Using the ARTMO toolbox for automated retrieval of biophysical parameters through radiative transfer model inversion: Optimizing LUT-based inversion

J. Verrelst [a], J.P. Rivera [a], G. Leonenko [b], L. Alonso [a] & J. Moreno [a]

[a]: Image Processing Laboratory (IPL), University of Valencia, Spain
[b]: College of Science, Swansea University, Wales UK.

*Jochem Verrelst
Image Processing Laboratory
(http://ipl.uv.es)
Universitat de Valencia, Spain
Jochem.verrelst@uv.es

1. Introduction

ARTMO, an Automated Radiative Transfer Models Operator toolbox

Radiative transfer (RT) models play a key role in earth observation (EO). They are needed to design and develop EO instruments, and to test and apply inversion algorithms. In the scientific community a number of often highly specialized leaf and canopy RT models has been developed, each of which emanates from a different set of original requirements. ARTMO (Automated Radiative Transfer Models Operator) is the first toolbox that brings a variety of leaf and canopy RT models together in one GUI. Moreover, ARTMO encompasses essential tools for EO applications such as defining your own sensor, plotting and exporting outputs and automated LUT-based model inversion. With ARTMO, maps of biophysical parameters can be rapidly derived from EO data. As the toolbox is constantly under development new features are presented here.

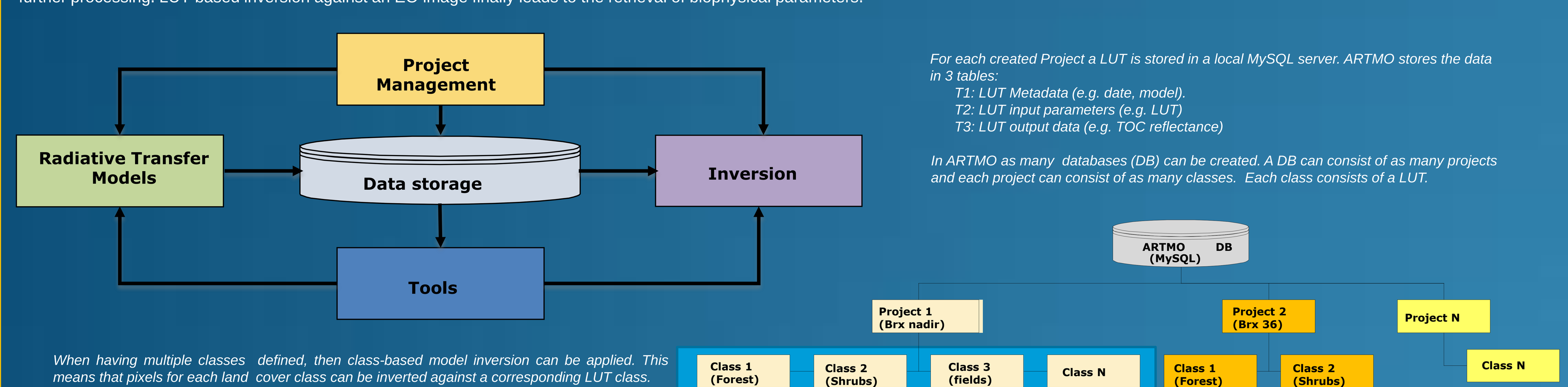
Objectives

The aim of this study was to expand ARTMO by offering new advanced functions for improved retrieval performances through model inversion. Specifically, the objective was to implement a new inversion module that provides a wide range of cost functions and regularization options.

A secondary objective was to test these cost functions and regularization options against a validation dataset (SPARC; Barrax, Spain) for the benefit of simultaneous mapping of multiple biophysical parameters over large areas.

2. Conceptual design

ARTMO is a toolbox written in Matlab that consists of a package of GUIs. ARTMO incorporates a variety of leaf and canopy radiative transfer models, which can be operated through the creation of' 'Projects'. Within a Project, Look Up Tables (LUT) can be created, which are then stored in a MySQL database (DB). These LUTs can then be called by various modules such as the Graphics module or the Inversion module for further processing. LUT-based inversion against an EO image finally leads to the retrieval of biophysical parameters.



For each created Project a LUT is stored in a local MySQL server. ARTMO stores the data in 3 tables:
T1: LUT Metadata (e.g. date, model).
T2: LUT input parameters (e.g. LUT)
T3: LUT output data (e.g. TOC reflectance)

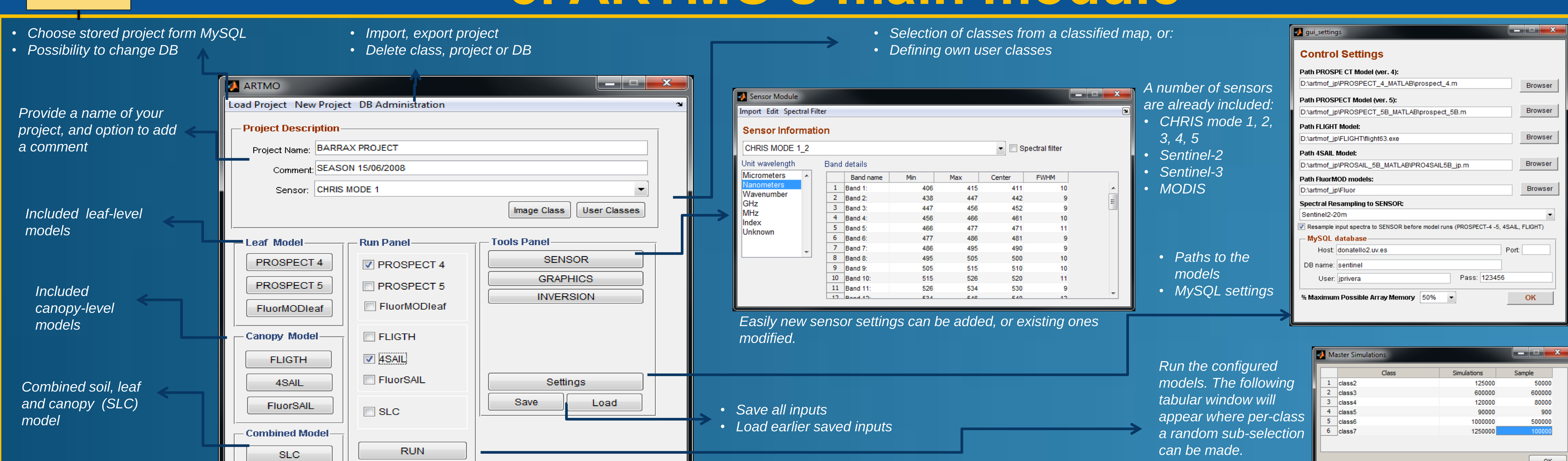
In ARTMO as many databases (DB) can be created. A DB can consist of as many projects and each project can consist of as many classes. Each class consists of a LUT.

When having multiple classes defined, then class-based model inversion can be applied. This means that pixels for each land cover class can be inverted against a corresponding LUT class.

3. ARTMO's main module

Project Management

- *Choose stored project form MySQL*
- *Possibility to change DB*
- *Import, export project*
- *Delete class, project or DB*
- *Selection of classes from a classified map, or:*
- *Defining own user classes*



Provide a name of your project, and option to add a comment

Included leaf-level models

Included canopy-level models

Combined soil, leaf and canopy (SLC) model

A number of sensors are already included:
- *CHRIS mode 1, 2, 3, 4, 5*
- *Sentinel-2*
- *Sentinel-3*
- *MODIS*

- *Paths to the models*
- *MySQL settings*

Easily new sensor settings can be added, or existing ones modified.

- *Save all inputs*
- *Load earlier saved inputs*

Run the configured models. The following tabular window will appear where per-class a random sub-selection can be made.

When selecting a sensor, all input data will be automatically resampled to the spectral settings of the selected sensor. This means that any type of spectra (e.g. from field spectrometer or from satellite observations) can be fed into the models (e.g. soil spectra). A warning message appears when ARTMO detects that spectral resampling is required. Any spectral settings can be defined by the user. This is helpful for simulations studies of new or upcoming sensors such as FLEX. Output data is then provided according to chosen sensor. By default spectral resampling will take place before running the models. In 'Settings' it can also be chosen to do the resampling after the simulations.

When a model has been configured it turns active in the 'Run Panel'. Any configured leaf model can be coupled with any configured canopy model. However note that FluorMODleaf needs to be coupled with FluorSAIL to simulate fluorescence emission at canopy level. When clicking on 'Run' then all combinations of the leaf and canopy LUTs will be simulated.

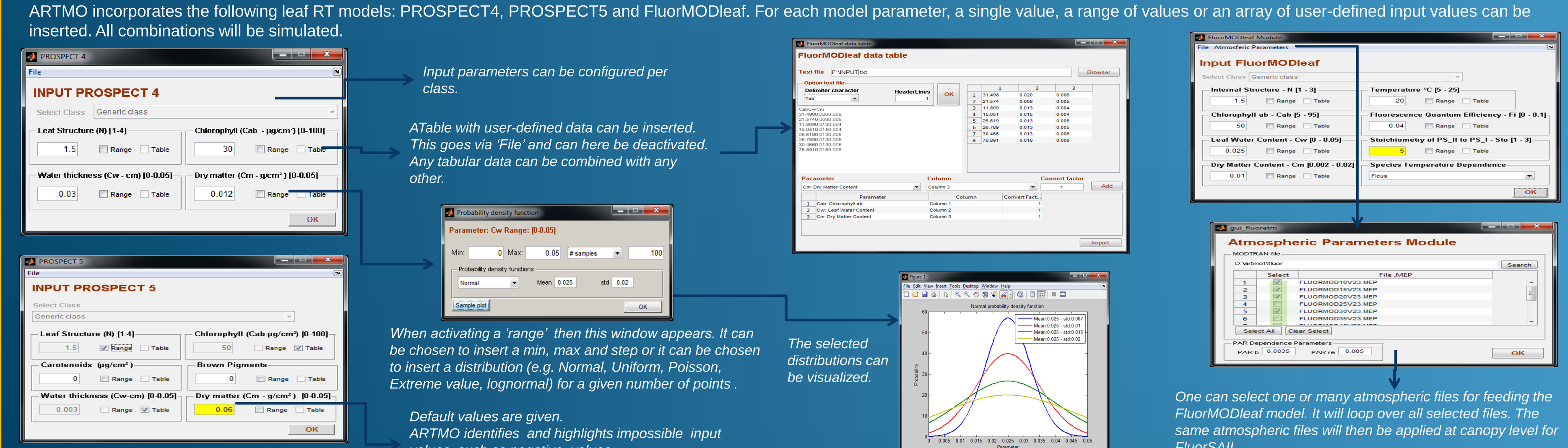
Input, output and meta data are directly stored in a MySQL data server.

On time-consuming tasks, such as forward simulations and inversion calculations, ARTMO provides progress bars of processing time and executed simulations or inverted pixels, respectively.

4. ARTMO's leaf-level models

Radiative Transfer Models

ARTMO incorporates the following leaf RT models: PROSPECT4, PROSPECT5 and FluorMODleaf. For each model parameter, a single value, a range of values or an array of user-defined input values can be inserted. All combinations will be simulated.



Input parameters can be configured per class.

ATable with user-defined data can be inserted. This goes via 'File' and can here be deactivated. Any tabular data can be combined with any other.

When activating a 'range' then this window appears. It can be chosen to insert a min, max and step or it can be chosen to insert a distribution (e.g. Normal, Uniform, Poisson, Extreme value, lognormal) for a given number of points.

The selected distributions can be visualized.

Default values are given. ARTMO identifies and highlights impossible input values, such as negative values.

One can select one or many atmospheric files for feeding the FluorMODleaf model. It will loop over all selected files. The same atmospheric files will then be applied at canopy level for FluorSAIL.

ARTMO can read in text files with model input values, e.g. coming from field measurements. Data in all kinds of formats can be read. Data columns can be linked to a corresponding parameter. Options to select the required column, to convert data, to skip header and to identify the delimiter character are provided. When a model parameter is being fed by data from this parameter is disabled in the main input window. This parameter can then be combined with inputs of the remaining parameters (single value, range or user-defined values).

Conclusions

ARTMO aims to implement essential models and modules required for terrestrial EO applications in a graphical user interface (GUI) toolbox. A new version (V2) is presented here. ARTMO allows the user:

I. To choose between various leaf and canopy RT models.
II. To choose between spectral band settings of various sensors, or to define own band settings.
III. To simulate a massive amount of spectra based on look up tables (LUT) and storing it in a relational database
IV. To plot simulated spectra of multiple models and compare it with measured spectra.
V. To evaluate over 60 different cost functions against a validation dataset.
VI. To run model inversion against airborne or spaceborne images given a chosen cost function, class-based LUTs, a best-evaluated cost function and accuracy estimates.

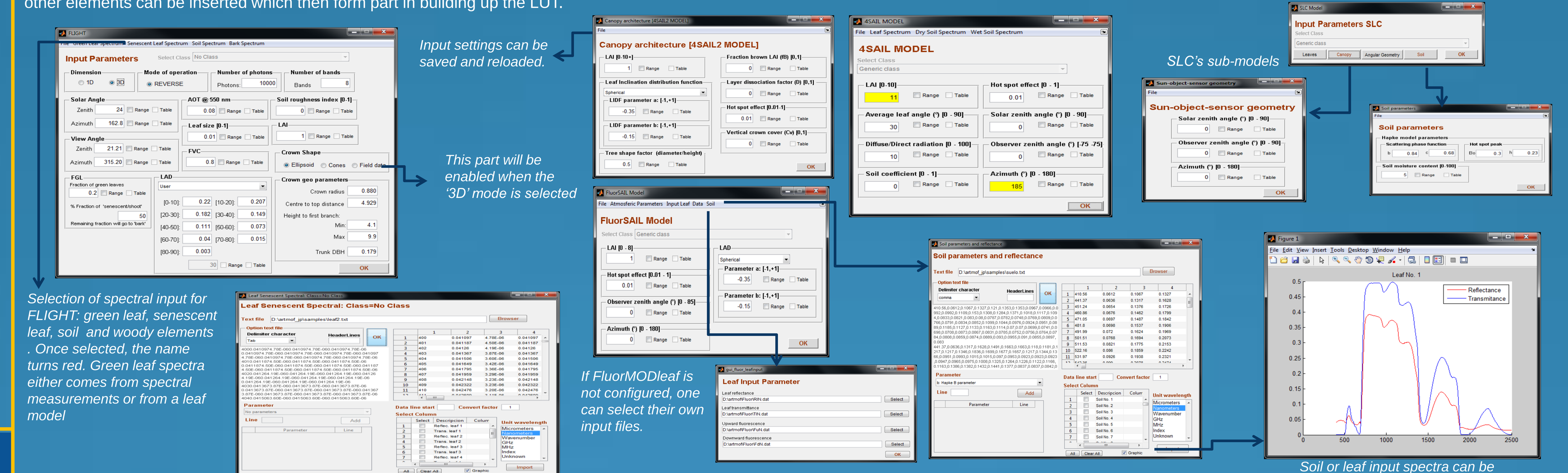
In this version (V2), the following new features have been implemented:
I. To all models, the otpion to insert input distributions (e.g., Gaussian, uniform, Poisson) next to stepwise ranges.
II. The ability to select a random sub-selection from all possible configured combinations.

The widely used RMSE was not evaluated as best performing cost function in LUT-based inversion when using the SPARC dataset (Barrax, Spain). Also opting for a single best solution appeared to be suboptimal. Alternative cost functions such as 'Power diverence measure', 'Logistic distribution Trigonometric' and 'K(x)=-log(x)+x' performed more robust. Taking the average of multiple best solutions in combination with added noise further improved the retrievals.

5. ARTMO's canopy-level models

Radiative Transfer Models

ARTMO incorporates the following canopy models: 4SAIL, FluorSAIL, FLIGHT and then the combined soil-leaf-canopy (SLC) model. Similar to the leaf models, for each parameter a single value, a range or distribution, or a text file with user-defined values can be inserted.
Further, in contrary to leaf models, canopy models need spectral inputs for their elements such as leafs, soil, bark and senescent leaves. Therefore, for each model spectral data can be inserted by clicking on the associated name in the top bar. An input window will appear. When also a leaf model has been configured then those simulated spectra will be used as leaf spectral input into the canopy model. Multiple spectra of other elements can be inserted which then form part in building up the LUT.



Input settings can be saved and reloaded.

This part will be enabled when the '3D' mode is selected

SLC's sub-models

Selection of spectral input for FLIGHT: green leaf, senescent leaf, soil and woody elements. Once selected, the name turns red. Green leaf spectra either comes from spectral measurements or from a leaf model

If FluorMODleaf is not configured, one can select their own input files.

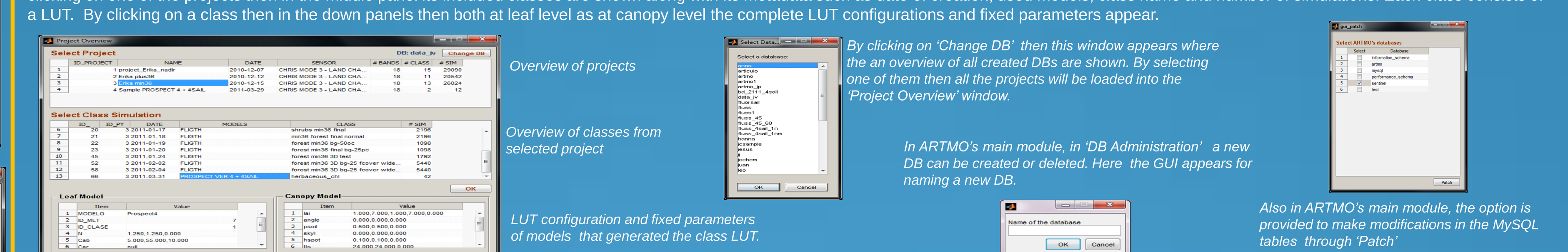
Soil or leaf input spectra can be visualized when selecting them.

One or various spectra can be selected as input in the canopy models. Any text file with columnar spectra can be read. Header lines can be removed and spectra can be converted to other units. Also different wavelength units can be chosen. The selected spectra can also be visualized by enabling the 'Graphics' button. As such it can be quickly viewed whether the right spectra is imported.

6. LUT access and metadata

Data storage

In ARTMO´s 'Project Overview' window an overview of all created projects and classes within the current DB are displayed. This 'Project Overview' can be accessed from ARTMO´s main module (click on 'Load Project') or via the 'Graphics' or 'Inversion' modules. The top panel shows all Projects from the current DB along with its metadata such as date of creation, sensor, number of bands, classes and simulations. By clicking on one of the projects then in the middle panel its included classes are shown along with its metadata such as date of creation, used models, class name and number of simulations. Each class consists of a LUT. By clicking on a class then in the down panels then both at leaf level as at canopy level the complete LUT configurations and fixed parameters appear.



Overview of projects

Overview of classes from selected project

LUT configuration and fixed parameters of models that generated the class LUT.

By clicking on 'Change DB' then this window appears where the an overview of all created DBs are shown. By selecting one of them then all the projects will be loaded into the 'Project Overview' window.

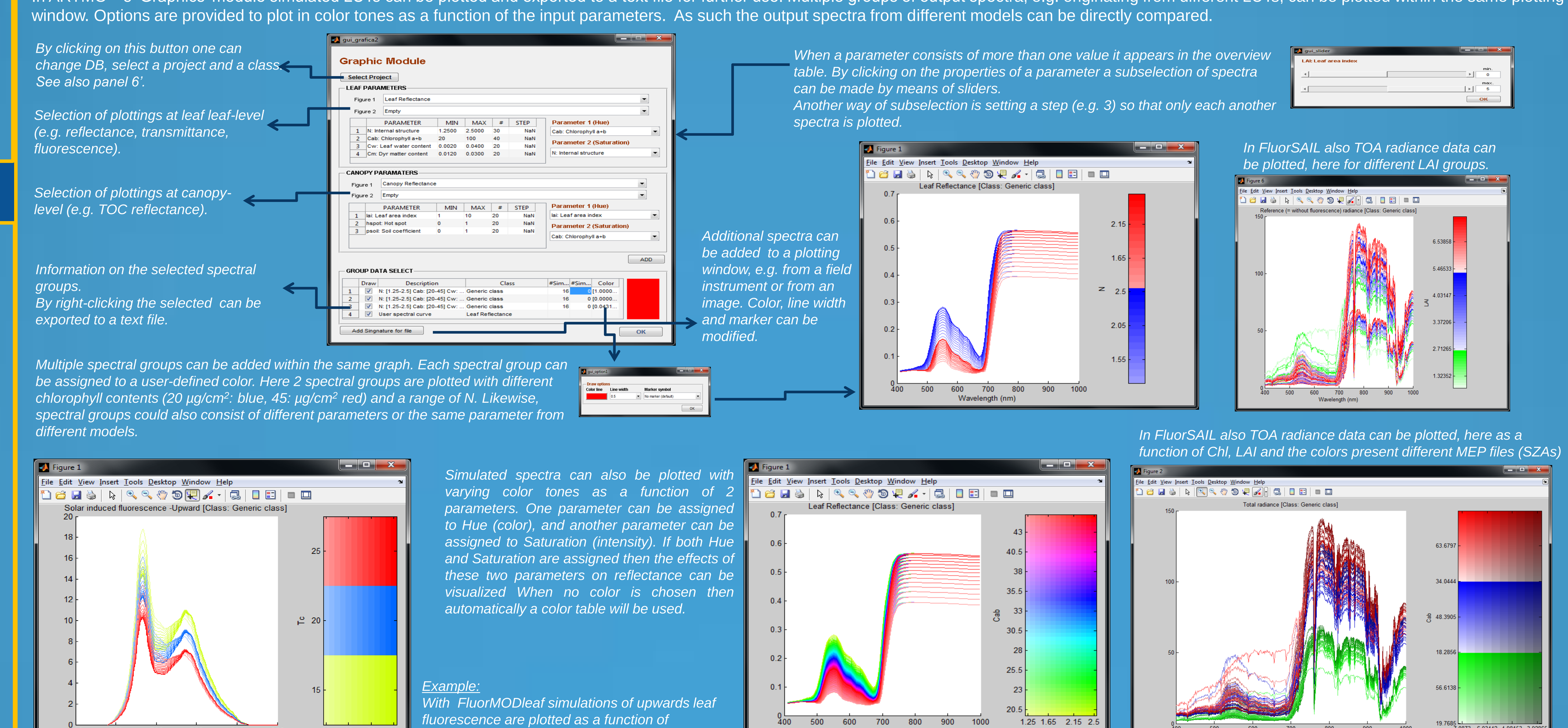
In ARTMO's main module, in 'DB Administration' a new DB can be created or deleted. Here the GUI appears for naming a new DB.

Also in ARTMO's main module, the option is provided to make modifications in the MySQL tables through 'Patch'

7. ARTMO's graphics module

Tools

In ARTMO´s 'Graphics' module simulated LUTs can be plotted and exported to a text file for further use. Multiple groups of output spectra, e.g. originating from different LUTs, can be plotted within the same plotting window. Options are provided to plot in color tones as a function of the input parameters. As such the output spectra from different models can be directly compared.



By clicking on this button one can change DB, select a project and a class. See also panel 6'.

Selection of plottings at leaf leaf-level (e.g. reflectance, transmittance, fluorescence).

Selection of plottings at canopy-level (e.g. TOC reflectance).

Information on the selected spectral groups. By right-clicking the selected can be exported to a text file.

When a parameter consists of more than one value it appears in the overview table. By clicking on the properties of a parameter a subselection of spectra can be made by means of sliders. Another way of subselection is setting a step (e.g. 3) so that only each another spectra is plotted.

In FluorSAIL also TOA radiance data can be plotted, here for different LAI groups.

Additional spectra can be added to a plotting window, e.g. from a field instrument or from an image. Color, line width and marker can be modified.

Multiple spectral groups can be added within the same graph. Each spectral group can be assigned to a user-defined color. Here 2 spectral groups are plotted with different chlorophyll contents (20 µg/cm²: blue, 45: µg/cm² red) and a range of N. Likewise, spectral groups could also consist of different parameters or the same parameter from different models.

Simulated spectra can also be plotted with varying color tones as a function of 2 parameters. One parameter can be assigned to Hue (color), and another parameter can be assigned to Saturation (intensity). If both Hue and Saturation are assigned then the effects of these two parameters on reflectance can be visualized. When no color is chosen then automatically a color table will be used.

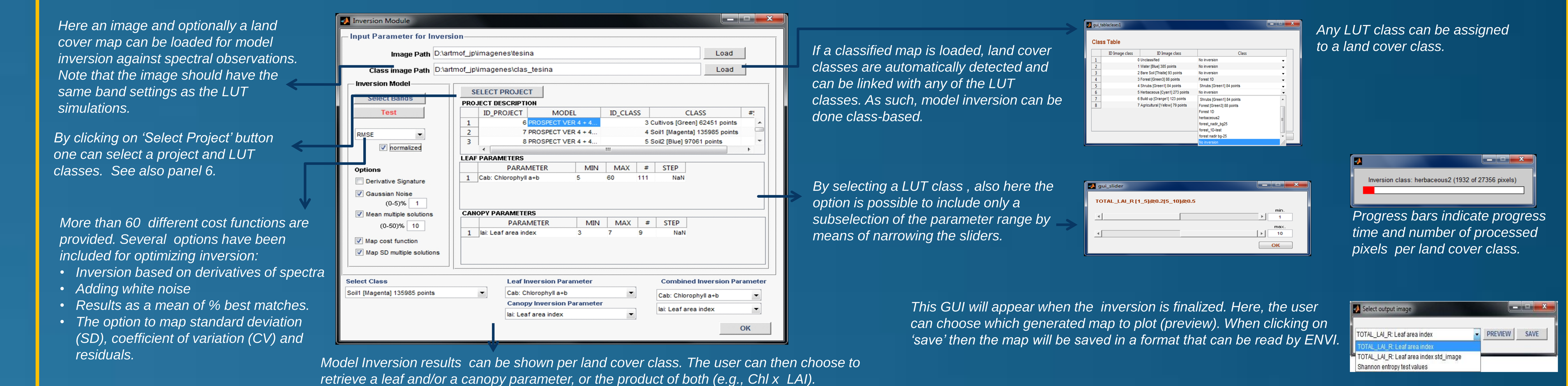
Example: With FluorMODleaf simulations of upwards leaf fluorescence are plotted as a function of chlorophyll content (Cab) and temperature (Tc).

In FluorSAIL also TOA radiance data can be plotted, here as a function of Chl, LAI and the colors present different MEP files (SZAs)

8. ARTMO's inversion module

Inversion

ARTMO's most advanced module is the 'Inversion' module. This module enables automated mapping of biophysical parameters from mulitspectral or hyperspectral imagery based on pre-computed LUTs. Several cost functions and optimization options are provided. Most importantly, inversion can be done class-based. This means that different land cover classes can be linked to different LUTs. For instance, homogenous land covers such as agricultural fields can be interpreted by a turbid model (e.g. SAIL) while heterogeneous land covers such as forests can be interpreted by a 3D model (e.g. FLIGHT).



Here an image and optionally a land cover map can be loaded for model inversion against spectral observations. Note that the image should have the same band settings as the LUT simulations.

By clicking on 'Select Project' button one can select a project and LUT classes. See also panel 6.

More than 60 different cost functions are provided. Several options have been included for optimizing inversion:
- *Inversion based on derivatives of spectra*
- *Adding white noise*
- *Results as a mean of % best matches.*
- *The option to map standard deviation (SD), coefficient of variation (CV) and residuals.*

If a classified map is loaded, land cover classes are automatically detected and can be linked with any of the LUT classes. As such, model inversion can be done class-based.

Any LUT class can be assigned to a land cover class.

By selecting a LUT class , also here the option is possible to include only a subselection of the parameter range by means of narrowing the sliders.

Progress bars indicate progress time and number of processed pixels per land cover class.

This GUI will appear when the inversion is finalized. Here, the user can choose which generated map to plot (preview). When clicking on 'save' then the map will be saved in a format that can be read by ENVI.

Model Inversion results can be shown per land cover class. The user can then choose to retrieve a leaf and/or a canopy parameter, or the product of both (e.g., Chl x LAI).

9. Provided cost functions

Inversion

In ARTMO about 60 different cost functions (also known as metrics, distances, or divergence measures) have been implemented. They can be clasified into three families.

1. First family is reffered to **information measures** and describes distances between two probability functions.
2. Second family is called **M-estimates**, and reflectance in this case is considered to be a nonlinear regression function.
3. Third family of **minimum contrast estimates** represents distances in the spectral domain. In this case reflectance is considered as spectral density function.

1. INFORMATION MEASURES

In order to apply some classes of distances between discrete distributions we assume that the reflectance data are normilised in the following way, where $R^*(\lambda_j)$ – satellite reflectance and $R_i(\lambda_j)$ – LUT reflectance. $R^*(\lambda_j), \lambda_j \in \Lambda$ and for $1 \le i \le N$ we introduce

$$Q=(q_1^*,\ldots,q_n^*)=\frac{R^*(\lambda_1)}{\sum R^*(\lambda_j)},\ldots,\frac{R^*(\lambda_N)}{\sum R^*(\lambda_j)},$$
$$P=(p_1^i,\ldots,p_n^i)=\frac{R_i(\lambda_1)}{\sum R_i(\lambda_j)},\ldots,\frac{R_i(\lambda_N)}{\sum R_i(\lambda_j)}$$

and $\sum q_i = 1, \sum p^i = 1$.

The class of distances can be written as follows: for a given strictly convex twice differential function f we define:

$$\Gamma_i[P,Q]=\sum_{l=1}^{n} q_l f\left(\frac{p_l}{q_l}\right),\ 1\le i\le N,\ \text{then } \Gamma_i[P,Q]\to \min \text{ iff } P=Q.$$

1. Power divergence $\Gamma_i[P,Q]=\sum_{l=1}^{n} p_l \frac{(p_l/q_l)^a-1}{a(a+1)}, a\in(-\infty,+\infty)$.

2. Cressie and Read power divergence $\Gamma_i[P,Q]=\left(\frac{1}{a+1}\right)\left[\sum_{l=1}^{n} p_l (p_l/q_l)^a - 1\right]$

3. Sharma - Mittal, $a \ne 0,1$: $\Gamma_i[P,Q]=\left(\frac{1}{(b-1)}\right)\left(\left[1+\sum_{l=1}^{n}(p_l/q_l)^a - a(p_l-q_l)-q_l\right]^{\frac{b-1}{a-1}}-1\right)$

4. Renyi, $a \ne 0,1$: $\Gamma_i[P,Q]=\left(\frac{1}{a(a-1)}\right)\left[\log\left(\sum_{l=1}^{n} q_l (p_l/q_l)^a - a(p_l-q_l)-q_l\right)+1\right]$

2. M-ESTIMATES

Let us consider BRF $R(\lambda_j,\bar{\vartheta})$ as nonlinear regression function which is observed at wavelength $\lambda_j \in \Lambda$ with some noise of complicated nature. In our notations $R(\lambda_j,\bar{\vartheta})$ is LUT reflectance.

The satellite observations can be represented as follows:
$$R_j^* = R(\lambda_j,\bar{\vartheta})+\varepsilon_j,\quad j=1,\ldots,n,$$
where $E\varepsilon_j = 0$, that is ε_j random noise, not Gaussian in general.
We use the M-estimates generated by a function of loss $\rho(x)$, $x\in\Re$.
Minimisation problem has the following form:
$$Q_n(\bar{\eta})=\sum \rho(R_j^* - R(\lambda_j,\bar{\eta})) \to \min_{\eta}$$
The classical LSE corresponds to the case when $\rho(x)=x^2$, where $x=R^*-R(\lambda_j,\bar{\vartheta})$.

1. LSE: $\rho(x)=x^2$.
2. Laplace estimator: $\rho(x)=|x|^p$, $1\le p\le 2$.
3. Alpha estimator: $\rho(x)=\frac{1}{2\alpha}-\frac{-e^{-\alpha x}}{2\alpha}$, $\alpha>0$.
4. Koenker and Basset $(0<c<1)$, $\rho(x)=\begin{cases} cx, & x\ge 0\\ (c-1)x, & x<0\end{cases}$
5. Trigonometric: $\rho(x)=\nu\left(x\arctan(sx)-\frac{\log(s^2x^2+1)}{2s}\right)$, $s,\nu>0$.
6. Tukey function $\rho(x)=\begin{cases}\frac{c^2}{6}(3x^2-3x^4+x^6), & |x|\le c\\ \frac{c^2}{6}, & |x|>c\end{cases}$

3. MINIMUM CONTRAST ESTIMATION

Let $\{Z_t\}$ be a stationary or harmonizable stochastic process with mean m and true spectral density $g(\lambda)$.
Indeed the BRF observations can be represented in the spectral domain in the form of periodogram $I_n(\lambda_k)$:
$$I_n(\lambda_k)=\frac{1}{2\pi m}\left|\sum_{j=1}^{N}(Z_j-m)e^{ij\lambda_k}\right|^2,\quad \lambda_k\in\Lambda.$$
We approximate $g(\lambda)$ by parametric family $f_\theta(\lambda)$ and a minimum contrast estimator minimizes
$$D(f_\theta,g)=\int_{\lambda\in\Lambda} K\{f_\theta(\lambda)/g(\lambda)\}d\lambda.$$
Function $K(x)$ is called contrast function should be a three times continuously differentiable on $(0,\infty)$ and it has a unique minimum at $x=1$. Then, $D(f_\theta,g)=0 \Leftrightarrow f_\theta = g$.

1. Let $K(x)=\log x + 1/x$, then $D(f_\theta,g)=\sum_{\lambda_j}\{\log(f_\theta(\lambda_j)/g(\lambda_j))+g(\lambda_j)/f_\theta(\lambda_j)\}$
2. $K(x)=-\log x + x$, then $D(f_\theta,g)=\sum_{\lambda_j}\{-\log(f_\theta(\lambda)/g(\lambda))+f_\theta(\lambda)/g(\lambda)\}$
3. $K(x)=(\log x)^2$, then $D(f_\theta,g)=\sum_{\lambda_j}\{\log(f_\theta(\lambda_j))-\log g(\lambda_j)\}^2$
4. $K(x)=x\log x - x$, then $D(f_\theta,g)=\sum_{\lambda_j} f_\theta(\lambda_j)g(\lambda_j)^{-1}\{\log(f_\theta(\lambda_j)g(\lambda_j)^{-1})-1\}$
5. $K(x)=(x^a-1)^2$, then $D(f_\theta,g)=\sum_{\lambda_j}\{(f_\theta(\lambda_j)/g(\lambda_j))^a-1\}^2$

As a first step we compared all cost functions for a given noise and by taking the mean of multiple best solutions.

Many cost functions performed alike, henceforth from each family of cost functions we chose one promising function for further evaluation:
- **'Power divergence'**
- **'Trigonometric'**
- **'K(x)=-logx+x'**

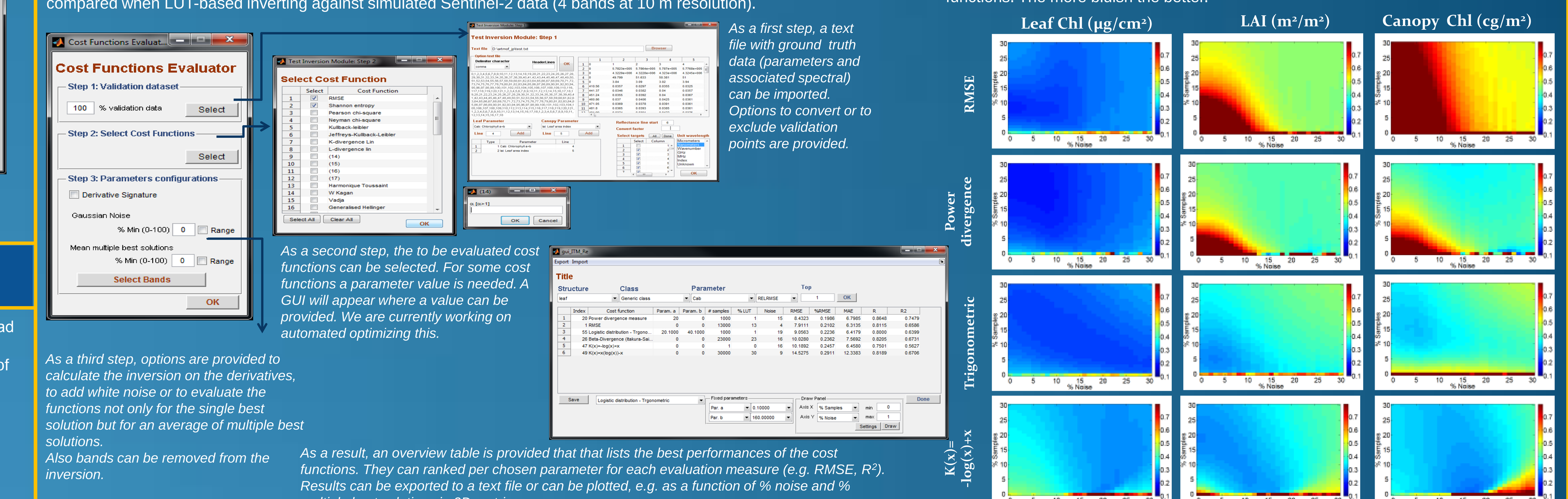
These functions were compared against the conventional **RMSE** (see below).

10. ARTMO's cost functions evaluator

Inversion

ARTMO offers the possibility to evaluate the range of included cost functions against validation data. By inputting a validation dataset (SPARC, Barrax, 2003) into ARTMO's cost function evaluator, the performance of all cost functions were compared when LUT-based inverting against simulated Sentinel-2 data (4 bands at 10 m resolution).

The LUT-based inversion was evaluated using the relative RMSE as a function of % Gaussian noise (X-axis) and % multiple best solutions (Y-axis) for the 4 chosen cost functions. The more bluish the better.



As a first step, a text file with ground truth data (parameters and associated spectral) can be imported. Options to convert or to exclude validation points are provided.

As a second step, the to be evaluated cost functions can be selected. For some cost functions a parameter value is needed. A GUI will appear where a value can be provided. We are currently working on automated optimizing this.

As a third step, options are provided to calculate the inversion on the derivatives, to add white noise or to evaluate the functions not only for the single best solution but for an average of multiple best solutions. Also bands can be removed from the inversion.

As a result, an overview table is provided that that lists the best performances of the cost functions. They can ranked per chosen parameter for each evaluation measure (e.g. RMSE, R^2). Results can be exported to a text file or can be plotted, e.g. as a function of % noise and % multiple best solutions in 2D matrices.

11. Final maps

Inversion

The cost function 'K(x)=-log(x)+x' performed most consistent over leaf chlorophyll content (*Leaf Chl*), leaf area index (*LAI*) and canopy chlorophyll content (*Canopy Chl*), and would therefore be an adequate candidate for realizing simultaneous retrieval of these biophysical parameters. Optimized accuracies were obtained by introducing 17% Gaussian noise and taking the mean of the 1% best solutions in the LUT-based inversion against a simulated Sentinel image at a spatial resolution of 10 m (4 bands). Along with the mean (μ) prediction, also its standard deviation (σ) and the coefficient of variation (CV: σ/μ) was mapped on a pixel-by-pixel basis. The CV maps allow comparison of the inversion performance of all three biophysical parameters. A lower CV means a greater uniformity across the 1% best solutions.
Most spatial variation in the mean prediction maps (Top) was obtained in the combined parameter *Canopy Chl*. The independent parameters *Leaf Chl* and *LAI* provided accurate results over the irrigated parcels but the dried-out areas were somewhat overestimated. Also the CV maps (Bottom) show that the inversion process had least difficulty with resolving *Canopy Chl* over the whole image. For *Leaf Chl* and *LAI* the inversion was better resolved over the irrigated areas than the dried-out areas. It should hereby be noted that the used LUT was not primary configured for these land cover types, but that can be easily done in ARTMO.
Moreover, ARTMO also enables to configure the inversion class-based, e.g. with different LUTs for different land cover types. These LUTs can be parameterized with different optical properties (e.g. for soil types) and structural features (e.g. coming from different models).