spectrum, and uniquely related to exactly one instance in each other entity. Vice versa, the relation between SPECTRUM and other instances is non-unique. In other words, SPECTRUM is linked to the entities GENERAL, POSITION, MODEL, SENSOR, TARGET TYPE, and LANDUSE TYPE by n:1 relationships, enforced by referential integrity constraints (foreign keys). Relations are in the third normal form to guarantee consistency and minimize redundancy of the data. This normal form requires for each entity compulsory key attributes (`not null`), specifically defined foreign keys (FK), and uniqueness constraints that apply to the most relevant attributes, as denoted by (*) in Fig. 2.

Spectral attributes as given in Fig. 2 were defined based on the scientific requirements, particularly in imaging spectroscopy applications, and the review of spectral data descriptions in existing spectral data collections (section 4).

Users can freely define instances in all entities, except for the specification of the TARGET

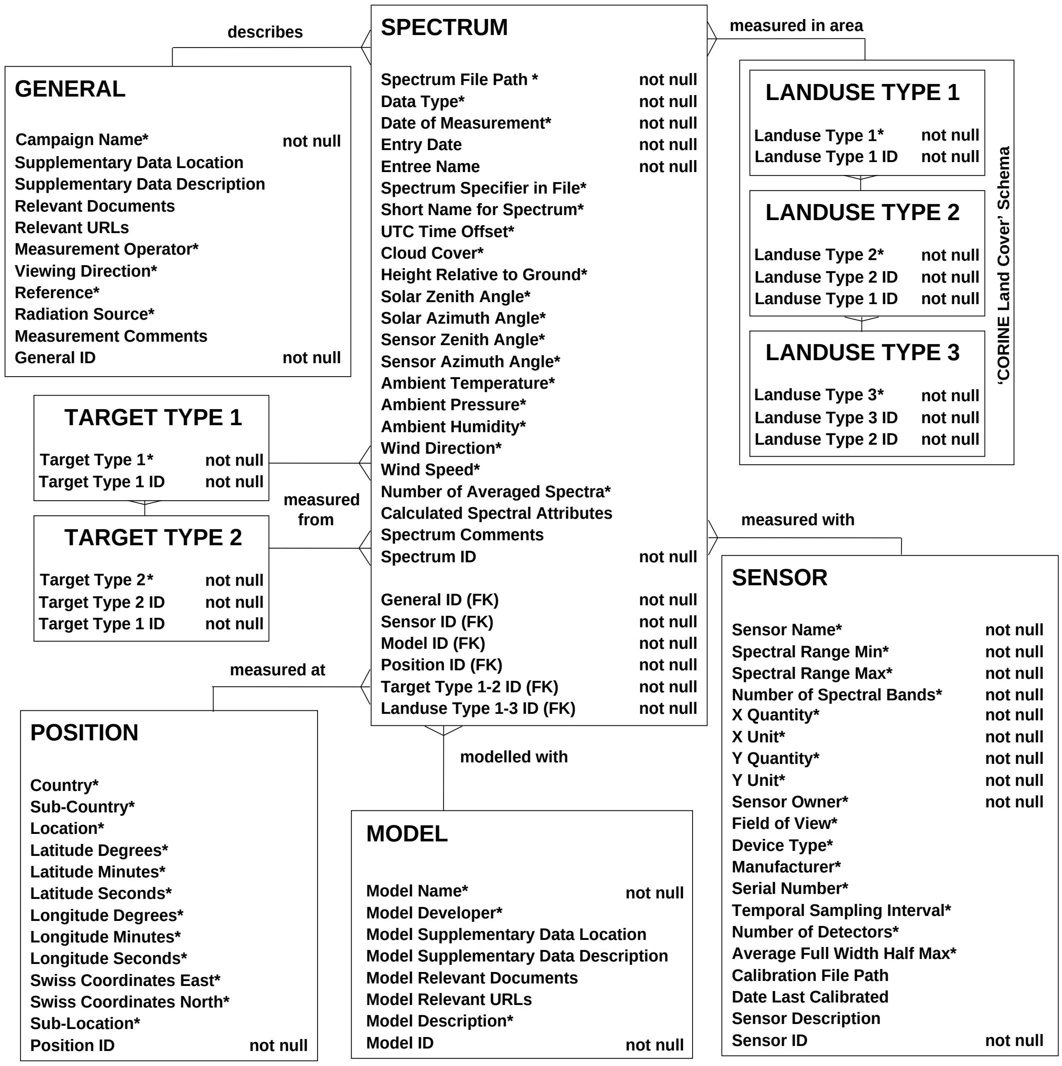

Figure 2: Data model of SPECCHIO expressed by an entity-relationship diagram, which describes the spectroradiometric aspect of reality. Identifiers (ID) uniquely define instances in all entities. SPECTRUM is related to other entities by referential constraints (foreign keys, FK) on respective IDs. Forks denote n:1 relationships, `not null` tags compulsory attributes, and (*) indicates attribute sets subject to uniqueness in each entity.

TYPE captured by the spectrum, and the LANDUSE TYPE. The target type describes the physical type of object or part of the Earth's surface, and is often referred to as land cover. Land use represents a subjective, anthropocentric view of a type of target, reflecting its value as natural resource in a spatial context. The two concepts 'land use' and 'land cover' are often used interchangeably, but shall hereafter be treated as defined above.

The target type can be specified on the lower hierarchy, subordered to a coarse classification of (bio-)physical surfaces on the Earth: artificial, vegetation, rocks/minerals, soil, and water. The pre-defined three-level hierarchy from the 'CORINE Land Cover' scheme (European Commission DG XI, 1993) was employed for the land use type and remains unmodified in the database.

Files that contain the actual spectral information physically reside on a disk, accessible by SPECCHIO on a local network, rather than as objects in the database itself. SPECCHIO locates files uniquely via the `spec_file_path` attribute. The separation of DBMS and file storage maintains the integrity of the files, keeps the implementation process simple, and enables swift upscaling of the database.

3.2 Data Formats

Information about the format of spectrum data is used by SPECCHIO for data display and output. Therefore, this information needs to be provided for input of new data. In principle, this functionality is independent of the data format itself. The interface design is flexible enough to incorporate user-defined display and output routines for any kind of spectrum data format.

A number of file formats for spectrum-type data exists, each of which adapted to certain fields of application. This implies specific ways of organizing data and descriptive meta data in the file structure. Examples are JCAMP-DX (McDonald and Wilks, 1988) in applied spectroscopy, HDF-EOS (Ullman, 1999) for airborne or spaceborne data, ENVI spectral library (Research Systems Inc., 2000a) for spectroscopy data, and certainly all flavours of instrument-specific ASCII file formats.

The implementation of SPECCHIO supports the ENVI spectral library (SLB) and columnar ASCII formats in the current version. SPECCHIO offers programs written in the Interactive Data Language IDL (Research Systems Inc., 2000b) that allow for the conversion of spectral data from spectral collections, field spectrometers, and modelling codes into formats supported by SPECCHIO, considering all pertinent meta data (cf. section 4). Once entered into the database, the spectral data can subsequently be queried, displayed, and exported. If a query results in a large number of hits, it is desirable for users to obtain the data in a compact form. The ENVI-SLB file matches that purpose, as it consists of two components: descriptive ASCII header, which contains all meta data, and binary body. It is therefore chosen as the standard output format. If the ASCII export option is selected, export files appear as columnar ASCII, bundled in a tar 'tape archive' file (section 3.4).

3.3 Technology

Main technical features of the SPECCHIO database application are depicted in Fig. 3. Web access to the Database Management System (DBMS) is generally being established by (1) an application programming interface that enables communication between a programming language and a database, and (2) a method to call executable programs on a web server. As for (1), the scripting language TCL (Ousterhout, 1994) with the Oratcl [2] database interface extension is used to process database queries that comply with the SQL-2 standard. (2) has been implemented using the Common Gateway Interface (CGI) (Gundavaram, 1996) for web servers as provided by the Webshell [3] web application interface extension for TCL. All of these programming tools except the Oracle 8i DBMS, are developed and distributed as Open Source software [1]. We chose the CGI for reasons of implementation speed and ease of maintenance. It uses the standard HTTP protocol for communication between client (user) and SPECCHIO server. No disk volume requirements are imposed on the client side, and the lack of precise session management is compensated by expected low transaction rates. Dynamically created web pages are coded in HTML4.0 and Javascript. Command line-based user interaction is carried out via pre-defined scripts directly over the local area network.

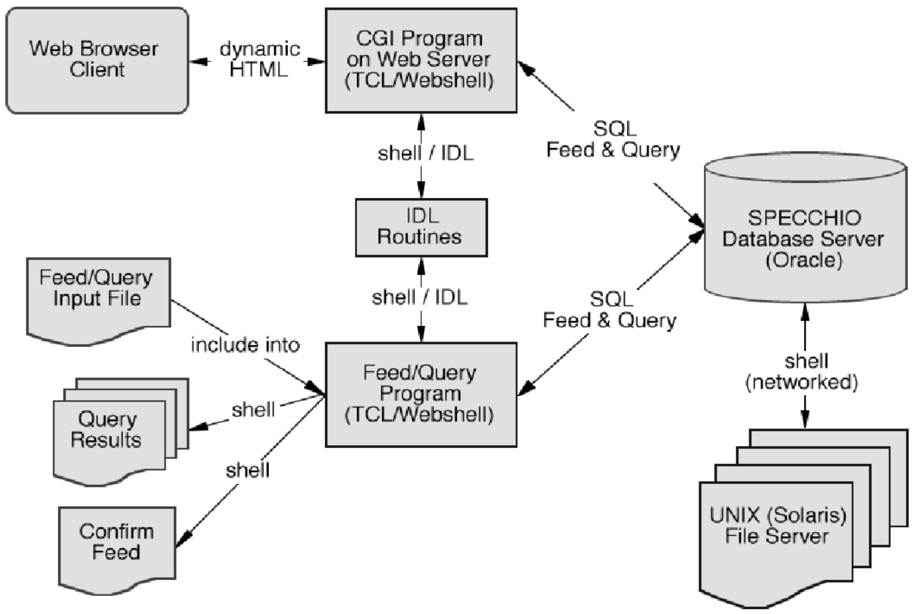

Figure 3: Technical layout of SPECCHIO. Two access interfaces are available: web browser-based (A), or script-based (B). The UNIX file server hosts the spectral source files.

These scripts can be incorporated into other scientific application programs, allowing the interaction with SPECCHIO at run time.

The DBMS capabilities in terms of backup, recovery, and constraint support are crucial for SPECCHIO. In principle though, any equivalent relational database software with an interface to TCL could be used here. Spectral files are stored on a UNIX file server integrated in the local environment of the database server.

Scripts written in IDL are executed at run time for dynamic plotting and exporting of spectrum data. Flexible adaptation of other data formats is possible by adding IDL programs with full display and output capability.

The software at large is server-based and runs on all platforms that support Webshell (e.g., UNIX Solaris, Windows NT).

3.4 Interfaces

Interfaces to a spectrum reference database have to be intuitive and widely accessible, i.e. suitable for laboratory work as well as in the field. Accordingly, access to the database is twofold: (1) by a standard web browser, and (2) by command line scripts. Users can input and query data via either alternative.

(1) The web interface offers

- online query and visualization of spectra,
- remote download of spectrum data and meta data,
- online views of database content, and
- input of single spectrum datasets and meta data.

(2) Command line scripts allow

- local network based input and query of spectra,
- input of large amounts of spectrum datasets and meta data, and
- embedding of SPECCHIO functionality into other spectral analysis applications.

Operational, frequent users prefer way (2) on the local network of the SPECCHIO installation. Remote interaction on a more infrequent basis, as well as visualization of the current database content is provided by option (1). The following two subsections explain both interfaces in detail.

3.4.1 Input Data

Input of new data into SPECCHIO currently requires user authorization for both interfaces, as control over data quality has to be maintained. Access to the database server's local network is necessary as well. The most important attributes to be given on input are

- the file name including full local network path information of the spectrum data file to be read,
- the data format (ASCII or ENVI-SLB), and
- the sensor specification that belongs to the spectrum.

New spectrum meta data can be stated on the web site (Fig. 4) in text boxes or clickable menus. Text boxes are used for attributes where high semantic variability is expected. Menus are given for cases with low variation in meta data, or pre-defined selections. A dynamic view of instances of a selected entity (e.g., SENSOR) is shown in the lower part of the main frame. Here, entries can be associated with the new spectrum, instead of defining a new instance (e.g., for the SENSOR part) in the upper frame. This saves time and reduces semantic redundancy in SPECCHIO. The web site is updated on every reload so that it always represents the current database content.

Through the command line-based interface, large amounts of spectra can be read with only one input text file, following a prescribed syntax which is exemplary given as follows:

day of measurement = 03.06.1999
time of measurement = 12 : 42|12 : 43|12 : 44|12 : 45
spectral file path = /data/rsl/barrax/spectrum.slb
ambient temperature =
sensor angle = 45|45|45|60

In this example, the spectral file contains four spectra which are assigned different time and sensor angle, identical day, and no temperature information. Generally, multiple attributes as stated in the example have to be consistent in number and are attributed to single spectra. Attributes stated exactly once or not at all apply to the entire set of spectra to be read in. Spectral attributes are divided into compulsory and optional parts. Completeness and consistency of attributes are checked by appropriate statements in the database application, and again verified by key constraints in the data model (Fig. 2). Concerning the target types in SPECCHIO, new entries can only be defined on the lower level of the target type hierarchical structure, and have to be associated with a pre-defined target type of the upper level. New definitions can be made online as well as script-based.

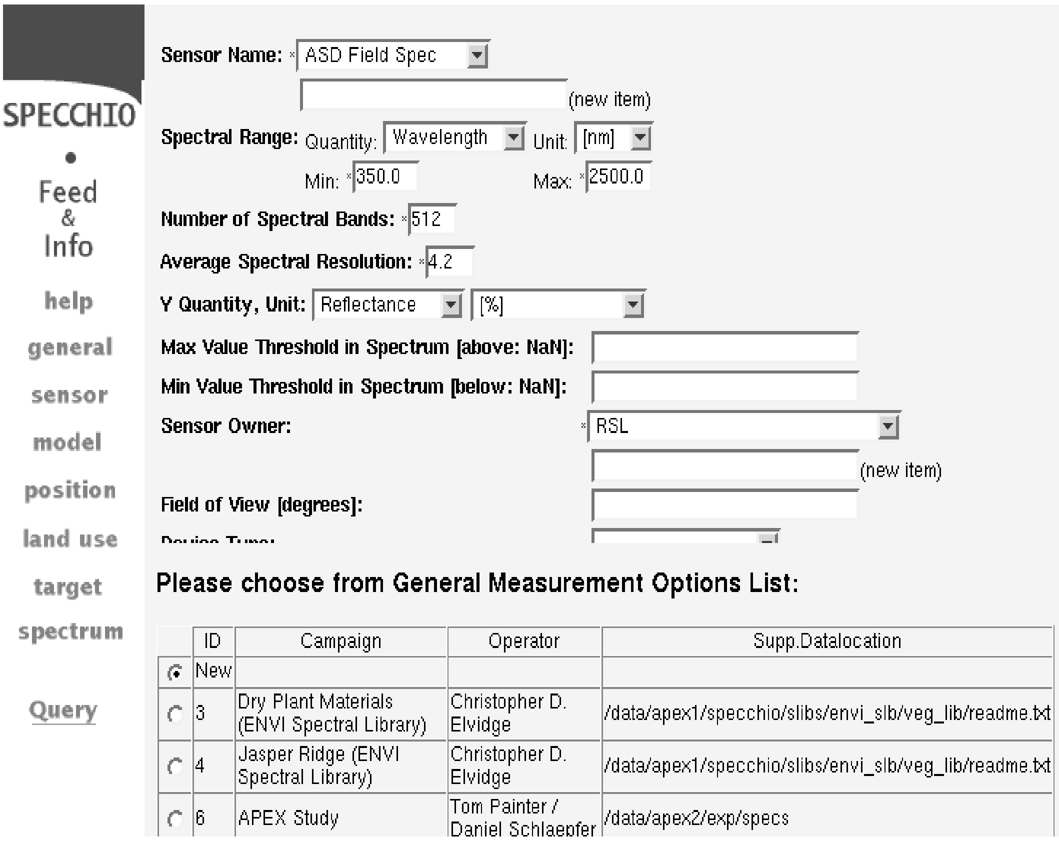

Figure 4: Web interface to feed data into SPECCHIO. The lower main frame of the web site also serves as a view on parts of the current database content.

3.4.2 Query Data

Querying spectral data using SPECCHIO is free of authentication and feasible for everybody on the web with ordinary browser software. A command line option for local use also exists using a query text file. After submitting the web query, a list of matching spectra is loaded into the browser window, offering previews of spectral plots, as well as the export of spectra in a tar 'tape archive' file (Fig. 5). The export dataset is created at run time. To save loading time, a maximum of 10 plots is shown at once. Meta data from each spectrum appear at the bottom of the preview list and are exported as well.

Via the command line interface, the application reads a text file in which a query is made using a particular syntax. This is illustrated by the following example:

country = Spain
day of measurement = ∗06.1999
operator = Beisl | Strub

This text file fragment results in a query that looks for spectra measured in Spain AND measured sometime in June 1999 AND collected by operators Beisl OR Strub. Generally,

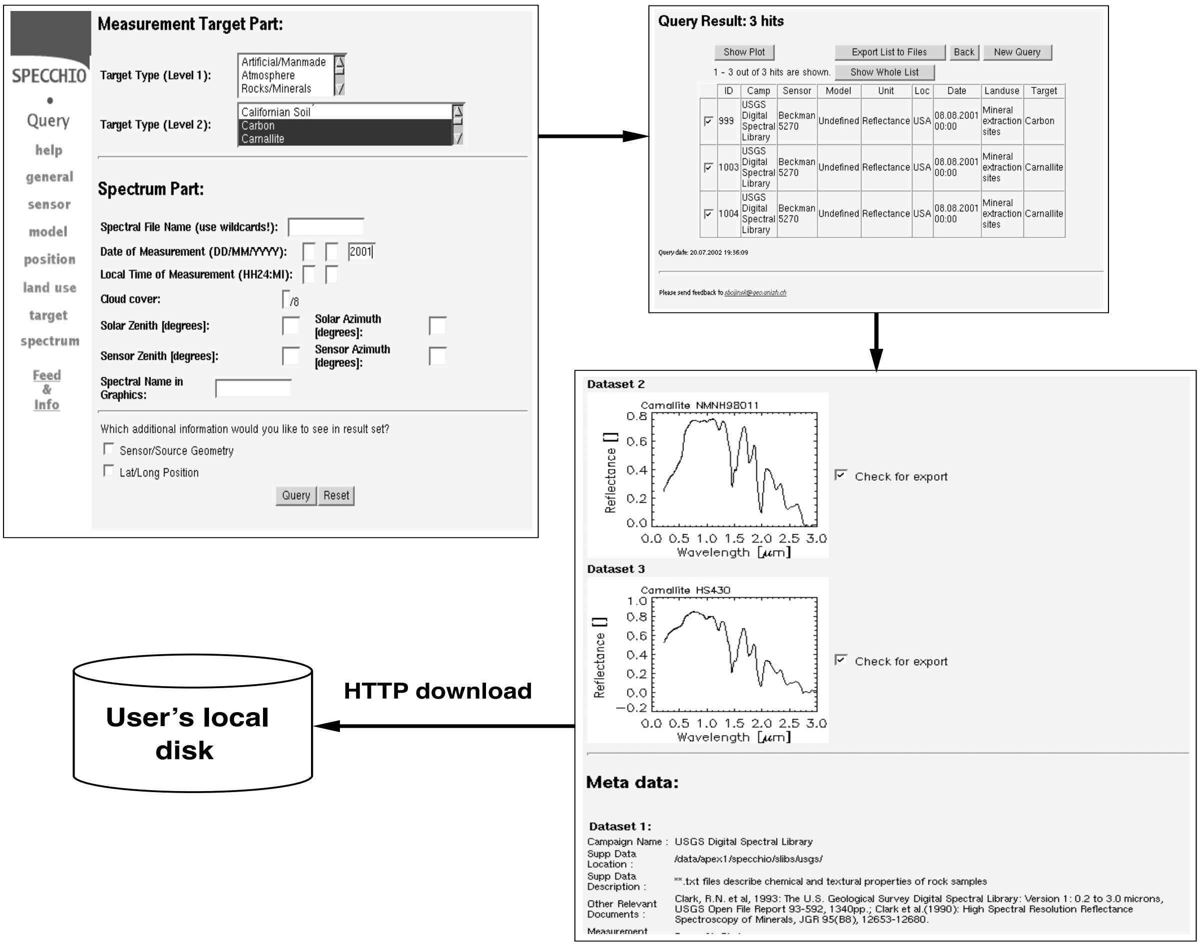

Figure 5: Web interfaces to query data from SPECCHIO. A suite of interactions leads to display and user download of spectral data. All associated meta data are included in the export datasets.

Boolean logic is coded by stating the appropriate attribute and using the operator syntax as given by the example. As a result of the query, users can load the matching datasets into their current working directory.

The granularity of SPECCHIO data output in ENVI-SLB format, i.e., the effective number of files that make up the result of a query, is determined by the Sensor definition of the matching spectra. This definition contains spectral resolution, physical units, and spectral range of the data, i.e. no resampling or rescaling is performed in the current version.

In case of ASCII output, the tape archive file contains each spectrum represented as a single file.

4 Examples for Input Data

In this section, the storage and access capabilities of SPECCHIO with regard to heterogeneous spectrum data is demonstrated. The flexibility of our data model is shown by trans-

Institution	Reference	Number of spectra	Target types
Johns Hopkins University	Salisbury et al. (1991)	617	Terrestrial, lunar, artificial
Jet Propulsion Laboratory	Grove et al. (1992)	430	Minerals
US Geological Survey Denver	Clark et al. (1993)	498	Minerals, vegetation
USDA Beltsville	Price (1995)	3257	Natural, artificial

Table 1: Spectral collections contained in SPECCHIO.

lating the characteristics of existing spectral library data, field campaign data, and modelled data into appropriate sets of meta data that are subsequently entered into SPECCHIO. The database is perfectly able to accommodate laboratory campaign data as well.

4.1 Spectral Library Data

The need for comprehensive and widely accessible spectral data collections has been addressed previously by several institutions and researchers, as listed in Table 1.

All these spectral collections have been entered into SPECCHIO, along with full documentation on sensors, measurement set-ups, operators, locations, and measurement targets. An example of data from the USGS Digital Spectral Library is shown in Fig. 5. Important attributes of the spectra in terms of variability are the target type and further description of the measured object, e.g., its chemical composition. Example code that has been used to enter these data into SPECCHIO reads:

```
new target type2 = Acmite | Adularia | ...
spectrum comments = Formula: NaFeSi2O6 | Formula: KAlSi3O8 | ...
```

4.2 Field Campaign Data

Spectral measurements carried out during field campaigns provide substantial information on the physical state of the Earth's surface that is required as ground truth in airborne or spaceborne imaging spectroscopy, as well as for the vicarious calibration of nadir-looking sensors. Two examples of campaign datasets are given in the next sections, from applications in limnology and vegetation analysis.

4.2.1 Limnology

In-situ spectral data were measured during a limnological study to investigate the water quality of inland lakes (Keller, 2001) using ground-based and airborne data. Measurements were carried out with a GER1500 spectroradiometer at several locations on different Swiss lakes. At each location, depth profiles of upwelling and downwelling radiance were measured in water, giving a handle on scattering and absorption properties of the water and dissolved constituents. From this set-up, it is obvious that defining descriptive attributes to these spectra are lake, measurement location, depth, and viewing direction of the sensor. Fig. 6 shows a sketch of the measurement set-up and part of the associated text file that was used to

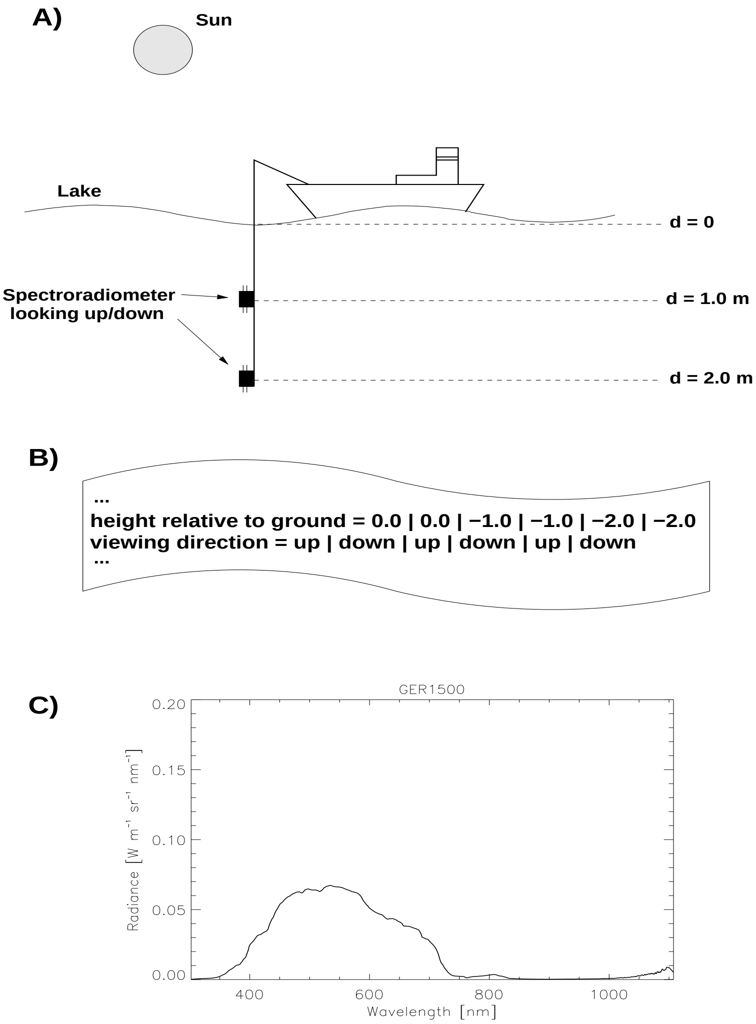

Figure 6: Typical measurement set-up for spectral measurement in lakes in the course of a limnology campaign (A) and part of the corresponding feed text file (B). (C) shows an example plot of downwelling radiance at lake water depth 1.0 m.

enter the spectra into the database. The limnological dataset is expected to be representative for the water optical properties of alpine lakes and rivers and can be used as a reference for other applications in that area.

4.2.2 Vegetation Analysis

Studying the spectral reflectance behaviour of vegetation constitutes an important part of agricultural and forestry analysis. Measuring the bi-directional angular reflectance of plants during a growing season gives information on growth status, vitality, and phenological stage. Spectral data were measured across a hemisphere with a goniometer set-up over an alfalfa canopy during a large-scale measurement campaign in Barrax (Spain).

In this case, attributes that make a distinction between individual spectra are the four angles specifying the sensor-sun geometry, as depicted in Fig. 7, and the local time of measurement. SPECCHIO can store all these attributes and allows detailed queries on

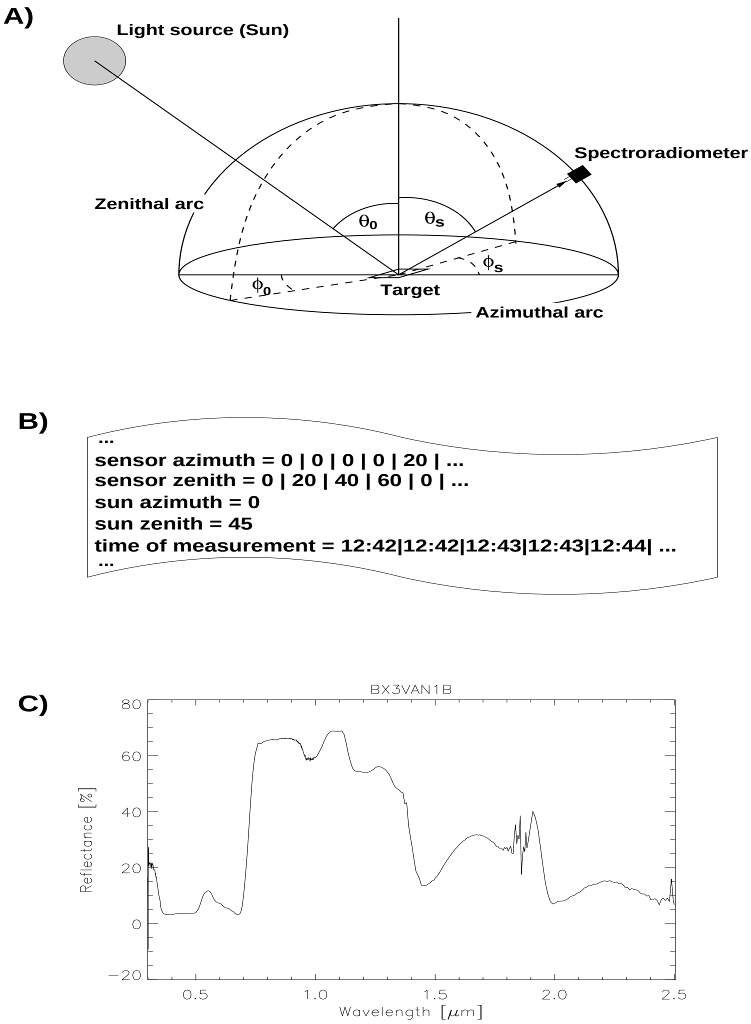

Figure 7: (A) Geometry of typical measurement for the study of bi-directional spectral reflectance of natural surfaces. ϕ_O, ϕ_s are solar and sensor azimuth angles, θ_0, θ_s are solar and sensor zenith angles, respectively. (B) Part of the feed script that describes this measurement set-up. (C) shows an example plot of green vegetation (alfalfa) reflectance for sensor zenith and azimuth angles 60 and 180 degrees, and solar zenith and azimuth angles 48 and 94 degrees, respectively.

individual spectra as well as parts of measured hemispheres.

4.3 Modelled Data

The use of modelled reference spectra is widely accepted in imaging spectroscopy, since complete field or laboratory spectral series are seldom available for parameters under investigation. Thus, series of reflectance spectra using established models were generated and stored in the database. One major series was created for generic vegetation canopies using the PROSPECT (Jacquemoud and Baret, 1990) and SAIL models (Verhoef, 1984). They include parameter variations for leaf area index, leaf chlorophyll and leaf water contents. A second reference series of reflectance data was modelled for snow analysis where the snow

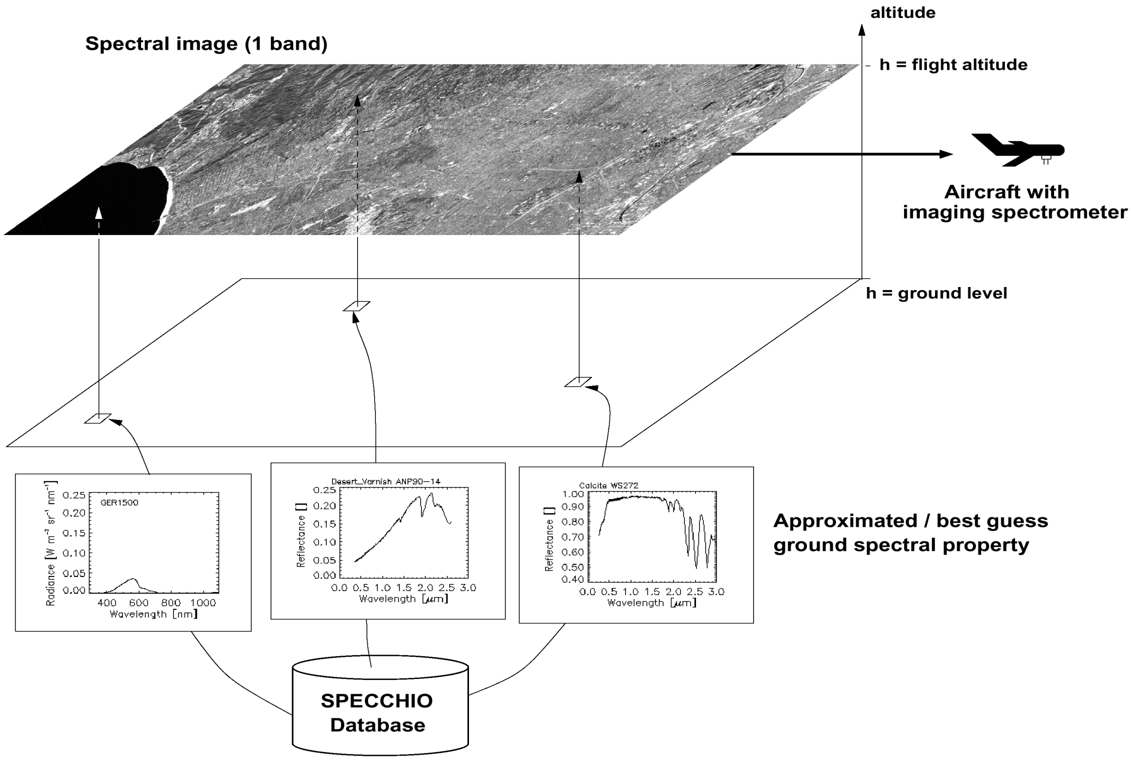

Figure 8: SPECCHIO providing surface spectral information to airborne or spaceborne imaging spectroscopy measurements, aiding in endmember selection for spectral unmixing of the image data.

optical thickness and its grain size have been varied systematically (Painter et al., 1998).

5 Application in Imaging Spectroscopy

A typical application of the SPECCHIO reference spectrum database arises from the need for surface reflectance approximations, when airborne or spaceborne downward looking spectral measurements are analysed (Fig. 8). The nadir-looking spectrometer mounted on a carrier platform continuously scans the Earth perpendicular to the flight direction, yielding an image cube in three dimensions. Contiguous pixels span in two spatial directions, the third spectral dimension is reduced to one image layer for the purpose of illustration.

Generally speaking, there are four driving factors to the shape of individual pixel spectra in the image: Optical properties of (1) the surface cover, (2) the atmosphere, (3) the sensor response, and (4) the extraterrestrial solar irradiance. SPECCHIO helps to better characterize both of these physical characteristics, as indicated in Fig. 8. Selected ensembles of spectra from the database represent a good first guess on spectral endmembers in an unmixing analysis. In case of missing in-situ ground spectral measurements especially, as is often the case in imaging spectroscopy, the use of region-specific or cover-specific spectral database information significantly improves endmember specification. For example, this results in more accurate geological mapping of minerals as well as better spatial characterization of soils.

If one is either interested in the removal of atmospheric optical influence, as necessary for case (1), or in atmospheric properties themselves (2), an approximation of the surface reflectance for certain spectral windows is required. This is particularly true over land surfaces (Kaufman et al., 1997). The atmospheric effect can then be isolated from surface radiative contributions and inverted to atmospheric parameters, such as optical thickness.

6 Conclusions

Concept, design, implementation, and parts of the content of the newly developed reference spectrum database SPECCHIO are presented in this paper. A comprehensive collection of spectral measurements from a variety of natural and artificial surfaces with intuitive user interfaces has been created. SPECCHIO contains field and laboratory campaign data, spectra from existing spectral collections, and modelled spectra. Due to the separation of database and spectrum data files, heterogeneous spectral data from a variety of sources can be stored. Web-based and command line-based interfaces allow user access to the database. Single and multiple spectral sets can be input and queried using these interfaces, including descriptive meta data.

The inversion of airborne and spaceborne imaging spectrometry data with respect to physical properties of the Earth-atmosphere system can be improved by spectral reference data from SPECCHIO. Missing in-situ surface spectral data can be replaced on an approximative basis. The database can also help to better classify spectral images by providing endmembers for spectral unmixing. Secondly, the database organizes and manages spectral data that depend on a high number of independent parameters, such as bi-directional reflectance field campaign data.

ASCII columnar and ENVI spectral library data formats are supported in the current version 1.0, and the flexibility to add other data formats is given. Input of spectral data is work in progress.

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