ARTMO: AN AUTOMATED RADIATIVE TRANSFER MODELS OPERATOR TOOLBOX FOR AUTOMATED RETRIEVAL OF BIOPHYSICAL PARAMETERS THROUGH MODEL INVERSION

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ABSTRACT:

The here presented Automated Radiative Transfer Models Operator (ARTMO) Graphic User Interface (GUI) software package provides a seamless link between inputs and outputs required for running a suite of reflectance models both at the leaf level and at the canopy level. ARTMO facilitates consistent and intuitive user interaction, thereby streamlining model setup, running, storing and output plotting for any kind of optical sensor operating in the VNIR range. The toolbox, developed in Matlab, allows the user: *i*) to choose between various leaf-level and canopy-level RT models, *ii*) to choose between spectral band settings of various air- and spaceborne sensors or defining own sensor settings, *iii*) to simulate and store a massive amount of spectra based on a look up table (LUT) approach in a spectral database, *iv*) to plot simulated spectra of multiple models and compare with measured spectra, and finally, *v*) given several cost options and accuracy estimates, to run model inversion against airborne or spaceborne images. Moreover, ARTMO is able simulate and run inversions per land cover classes. As such fragmented landscapes can be more realistic handled: homogenous land covers (e.g. agricultural land) can be simulated with a 1D model, while heterogeneous surfaces (e.g. forest) can be simulated with a 3D model. Examples of all relevant modules and an inversion application are provided.

1. INTRODUCTION

Radiative transfer (RT) modeling plays a key role for earth observation (EO) because it is needed to design EO instruments and to develop and test inversion algorithms. In the scientific community a number of often highly specialized leaf and canopy RT models has been developed over the last three decades, each of which emanates from a different set of original requirements. During the development of RT models a tradeoff has to be made between the invertibility and accuracy of the model, leading to large diversity of models with varying degrees in complexity. It led to that a whole spectrum of reflectance models have been published, ranging from 4-parameter turbid medium models until the rendering of complicated 3D scenes where each single element can be controlled.

While a wide range of models have been published, in reality not all of them are easily available. Often a model is kept within a research group, or is not available for free. On the other hand, some models are freely distributed throughout the community, thereby becoming a benchmark in EO research (e.g. the SAIL model). Over the past, efforts have been undertaken in evaluating a wide range of models in the RAdiation transfer Model Intercomparison (RAMI) exercises (Pinty, et al., 2001), but no facilities are currently available that bring all these models together in an accessible toolbox. One undertaken initiative in this direction is the so-called RAMI On-line model checker (ROMC) (Widlowski et al., 2008) which allows the user to evaluate the performance of a newly developed canopy reflectance model against a set of reference data obtained from RT models that, in turn, were identified during the 3rd phase of the RAMI exercise. Although ROMC provides a benchmark for developers of new models, however, the majority of the community does not develop new models but instead uses models that already have proven their functionality.

A common practice is opting for the model that is in-house available, regardless of evaluating whether the used model is best prepared for correctly representing the area of study. For instance, literature reveals that the well-known and freely available turbid medium model SAIL, designed for simulating homogeneous plant surfaces (e.g. agricultural fields) is often applied in inversion exercises of forests (e.g. Gond et al., 1999; Soudani et al., 2000; Zang et al., 2005, 2006; le Maire et al., 2008). Nevertheless, SAIL does not simulate 3D structures of trees and associated shadowing. Hence, when applying SAIL to forests the risk of oversimplifying the RT processes is introduced and so increasing the likelihood of propagating errors in the inversion.

Along with the absence of having several models accessible in one toolbox, another faced inadequacy is that currently no standardized model inversion procedure is offered in a software package. While in the scientific literature many inversion strategies have been proposed, though when it comes to mapping applications often the same sequence of steps is

undertaken. It would therefore be of interest to bring these steps together in a toolbox so that model inversion can be streamlined. Given the above, it underlines the need for developing a toolbox that: i) brings a wide range of leaf-level and canopy-level models together, ii) is plug-n-play and simply usable, iii) allows easy comparison and evaluation of different models, iv) streamlines model inversion to retrieve biophysical parameters, and v) is freely available.

There have been a few earlier attempts undertaken in building modules that automate model inversion. An example in this respect is CRASh (Dorigo et al., 2009), which was designed for the concurrent retrieval of biophysical parameters from high resolution EO data. CRASh is based on the inversion of the combined PROSPECT+SAILh RT model and explores the benefits of combining semi-empirical and physically-based approaches. Although CRASh only includes one leaf-level and one canopy-level model, an interesting feature of this module is that the inversion takes place class-based, thereby allowing configuring the model depending on the specific land cover. The fundamentals of CRASh inspired to develop a toolbox that includes various leaf-level and canopy-levels models and allows class-based model inversion.

This paper provides a description of a Graphic User Interface (GUI) toolbox for automated leaf and canopy model reflectance data generation and inversion against actual spectral observations from air- or space-crafts. This toolbox hereafter referred to as Automated Radiative Transfer Models Operator (ARTMO), can facilitate the testing of various remote-sensing detection scenarios for future airborne and spaceborne optical and fluorescence missions. ARTMO (V1.0) is developed in Matlab in interaction with MySQL to run under Microsoft Windows operating system. In the following sections the main modules of ARTMO will be explained, being: i) the main module, ii) module with the leaf-level models, iii) graphic module, and finally, iv) the inversion module.

2. MAIN MODULE

ARTMO's main module can be seen in figure 1a. All ARTMO's functionalities are started by entries in this window. It controls all data processing modules, and enables the running of a leaf model or a canopy model independently, or both linked together. Most important functions of the main module are (*i*) the leaf-level models, (*ii*) the canopy-levels models, (*iii*) the run panel, (*iv*) the 'sensor' module (*v*) the 'graphics' module, and (*vi*) the 'inversion' module.

In the top panel it provides the entries where a new project can be initiated or an existing one loaded. A new project can be created by providing a new name, and additionally a comment can be provided, such as a project description (e.g. 'Barrax 2011'). By scrolling down the sensor list, the user can select the band settings of a list of predefined sensors (e.g. 5 different CHRIS modes, Sentinel-2). Alternatively, the user can also define its own sensor configurations. This is arranged within the 'sensor' module. In this module (figure 1b) any kind of band settings can be configured. This can be done either manually, e.g. by providing for each band the min, max, center and bandwidth (in fact center and bandwidth already suffice). Or it can be done by loading in band settings, e.g. via a spectral filter file, or via an ENVI header file. By loading a header file ARTMO reads in information on band center and bandwidth of the associated imagery. As such a quick and convenient way is provided to set the spectral settings for any kind of sensor. When saved, these spectral settings automatically appear in the sensor list of the main module. All input and subsequently output spectral data are directly resampled according to the selected sensor. Hence, because ARTMO takes care of the spectral resampling it implies that the user can enter any kind of spectra.

Another important button within ARTMO's main menu is the 'Settings' button (figure 1c). Its associated window controls the paths towards the included models. It is important to note that the models itself were not touched. Essentially, all GUIs were programmed as a wrapper around the models, thereby keeping the flexibility that current model versions can be simply replaced, e.g. by newer ones. Further, the settings for accessing the MySQL DB are also controlled here.



Figure 1a: ARTMO's main module (left), 1b: sensor configuration module (middle), 1c: control settings module (right).

Once having a project and sensor either created or selected, the following step is to decide whether a project should exist of classes or not. A class is basically nothing more than creating a lower level project and can hold any configuration (e.g. with respect to a land cover class, a specific sun-target-sensor geometry, another test). Its advantage lies in adding another level of hierarchical grouping and, above all, it allows class-based model inversion in the 'inversion' module (c.f. 'inversion' module). Classes can be either manually defined, i.e. by providing the number of classes and class names, or can be automatically defined, i.e. by reading in an ENVI header file of a classified image. When having multiple classes introduced, the user will be invited assigning model configurations for each class.

With the introduction of classes ARTMO's data structure is hierarchically organized at three levels. At main level there is the initially defined database. A database can exist of as many projects, with new projects created though ARTMO's main module. Finally, a project can exist of as many classes. An existing class can be anytime deleted while a new class can be anytime created. The hierarchic data structure is schematically exemplified in figure 2a. This hierarchy is also reflected in ARTMO's 'project overview' window. This window appears when clicking on the 'Load project' button at the left top in ARTMO's main module. This window provides an overview of all metadata of all projects (see figure 2b). A database can be chosen within the 'change DB' button. All projects of a DB are shown in the top tabular panel of the GUI window. For each class the following information is provided: i) ID, ii) name, iii) the date of creation, iv) included sensor, v) number of bands, vi) number of classes and, vii) total number of simulations. A project is loaded into the main module by selecting a project and then clicking on the 'Ok' button. Further, by clicking on a project, information of its included classes will appear in the middle tabular panel. For each class the following information is provided: i) ID, ii) project ID, iii) date of creation, iv) included models, v) class name, and vi) number of simulations. Note hereby that the date of class creation does not have to be the same as the date of project creation. Any time a new class can be added to a project. Finally, by clicking on a class all input configuration data appears into two down panels, one for leaf models (left) and one for canopy models (right). By scrolling down one of those provided lists all model input data is provided, including all ranges with its min, max and step.



Figure 2a: ARTMO's hierarchical data storing organization (left), 2b: ARTMO's data overview module (middle), 2c: ARTMO's flow chart (right).

An overview of ARTMO's functionality is schematically displayed in the flow chart of figure 2c. In short, once having either one (leaf or canopy) or two (leaf and canopy) models configured they can be run by clicking on the 'run' button in ARTMO's main module. The models start with the simulations by looping over the generated LUT's, thereby automatically updating the required input data. Each simulation is immediately stored into an underlying spectral database while keeping a link with its associated metadata. The database was implemented on a MySQL Version 5 database server. The advantage of having the spectra stored in a relational database with associated metadata files is that these data can any time be invoked flawlessly by the 'graphics' or 'inversion' modules.

Apart from 'Load Project', other functionalities in the top Menu bar are found within 'DB Administration' wherein the user has the possibility: i) to delete a class, a project or an entire DB, ii) to import a DB created by an ARTMO version on another pc, iii) to export the current DB to a text files so that it can be imported by another ARTMO version, and iv) the possibility to change the DB. When a DB is imported, it is automatically considered as a new DB and being the current working DB.

Finally, in ARTMO's main module, a button is provided to save all inputted data during a current session. Another button reloads earlier saved settings. The leaf and canopy models, graphics and inversion module will be described in detail in the following sections.

3. LEAF- LEVEL MODELS

ARTMO's 'leaf models' module currently consists of a suite of models from the PROSPECT family. The following models have been implemented: PROSPECT 4 (Feret et al., 2008), PROSPECT 5 (Feret et al., 2008) and the recently published FluorMODleaf (Pedrós et al., 2010), which is an extension of PROSPECT and also includes fluorescence emission. When selecting on one of these models, a window will appear where the model input parameters can be filled in (e.g. see figure 3a). Any model follows the same logic of reading in input data. There are three ways to read input data. First, the user can simply provide one single value in the active parameter box, which is the most straightforward way. Second, the user can also activate the range icon that enables to provide a starting and ending value, and a step. As such a range of simulations are initiated. Any parameter can be turned into a range and any range can be combined with other ranges. By adding ranges, internally all possible combinations will be calculated in a so-called look-up table (LUT). Third, within the top-left 'file' button, the user is also provided the possibility to load in its own values (figure 3.b). A new GUI will then appear that allows the user to read in a text file and then select a column and attach it to the desired model parameter (figure 3.c). With this, multiple parameters can be assigned to user-defined input data. This parameter is subsequently disabled in the model window but any combination with other activated ranges is possible. Again, a LUT of all possible combinations is internally generated.

Further, it is also worth mentioning that within the top-left 'file' button the inputted model settings can be saved or reloaded. Another inbuilt feature is that when an impossible value is inputted, the active text block will turn yellow (e.g. see figure 3.a). As such the user is invited to change the given value to a more realistic input.

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✓ Range Start: -20 End: 45 Step: 0.5	Leaf Structure (N) [1-4]	FluorMODieaf data table
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Dry matter (Cm - g/cm ²) [0-0.05]	Range	Column Convert Pact. Column Convert Pact. Column 1 1
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Figure 3a: PROSPECT 5 input window (left), 3b: PROSPECT 4 input window (middle), 3c: control settings module (right).

4. CANOPY-LEVEL MODELS

ARTMO's 'canopy models' module consists currently of a suite of leaf-level models from the SAIL family and a ray tracing model, FLIGHT. The following SAIL models are included: 4SAIL (Jacquemoud et al., 2009), FluoSAIL (Verhoef, 2005) and then the combined soil-leaf-canopy SLC model (Verhoef & Bach, 2007), which combines the Hapke soil model with PROSPECT and with 4SAIL2 (Verhoef & Bach, 2007).

Regarding FLIGHT, this model can either be configured in 1D or in 3D mode (see figure 4a). When the 3D mode is selected crown geo parameters are enabled such as: *i*) crown radius, *ii*) centre to top distance, *iii*) height to first branch, *iv*) max height, and, *v*) DBH. Apart from the input parameters, FLIGHT requires optical properties for green leaves, brown leaves, bark and soil. Optical properties of green leaf can either be inputted by the user, or if activated, can directly come from a leaf-level model. By clicking on the icon of the optical properties at the top left corner a GUI window appears where the user is invited to read in a text file with spectral data. This window also provides options to select the required column, to convert the data, and to discard header lines. Furthermore, once a spectrum is selected the icon will be boxed red.

Regarding the hybrid SLC model, 4 sub-modules need to be filled in: *i*) leaf, *ii*) canopy, *iii*) angular geometry, and *iv*) soil. For all sub-modules, the same input philosophy as for the other models has been implemented (single value, range or user-defined input). Once a sub-module is configured the associated button will switch green. Regarding the soil sub-module, a default soil file that consists of spectra of a wide range of soil types is provided, but any other file with soil spectra can be loaded. Having multiple soil spectra available, the flexibility is provided to activate each of them whereby they are automatically included within the loop (figure 4b).

With FluorSAIL TOC reflectance either with or without fluorescence emission can be generated. Other outputs options include solar irradiance and sky irradiance on ground. For more information about FluorSAIL outputs, see Zarco-Tejada et al. (2006).

When input values of a leaf or a canopy model are given, the model turns active in ARTMO's main menu. In its middle 'run' panel any activated model can be run or an activated leaf-level model can be combined with an activated canopy-

level model. As such, the leaf-level LUT will be coupled with the canopy-level LUT so that all possible leaf-canopy combinations will be simulated. Finally, by clicking on the 'run' button in the run panel the forward simulations will begin. Automatically, outputs from a leaf-level model required as inputs for a canopy-level model are internally updated. A process bar will appear that keeps track of the number of simulated spectra and estimated process time.



Figure 4a: FLIGHT input window (left), 4b: soil input window for the SLC model (right).

5. GRAPHICS MODULE

By clicking on ARTMO's 'graphics' button, a new module appears where the user has the possibility to visualize their simulations within the same plotting window, such as all spectra of a class (figure 5a). Within the appeared graphics module a first step to do is selecting a class for visualizing its containing spectra. By clicking on 'Select Project' the same overview window appears where any kind of project and class can be selected. When a class is selected those parameters that consist of more than one value (i.e. range) are shown in graphics module. Automatically the parameters are organized according to the leaf parameters and canopy parameters. Within the tabular parameter window the following information is provided for each parameter: *i*) minimum, *ii*) maximum, *iii*) total number of simulations, and *iv*) an option to add a step. The latter allows the user to select each other simulation in the plotting. Another way to realize a sub-selection is on clicking within the row of a parameter. A slider window will pop up that gives the user the possibility to narrow down the simulations by increasing the minimum or decreasing the maximum value of its range (figure 5b).

Two plotting windows are provided, both at leaf level and at canopy level. It was decided to provide two plotting windows because some models provide next to reflectance (or transmittance) additional output such as fluorescence emission. At leaf level, the option is provided to plot reflectance or transmittance within the first plotting window. At canopy level, different types or TOC reflectance can be plotted depending on the model, e.g. hemispherical reflectance or directional reflectance (SLC model) within the first plotting window. In case of FluorSAIL additional fluorescence radiance on ground level can be visualized in the second plotting window.



Figure 5a: ARTMO's graphics module (left), 5b: sliders for invoking parameter-based sub-selection of a spectral class (right).

When a selection of the spectra is made, it can be added to the plotting windows by clicking on the 'Add' button. The selected class will appear in the down panel where added spectra can be visualized. In this panel the following information about the parameter can be consulted: *i*) its boundaries, *ii*) class name, *iii*) the number of included simulations and, *iv*) the preferred color. Moreover, this panel provides the option to include or exclude this class in the plotting window by activating or deactivating it. An interesting feature hereby is that as many classes can be added to the same plotting window, even from different projects, each of them with their own sub-selections. As such the graphics module provides all the tools to the user for enabling easy comparison of different simulation scenarios (e.g. simulations of one model against simulations of another model).

There have been two color options programmed on how to visualize the simulated spectra. A parameter can be either assigned to color hue or to color saturation. When two different parameters are assigned to hue and saturation then the effects of both parameters can be visualized within the same plot. An example of this two-parameter combination is provided in figure 6a. Alternatively, when only one parameter is assigned to color hue then any color tone can be chosen by the user itself. This can be useful, especially when combining spectra from different classes, e.g. for comparison the performance of different models. An example of a plotting window with different spectral groups is provided in figure 6b.



Figure 6a: plotting window with 2 parameters assigned to hue and saturation (left), 6b: plotting window with the same parameter of 2 classes assigned to different colors (right).

Also the possibility to add external spectral data (e.g. from a field spectrometer or from observations from air- or spacecrafts) is provided for sake of comparison. This option is provided via the 'Add Signature' option. A window will appear to read in a text file and several conversion and drawing options are available. Another important feature is that the graphics module enables to export the selected simulations to a text file for further use. We felt that the graphic module is the most convenient module for exporting data because here the user can visualize the simulations and judge on its quality. Exporting data is possible by right-clicking on an added class module. A browser window will appear where the path and filename can be chosen. Two text files will be created. One file consists of the data itself. It is organized as a 2D matrix so that the data can be easily read by other software packages for further processing. The second file consists of all meta-data, which not only includes explanation of the row and columns, but also includes all model input data.

6. INVERSION MODULE

ARTMO's 'inversion' module is probably the most exciting module of the toolbox (figure 7a). This module handles the inversion of multispectral or hyperspectral imagery into biophysical products by matching the simulated spectra against actual spectra with a cost function. Two input types are required here. On one hand it needs actual spectral observations, e.g. an imagery from an air- or spacecraft, while on the other hand it needs the earlier generated simulations. The latter is available in the spectral DB and can be loaded into the module in the same way as in the graphics module. By clicking on the 'Select Project' module the same overview window as in 'graphics' appears where projects and classes can be selected. Again, those parameters that contain more than one value will appear in the tabular panels, both at leaf and canopy level. Also here, a slider bar will appear when clicking on a parameter so that the included simulations can be narrowed down.

In case a single class is selected then inversion will take place only against that class, however in case a project is selected then all included classes are possible for class-based model inversion. Class-based model inversion signifies that model inversion per pixel takes into account class-specific information. This is made possible when the user loads an additional land cover class map. If this land cover map originates from ENVI then the associated header file will be read. A new window will appear where the user can link the land cover classes with the simulation classes (figure 7b). As such each land cover class is linked with a class of simulations with own configurations. The user can choose either employing inversion of all classes or one single class. Similarly, the user can choose which model parameter to be inverted, both at leaf and canopy level, or select concurrent retrieval of all parameters. A progress bar will appear that keeps track on the performed inverted pixels and estimated time per land cover class (figure 7c). Until now only one cost function is included to search for matching simulated spectra against an actual observation, being root mean square error (RMSE), but efforts are underway to implement more cost functions. By searching pixel-wise for the minimum RMSE against all selected simulations, its associated parameters are returned for mapping. Several options are provided to optimize this cost function. Instead of using absolute spectra the user can select its derivative whereupon inversion will be applied on. Further, the option is provided to add a percentage of white noise. Another common practice in model inversion is not to take the single lowest RMSE but a percentage of best matches. Here, the mean or the median can be chosen. Also the SD of the associated mean can be mapped, as well the minimum RMSE as a spatial indicator of the inversion performance. When the inversion is done the map will appear, whereby the user has the ability to save the generated maps for further use, e.g. in ENVI.



Figure 7a: ARTMO's inversion module (left), 7b: soil input window for the SLC model (right), 7c: inversion progress bar (top right).

7. APPLICATION

With ARTMO the possibility is provided that homogenous land cover types such as agricultural field can be inverted against simulations from 1D models (e.g. SAIL), while heterogeneous land cover types such as forest can be inverted against simulation from 3D models. An example of class-based retrievals is provided in figure 7. The study site is the floodplain 'Millingerwaard' (51° 84' N, 5° 99' E) along the river Waal, which is the main branch of the river Rhine in the Netherlands. Prior to vegetation density retrieval in canopies comprised of a heterogeneous mix of vegetation types, these vegetation types need to be identified so that the RT model can be parameterized accordingly. To do so, by using maximum likelihood classification and ground truth data a map was created that included eight major land cover classes (figure 8a). The vegetated classes consisted of 'bare and pioneer communities'; 'grasses and herbaceous vegetation'; 'herbaceous and low woody vegetation'; 'shrubs'; and 'forest'. In fact, such a patchy heterogeneous landscape, with fragments of homogenous agricultural lands next to heterogeneous semi-natural areas such as forest is common throughout the world. Thanks to ARTMO's class-based simulations a more realistic representation of reality can be achieved when inverting the models. Here inversion was done for retrieving leaf area index (LAI). Pixels assigned to 'grasslands' and 'shrubs' were simulated and inverted with 4SAIL, while pixels assigned to 'forest' were simulated and inverted with FLIGHT. ARTMO provides also associated minimal RMSE maps to give the user an idea about the performance of the retrieval. Overall, apart from a few agricultural lands with poor performances, the inversion performance occurred in the same order of magnitude throughout the different classes.



Figure 8a: Land cover map (left), 8b: LAI inversion map (middle), 8c: associated minimum RMSE map (right).

8. CONCLUSIONS

The here presented ARTMO toolbox aims to implement all the necessary models and features required for terrestrial EO applications in a graphical user interface (GUI). The toolbox, developed in Matlab, allows the user:

- 1. to choose between various leaf-level and canopy-level RT models
- 2. to choose between spectral band settings of various sensors, or to define own band settings
- 3. to simulate a massive amount of spectra based on a look up table (LUT) approach and storing it in a spectral database
- 4. to plot simulated spectra of multiple models and compare it with measured spectra
- 5. to run model inversion against airborne or spaceborne images given land cover classes, several cost options and accuracy estimates.

Finally, it has to be noted that the toolbox presented here is still a beta version. We are currently working on testing its robustness with large hyperspectral datasets and its compatibility to other platforms. As soon as we feel sufficiently confident about its stability we will release information on a dedicated website on how to obtain ARTMO.

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