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Abstract: SPECTRA (Surface Processes and Ecosystem Changes through Response Analysis) is a planned spaceborne multiangular hyperspectral and thermal imaging spectrometer in phase A early design led by ESA’s earth observation group. Its mission is to describe, understand and model the role of terrestrial vegetation in the global carbon cycle and its response to climate variability. Even though the project has been terminated in November 2005, many results of the phase A studies are considered to be useful as input to future missions. The SPECTRA end-to-end simulator is intended to be used to test different aspects of the SPECTRA mission concept and for tuning the retrieval algorithms as well as assessing their performances. The intention of this ESA-commissioned study was not to build an actually working simulator, but to conceive an architecture for a simulator to be built during phase B of the SPECTRA design, as well as perform a limited validation of this architecture. The software architecture for the future SPECTRA end-to-end simulator has been designed to be modular, flexible and distributed. It consists of a central control unit with associated database, which is controlled and monitored via an internet-accessible web interface, and a flexible number of modules performing the actual calculations. The list of simulator modules currently includes but is not limited to state-of-the-art developments in radiative transfer (Onera), instrument modelling (ESA), atmospheric correction (Onera), and various level 2 algorithms (Alterra). Assimilation models and global carbon flux models are linked to the simulator via the SPECTRA field segment database (RSL and Princeton), for which a high level schema has been defined. The simulator structure has been validated using full end-to-end simulations from ground data to top-of-atmosphere, through the SPECTRA instrument simulator provided by industry, and back again. Test data from the Barrax field site are used for this purpose (University of Valencia).
DESIGN AND PROTOTYPING OF THE SPECTRA SIMULATOR ARCHITECTURE

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INTRODUCTION

SPECTRA (Surface Processes and Ecosystem Changes through Response Analysis) is a planned spaceborne multangular hyperspectral and thermal imaging spectrometer in phase A early design led by ESA's earth observation group. Its mission is to describe, understand and model the role of terrestrial vegetation in the global carbon cycle and its response to climate variability. Even though the project has been terminated in November 2005, many results of the phase A studies are considered to be useful as input to future missions.

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The software architecture for the future SPECTRA end-to-end simulator has been designed to be modular, flexible and distributed. It consists of a central control unit with associated database, which is controlled and monitored via an internet-accessible web interface, and a flexible number of modules performing the actual calculations. The list of simulator modules currently includes but is not limited to state-of-the-art developments in radiative transfer (Onera), instrument modelling (ESA), atmospheric correction (Onera), and various level 2 algorithms (Alterra). Assimilation models and global carbon flux models are linked to the simulator via the SPECTRA field segment database (RSL and Princeton), for which a high level schema has been defined. The simulator structure has been validated using full end-to-end simulations from ground data to top-of-atmosphere, through the SPECTRA instrument simulator provided by industry, and back again. Test data from the Barrax field site are used for this purpose (University of Valencia).

SOFTWARE ARCHITECTURE

A critical component of the proposed SPECTRA simulator is the architectural framework to support the simulator given both technical (e.g. high bandwidth) and non-technical (e.g. intellectual property protection) constraints. From the various requirements that apply to the simulator, modularity emerged as the most important one. The architecture consists of a central control unit with associated database and a configurable set of modules which do the actual calculations. Figure gives an overview of one possible realization of such a chain of modules and the currently used module naming convention. Module A and C refer to the forward and inverse models (of which currently only the RTM parts dubbed A2 and C2 have been implemented as working modules), Module B is
the instrument simulator (two implementations resulting from two independent industry studies (i))
and module D refers to the SPECTRA field segment (ii). Effort has been made to ensure that the
upgrading (including versioning) or changing of modules and the addition of new ones is easy and
flexible. In order to meet these requirements, each module is bracketed by two converters and a
database is placed between converters as shown. Scientific data and simulator management data
are kept in a centralized relational database management system to ensure repeatability and facili-
tate dynamic configuration and flexibility. The system allows for the remote execution of any mod-
ule and is controlled and monitored via a web interface. Figure gives an overview of the top-level
software architecture for the CCU and external modules (“slaves”).

The simulator design report (iii) includes a full description of the simulator data model, which is
designed to support management of the highly modular architecture, the simulations and the scien-
tific datasets. Remote execution of modules is addressed with respect to security-related deploy-
ment issues, data exchange and format conversions. Other issues related to the development and
the maintenance of the simulator are addressed as well. The proposed concept of a simulator
framework with modular and distributed architecture has also been illustrated by a working demon-
stration prototype. The flexibility of this architecture allows it to be used for virtually any future
simulator consisting of any number and kind of modules.

Figure 1: Overview of modules, converters and databases
MODELLING OF TOA IMAGES (MODULES A1 AND A2)

Module A1, dedicated to the creation of TOC data as input to an RTM model, has been out of scope of this study. This gap could be filled using the results obtained from other studies [e.g. (iv)]. Module A2 is devoted to a physical model implemented to compute the forward path (i.e. natural path) of the signal up to the observer. The model is actually an improved version of an existing model called Comanche, which was developed by ONERA in order to deal with a flat target of a given size surrounded by an homogeneous flat background. This new version has been developed to fulfill SPECTRA simulator requirements and is able to deal with a flat heterogeneous ground surface and directional effects.

Comanche, in its "2D" version, is based on the MODTRAN radiative transfer code and operates from the visible to the thermal infrared spectral domain (0.4 – 14 µm). It is able to produce sensor level radiances with proper environment effects consideration. These effects are modeled using specific Monte Carlo modules producing the typical environment functions. In addition, Comanche can consider directional effects of reflectance and emissivity of the ground surface.

ATMOSPHERIC CORRECTION AND SPECTRA LEVEL 2 PRODUCTS (MODULES C2 AND C1)

The downward path (from the SPECTRA instrument to the Top of Canopy) is dealt with by the "Cochise" Model. Cochise is the reciprocal modelization of the calculations performed by Comanche, which is used for the direct upward path. It is able to retrieve the ground spectral reflectance from sensor level hyperspectral radiances. Cochise does not yet completely fulfill the SPECTRA requirements (automatic atmosphere characterization and temperature retrieval from thermal infrared measurements), but still allows to validate the global simulator concept. Similarly to Comanche, Cochise computes atmospheric coefficients with MODTRAN and environment functions using specific Monte Carlo modules. The ground reflectances, currently assumed lambertian, are retrieved using an iterative method: the first step is performed by simply reversing the direct analytical model, considering for each sensor pixel that the ground is homogeneous; for all next steps, the results of the previous one are used to compute the environment components. Total water vapour contents may also be retrieved if adequate spectral bands are available (typically around 940 or 1013 nm). In the final report of this study (iii), a validation of both Comanche and Cochise is presented, using both simulated and measured datasets.

The second part of the inversion deals with the SPECTRA level 2 products. The final study report (iii) presents the ATDBs (Algorithm Theoretical Basis Documents) of several bio-physical variables including LAI, leaf chlorophyll, fAPAR, fractional cover, soil and foliage temperatures using SPECTRA multi-spectral and multi-angular radiance measurements.

The architecture of terrestrial vegetation and the biochemical composition of canopy elements, as described by the key variables listed above, are known to determine an information-rich radiance field in the optical (visible, near-and mid-infrared) as well as thermal infrared region of the spectrum. Some of the geophysical variables of interest, such as radiative fluxes or surface albedo,
correspond to integral quantities; they can be estimated directly from the radiation measurements, provided a sufficient number of representative observations are acquired. All other biophysical variables are derived from a further detailed analysis of the spectral and directional signatures of the observed radiance fields. Models provide a link between the radiometric data and the variables and processes controlling the spectral and directional observations. Various techniques have been developed to carry out model inversion to provide accurate estimation of canopy biophysical variables from radiance measurements. Our algorithms are based on model inversion by optimization, Look-Up Table (LUT) search, and Artificial Neural Network (ANN), and their interfaces to the SPECTRA end-to-end simulator.

For the estimation of LAI, leaf chlorophyll, fAPAR and fractional cover, a LUT method using multi-spectral and multi-angular reflectance measurements at top of canopy was developed. For each of the four biophysical variables considered, less than six directions are required. The number and combinations of directions of measurements resulted to be variable-dependent.

Soil and foliage temperatures can be retrieved from directional measurements of exitance, provided that the fractional cover of vegetation is known at all view angles. The algorithm was evaluated using TOC measurements of directional brightness temperature and of component temperatures. At moderate LAI level, i.e. LAI = 1.5, the retrieved soil and foliage temperatures have good agreement with the measured ones, with RMSE 1.1 K for soil temperature and 1.4 K for foliage temperature. At higher LAI level (LAI=2.5), less accurate estimates have been obtained with RMSE 1.9K for soil temperature and 2.0 K for foliage temperature.

SPECTRA FIELD SEGMENT (MODULE D)

We propose to realize Module D (the field segment) of the SPECTRA simulator in the form of a data-base which will provide a link not only between the SPECTRA field sites and the simulator, but also takes the associated Regional Models (e.g. assimilation) and Global Models (e.g. carbon flux) into account. Since all of these elements of the SPECTRA mission are expected to evolve in the future, and new elements might be added, the focus of this proposed SPECTRA field segment database (SFSDB) is on flexibility.

Users of the SFSDB include field site investigators, SPECTRA end-to-end simulator users, as well as developers of regional and global models that rely on data from SPECTRA and its associated field sites.

The final report (iii) also gives an overview of existing Global Carbon Flux Models and recommends the Ecosystem Demography (ED) model to be used with SPECTRA products in order to reduce the uncertainties of carbon pool size estimation.

The input requirements of the Global Carbon Flux Models and of the SPECTRA simulator have been checked against the list of variables provided by FLUXNET, which is currently taken as standard for the SPECTRA field sites. The comparison yields some important variables which are not covered by FLUXNET. We also propose a minimal list of metadata that should be included along with the data to be stored in the SFSDB, the usage of HDF5 as standard format, minimal requirements for the user interface, as well as data quality, integrity and security requirements.

As most likely path towards the realization of the SFSDB, we envisage a step-wise, evolutionary merging of the capabilities and data contents of the Oak Ridge National Laboratory Distributed Active Archive Center (ORNL DAAC), which contains the FLUXNET data, and the extended ESA Campaign Database (CDB) at NILU.

A limited validation of the SFSDB concept has been performed within the context of the validation of the SPECTRA Simulator Architecture using Barrax data (see below).

Finally, the study report (iii) lists some psychological and political problems, such as data policy, fear of data misuse, benefits for researchers who are asked to upload but have not much interest in downloading, and so on. Some of these issues might become highly important and we recom-
mend to collect the opinions of potential SFSDB users well before the realization of such a database. In our report, we therefore also propose a questionnaire serving this purpose.

Figure 3: Schematic overview of the SPECTRA Field Segment Database and its interfaces

VALIDATION OF THE SIMULATOR

The role of the final task of this study was to check that the overall architecture of the simulator is compatible with the requirements and that all the modules that compose the simulator perform correctly.

A synthetic image derived from a Daedalus image over Barrax, as shown in Figure 4, has been used as input for a test calculation through Comanche, Module B and Cochise. Each surface type has been provided with realistic BRDF and emissivity as observed during the DAISEX campaigns.

The end-to-end simulator has undergone a full run to test its robustness. All modules have behaved well demonstrating the correctness of the data flow design and the simulator design.

Modules A2 and C2 are based on well-known algorithms and procedures, because they are based on the MODTRAN code and simulation tools already used in other studies. Then, the validation has been focused on Module B (the instrument simulator) and the links between Module A to Module B, Module B to Module C and mutual consistency between Modules A and C.

Module B is the most specific for the mission, as it is where all the characteristics of the sensor and the platform are implemented. The validation process has focused primarily in testing the performance and consistency of this module. The validation of Module B has dealt with three aspects: testing on realistic results, determining how close the output of the simulation is to real world val-
ues (e.g. radiance levels, angular effects); testing the compliance with SPECTRA system requirements (e.g. noise levels, focal planes alignment); and testing that all the steps to get from L1a to L1c products are consistent with the definitions.

The overall performance of Module B is satisfactory, accomplishing the requirements. Only two aspects need revision: first, the selection of programmable observation angles is not specifically optimised to have an acquisition in the solar principal plane, which is the most relevant in BRDF studies. Second, the georectification of L1c products achieves a subpixel accurate registration between VNIR and SWIR bands, but TIR bands are displaced up to 2.5 pixels at the larger observation zenith angles. In any case, the good results found in the validation are very encouraging and probe the simulator to be very useful in mission planning and design.

Figure 4: Original Daedalus image on the left, resulting synthetic image with five surface types: alfalfa (green), wheat (blue), light soil (yellow), fair soil (orange) and dark soil (brown). This image was used for the simulator validation.

References

i  SPECTRA - Reports for mission selection - The Six Candidate Earth Explorer Missions - Technical and Programmatic Annex, ESA-ESTEC, April 2004

ii  SPECTRA - Reports for mission selection - The Six Candidate Earth Explorer Missions, ESA-ESTEC, April 2004
