Gap Analysis for Integrated Atmospheric ECV CLImate Monitoring

WP5: Creation of a "Virtual Observatory" visualization and data access facility

D5.5: "Virtual Observatory Product User Guide and Implementation Description"

A Horizon 2020 project;

Grant agreement: 640276

Date: 22 December 2017

Lead Beneficiary: TUT

Nature: R

Dissemination level: PU

Work-package	**WP5 (Creation of a "Virtual Observatory" visualization and data access facility)**
Deliverable	D5.5 Virtual Observatory Product User Guide and Implementation Description
Nature	R
Dissemination	PU
Lead Beneficiary	TUT
Date	22/12/17
Status	Final
Authors	Kalev Rannat (TUT), Stephanie Guedj (EUMETSAT), Arndt Meier (EUMETSAT), Kuldar Taveter (TUT), Hannes Keernik (TUT), Merik Meriste (TUT), Neeme Loorits (TUT), Tonis Kelder (TUT), Jüri Helekivi (TUT), Marie Doutriaux Boucher (EUMETSAT), Jacques Descloitre (Univ. Lille), Pekka Kolmonen (FMI), Fabien Carminati (Metoffice)
Reviewers	Jörg Schulz (EUEMTSAT), Peter Thorne (NUIM), Anna Mikalsen (NERSC)
Contacts	kalev.rannat@gmail.com, Arndt.Meier@eumetsat.int, Stephanie.Guedj@eumetsat.int
URL	http://www.gaia-clim.eu

This document has been produced in the context of the GAIA-CLIM project. The research leading to these results has received funding from the European Union's Horizon 2020 Programme under Grant Agreement n° 640276.

Version	Author(s) /Reviewers	Date	Changes
0.1	Kalev Rannat, Stephanie Guedj (EUMETSAT), Arndt Meier, …	2017-09-18	1st draft
0.2	Kalev Rannat	2017-09-19	2nd draft, merging intro and added AERONET + HTTP-queries (appendix)
0.3	Arndt Meier(EUMETSAT), Stephanie Guedj (EUMETSAT), Kalev Rannat (TUT), Neeme Loorits (TUT), Pekka Kolmonen (FMI)	2017-09-19	3rd draft, major restructuring in chapter 2, adding chapters 3, 4, 5, and appendices.
0.4	Arndt Meier(EUMETSAT), Stephanie Guedj (EUMETSAT), Kalev Rannat (TUT)	2017-09-21	Major revision of chpt. 3, 4 and 5 by Kuldar Taveter
0.4	Peter Thorne, Joerg Schulz	2017-09-25	Major reviews, structure need to be update
0.5	Stephanie Guedj	2017-09-27	Major Restructuration, major rewriting and full revision
0.6	Kalev Rannat	2017-10-05	
0.7	Kalev Rannat, Arndt Meier	2017-10-06	Final review, language check
0.8	Marie Doutriaux Boucher, Stephanie Guedj	2017-10-23	Minor Reviews
0.9	Kalev Rannat, Kuldar Taveter	2017-10-30	Total revision
1.0	Jörg Schulz, Peter Thorne, Anna Christina Mikalsen	2017-12-22	Final reviewed version

Executive summary

The Gap Analysis for Integrated Atmospheric ECV CLImate Monitoring (GAIA-CLIM) project is funded by the European Commission Horizon 2020 programme.

A key outcome the GAIA-CLIM project is to provide a Virtual Observatory (VO) that is an internet service permitting end-users to discover, select, interrogate, extract, visualise and analyse co-located observations from satellites and high-quality non-satellite reference networks. These co-locations shall include traceable uncertainty estimates for the measurements and a characterisation of space-time mismatch and scale-smoothing uncertainties. The main application of the VO is the characterisation of the satellite products both at geophysical product level (Level-2) but also for satellite radiances (Level-1) that is achieved by applying a radiative-transfer model to the non-satellite reference measurements, transferring them into the satellite-measurement space. The VO contains built-in statistics and error-propagation tools for all products, making it a unique and powerful tool for users.

This User Guide provides an overview of the VO, the data in the VO, major functionalities and controls in the VO, usage limitations, and access point to the VO and how to get user support.

Contents

1 Introduction

1.1 Background

The Gap Analysis for Integrated Atmospheric ECV CLImate Monitoring (GAIA-CLIM) is a European Commission Horizon 2020 programme project.

The GAIA-CLIM project aims to improve our ability to make full use of non-satellite reference measurements for the characterisation of satellite measurements and derived products. Satellite products from current and future satellites are designed to provide crucial information related to a number of atmospheric Essential Climate Variables (ECVs), such as temperature, humidity and key atmospheric composition gases, such as ozone, methane, carbon dioxide and other greenhouse gases and aerosol.

However, the access to the different observations is scattered over numerous access portals, each with a different user interface, data formats, metadata descriptors and typically non-existent, incomplete or at least non-transparent uncertainty descriptors and data policies. The consequence is that products cannot generally be compared directly. GAIA-CLIM is providing a unified platform for co-located measurements, with built-in error propagation and statistics tools for both level - and level-2 products, making it a unique and powerful tool for users.

The Virtual Observatory (VO) is one of the main outputs of the GAIA-CLIM project, permitting end-users to discover, select, interrogate, extract, visualise and analyse co-located observations from satellite and high-quality non-satellite reference networks. A 3D-metadata platform has been integrated into the VO and provides an additional data discovery tool, not limited to the observational data ingested into the VO, but comprising almost all ongoing atmospheric measurements by high quality measurement infrastructures.

1.2 Purpose and scope

This document is prepared to help users from the general public, R&D, academia, satellite agencies or any other science-related sectors to use the current functionalities and data available in the VO. This version of the User Guide represents the status of the VO as of September 2017. An update is foreseen at the end of the project.

This User Guide provides an overview of the major functionalities and controls in the VO, usage limitations, access point guidance to the VO, and how to get user support. Specific examples for usage are available online in a series of YouTube video tutorial[1]s that can be reached via the Graphical User Interface by clicking on Tutorials. These on-line tutorials supplement the current guidance and will be updated on a regular basis until the project ends.

1.3 Structure of the document

The VO User Guide is structured in 5 sections to help the user to navigate into the VO, to find the data that are needed and to use the functionalities to visualise or extract these data.

- Section 1 (the current Section) provides the Introduction;
- Section 2 provides an overview of the VO;
- Section 3 describes the available data for the VO;

[1] The VO tutorials are available under: http://193.40.13.83/vo/#/tutorials

- Section 4 presents an overview how to work with the VO using the functionalities provided;
- Section 5 specifies current limitations;
- Section 6 describes access to the VO and its support;
- Annex A provides an overview of the acronyms used;
- Annex B provides suggestions for further reading on the topic;
- Annex C presents a preliminary list of data ingested into the VO;
- Annex D provides short descriptions of the ground-based reference networks from which data are used.

2 Virtual Observatory

2.1 Overview

The Virtual Observatory (VO) enables users to discover, select, interrogate, extract, visualise and analyse satellite to non-satellite data comparisons including all relevant uncertainties for such a comparison. Currently, the VO considers comparisons for the following Essential Climate Variables (ECVs):

- Atmospheric temperature and humidity profiles,
- Ozone total column and profiles, and
- Estimates of the aerosol optical depth.

These variables can be derived from various satellite measurements operating in the visible, infrared and microwave spectral regions. The satellite estimates are compared to ground-based measurements from various networks.

The VO takes into account the systematic and random uncertainties of each of the measurements, the smoothing errors (random and systematic), and the co-location mismatch error due to atmospheric variability, depending on the distance in time and space between the compared measurements that form a co-located observation pair. Mismatch uncertainties between satellite and non-satellite observations have been described in detail in other GAIA-CLIM documentation as listed in Section **Error! Reference source not found.**.

It is helpful to define the observation spaces before explaining how the VO works, as this is a unique facet of the VO. The geophysical (Level 2 or L2) parameter space is the space in which a physical quantity is observed directly. A thermometer shows the temperature of its direct surroundings providing temperature “in-situ”. This is the observational space we can usually perceive directly with our senses. It also includes the concentration profiles of atmospheric constituents like ozone, water vapour, methane, etc. However, remote sensing instruments, which include all satellite instruments and a subset of non-satellite instruments, measure the amount of radiation received, often as a function of wavelength with varying degrees of spectral resolution. The radiation received originates typically from one or more of the following sources: self-emission, solar (or lunar) absorption using the celestial body as light source, or reflection. With an inverse model of the atmosphere, sometimes including surface conditions, one can calculate the geophysical parameter from the observed radiances. In the processing chain of satellite observations, the radiance-space data is also known as Level-1 data (L1 data).

Traditionally, in satellite to non-satellite comparisons, geophysical (L2) products are derived from satellite observations and compared to measurements from non-satellite reference or other data. This is not necessarily favourable to characterise the quality of the satellite data as in such cases

measurement and retrieval errors always appear combined in the comparison and it is difficult to characterise the satellite measurement uniquely as a result. Theoretically, a very large number of geophysical profiles can satisfy a unique radiance signature at the top of the atmosphere. Typically, a priori information is required to convert a radiance to an equivalent geophysical profile. Thus, comparisons are complicated by the non-uniqueness and the dependence upon either models or other assumptions.

Nevertheless, satellite data are preferably analysed in radiance space, which is reasonable, for example, to ensure the continuity of a data record when one satellite is being replaced with a newer one (see www.fiduceo.eu for more details on this). On the other hand, radiance observations are usually not absolute values, directly traceable to a physical standard. Therefore, climate change research mostly considers geophysical parameters rather than radiances. This is also reflected in the list of ECV (GCOS, 2016)[2]. Reference networks such as GRUAN, NDACC, TCCON, EARLINET, AERONET, etc. aim to provide high-quality long-term observations of many of the ECVs. If satellite data is being used for deriving climate data records of ECVs, then full traceability must be established for the Level-2 products. Thus, the VO allows L2 comparisons.

Uniquely, the VO provides the capability to compare Level-2 reference network data with Level-1 satellite data relevant for temperature and humidity profile information as a proof of concept. The so called “GRUAN processor” converts the pressure, temperature, humidity profiles measured by a radiosonde into a brightness temperature as a satellite detector would see it at the top of the atmosphere (TOA) along the actual flight path of a GRUAN radiosonde. The GRUAN processor uses the EUMETSAT NWP-SAF radiative transfer model (RTTOV) modelling the specifics of a chosen satellite instrument. This forward model typically introduces smaller uncertainties as compared to the inverse model necessary to derive a Level-2 product from a satellite radiance product. This is a powerful feature of the VO, which could be extended in future to include further satellite radiances arising from further ECVs and ECV combinations.

2.2 Design

The VO has been designed and developed as a traditional client-server application (see Figure 1). Visible to the user is the Graphical User Interface (GUI) that allows the user to interact with the components of the VO. The GUI is used to send queries to retrieve data that result in graphical displays described later in the document. The data themselves are stored in a non-relational database that holds all the data including the uncertainties of the measurements and the co-locations available in the VO. The non-relational data base is very suitable to add new data of various types to the VO and makes extensions in the future relatively simple, should the VO be further developed and made operational.

Around the VO exist a number of support tools, the major ones are:

- tools to reformat all incoming data to a unified format,
- the GRUAN processor that performs the above described radiative-transfer calculations, and
- the co-location engine that precomputes the co-locations between the satellite and the reference data.

[2] GCOS, 2016: The Global Observing System for Climate: Implementation Needs. GCOS-200 [available under: https://unfccc.int/files/science/workstreams/systematic_observation/application/pdf/gcos_ip_10oct2016.pdf].

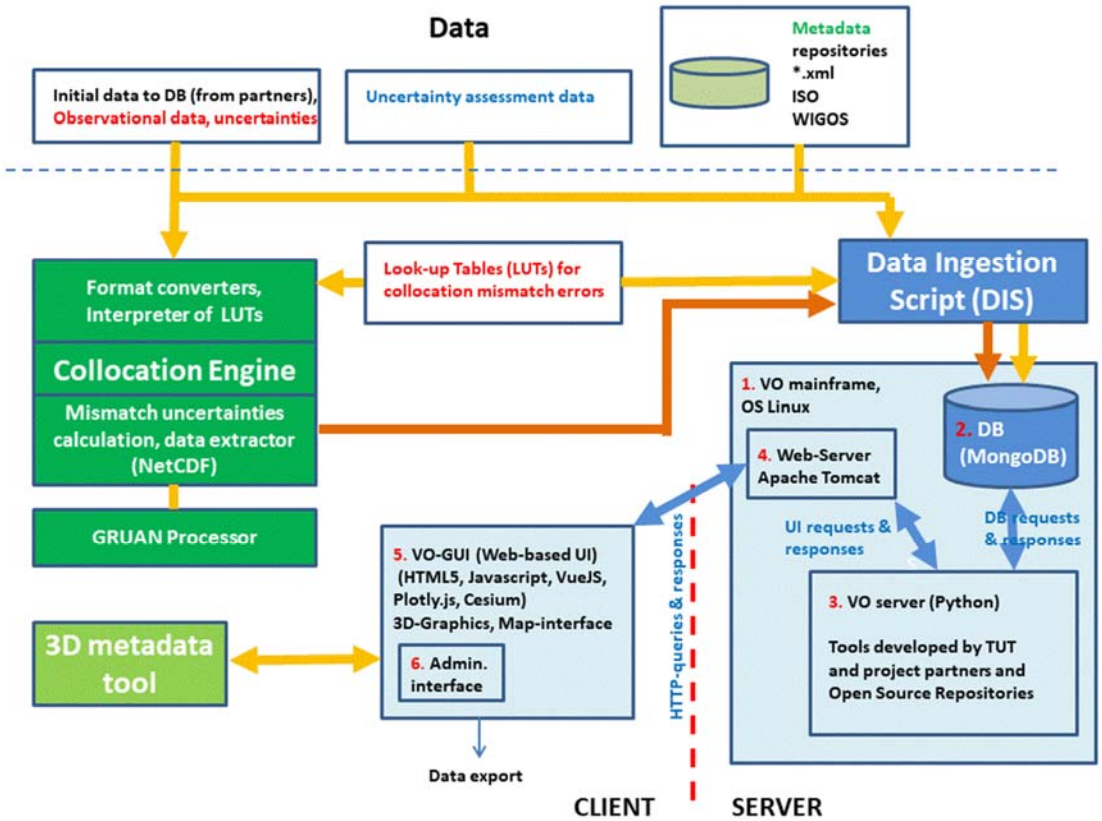


Figure 1: Architecture of the VO, consisting of the front end (client) and back end (server)

The main paradigm of data handling in the VO is searching for and accessing observational data by its metadata. Working directly with discovery metadata is supported by the online 3D metadata tool developed by CNR, which has been integrated with the VO (see section 4.2).

The 3D metadata tool has been designed to read the metadata from its own database, check for the availability of specific observations or observation locations, and, if data are available, visualise the data interactively through the GUI of the VO.

3 Data in the Virtual Observatory

The VO is intended to provide the user with access to both metadata and observational data from different ground-based reference networks with co-located satellite data. Appendix C presents an overview of ground-based reference networks used as data sources for the VO.

The GAIA-CLIM project addressed a specific selection of GCOS-ECV products for the development of the VO, which are:

- Temperature profiles;
- Humidity profiles;
- Ozone (total column and profiles);
- Aerosols optical depth.

The VO database consists of metadata in the VO's internal metadata format, which has been derived from the headers of the NetCDF-formatted and pre-co-located observational data. Metadata in the database of the VO is used for searching observational data from the database. The metadata is accessed by the 3D metadata tool that is described in Section 4.

The VO user can access and view the metadata by using the 3D metadata tool, which can be accessed through the GUI of the VO. This data currently cannot be extracted from the VO, but this functionality is foreseen to be added in subsequent developments.

The GUI offers the user different options to select and filter data and to visualise it online. During a given online session, everything the user has selected during the session can be downloaded for later use. User-selected data forms a temporary dataset in the VO and is deleted after the user has left the VO application.

4 Working with the VO

4.1 Access to the Virtual Observatory

The VO can be accessed online under: http://193.40.13.83/vo/#/ that brings the user to the main entrance page of the VO (Figure 2).

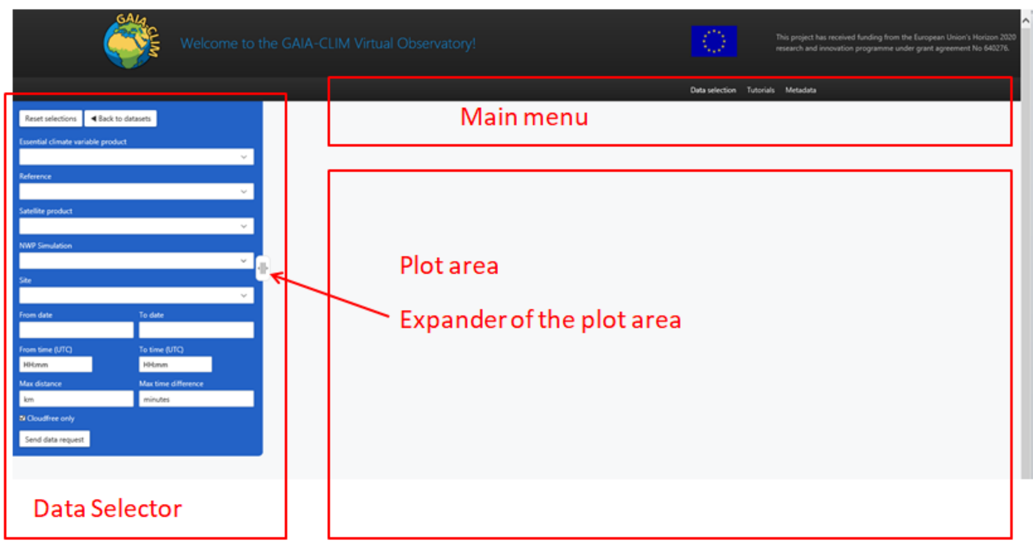


Figure 2. Main window of the VO

The main window of the VO is depicted in Figure 2. The main window comprises the main menu, data selector and plot area.

The purpose of the main menu is to enable the user to switch between "Data selection", "Tutorials" and "Metadata". The procedure for data selection is described in Section 4.3. "Tutorials" opens a window with links to online tutorials, which are intended to provide a user with an accessible overview about the VO and the 3D tool and their practical usage. "Metadata" opens the 3D metadata tool. The 3D metadata tool with general instructions is described in Section 4.2.

The data selector tool is for choosing the data for a given ECV and sending a data request. For temperature and humidity profiles, also the simulated brightness temperature from a subset of HIRS

measurements is accessible. Currently, the brightness temperatures can be shown when the ECV "Humidity" is selected.

The plot area is used for plotting the graphs according to the user's choices. The plot area can be expanded to full screen by selecting the expander of the plot area.

4.2 The 3D Meta Data Viewer

The mapping of geographical capabilities is described in detail in the GAIA-CLIM project deliverable D1.9[3]. The 3D-visualization tool is accessible from the main menu of the VO.

The meta data viewer covers non-satellite measurement networks and satellite platforms of 11 atmospheric ECVs, originating from almost 50 in-situ networks and 23 instruments on board 8 satellites. The station-discovery metadata has been collected using official documentation available online and following the recommendations provided by the network PIs and data managers.

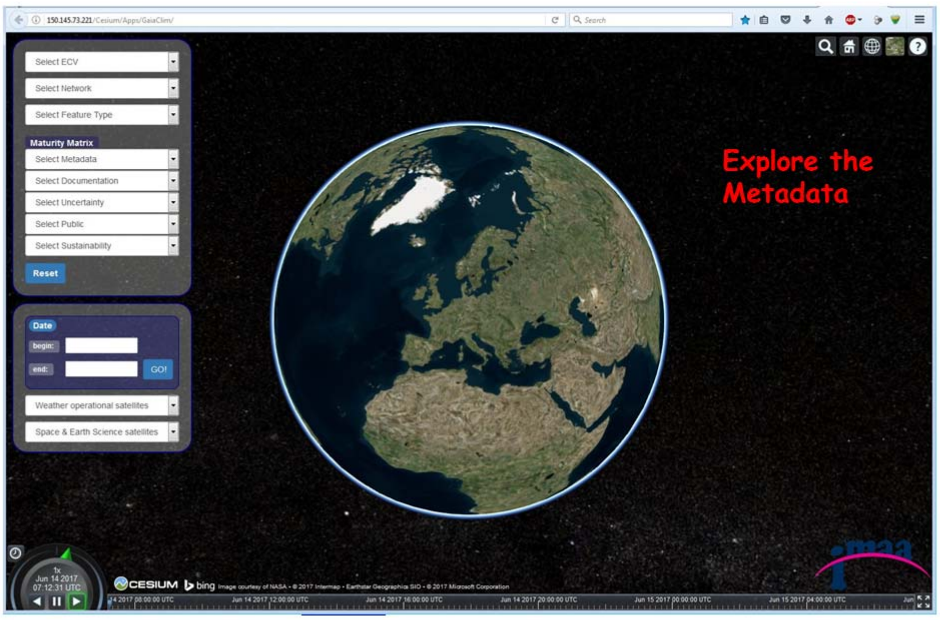


Figure 3: The main menu for exploring the metadata

The GUI of the meta data viewer, as it appears to the user, is shown in Figures 3-7. The main menu for exploring the metadata is represented in Figure 3**Error! Reference source not found.** where the left part of the screen contains the filters for network stations and satellites. The middle part of the screen shows the virtual globe in which stations are located and satellite paths are drawn. This globe can also be shown for 2-D projections. The user can zoom in, change the projection and apply some standard operations to improve the presentation. On the right side of the screen, all available information related to the chosen station and/or network is displayed, such as its latitude, longitude and instrument types.

[3] D1.9 and all other project deliverables are available from: http://www.gaia-clim.eu/page/deliverables

Figure 4 is displaying the result for the selection of the ECV water vapour, showing all stations at the ground that measure one of the specific ECV water vapour products as defined by GCOS (GCOS, 2016)[4]. The search can be further refined by choosing a network such as GRUAN as shown in Figure 5.

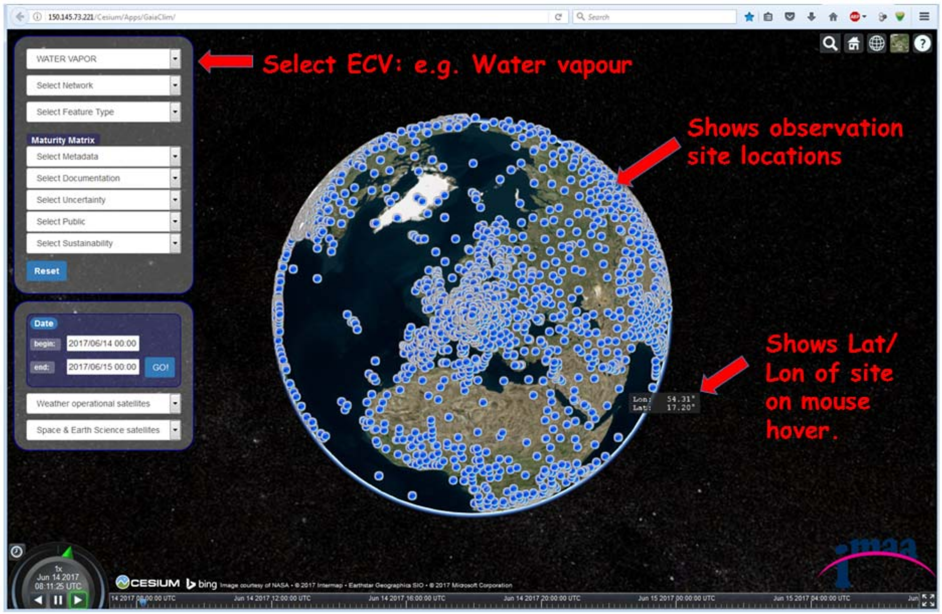


Figure 4: Selecting ECVs.

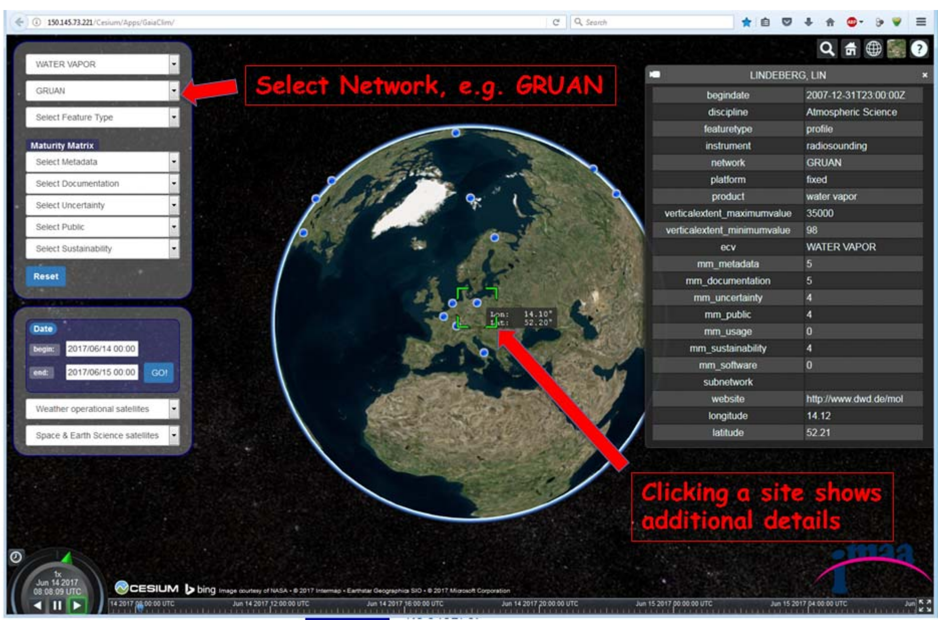


Figure 5: Selecting a reference network

In a next step, the user can explore which satellite measurements to be co-located to the chosen reference network by selecting a satellite platform and instrument. The meta data viewer shows the satellite overpass on top of the map, which allows the user also to get an overview at what times of

[4] GCOS, 2016: The Global Observing System for Climate: Implementation Needs. GCOS-200 [available: https://unfccc.int/files/science/workstreams/systematic_observation/application/pdf/gcos_ip_10oct2016.pdf].

the day which station of the reference network may have a co-location of measurements available, depending on choices of space and time coincidence tolerances for the measurements. Figure 6 shows as an example the overpass for the HIRS instrument aboard the EUEMTSAT Metop-A satellite and Figure 7 shows a selection of the ozone measurements with the GOME-2 instrument aboard the EUMETSAT Metop-B satellite. In Figure 7 also additional information on performance measures for the ground-based network is displayed. Information on the categorisations for the performance can be found in Thorne et al. (2017)[5].

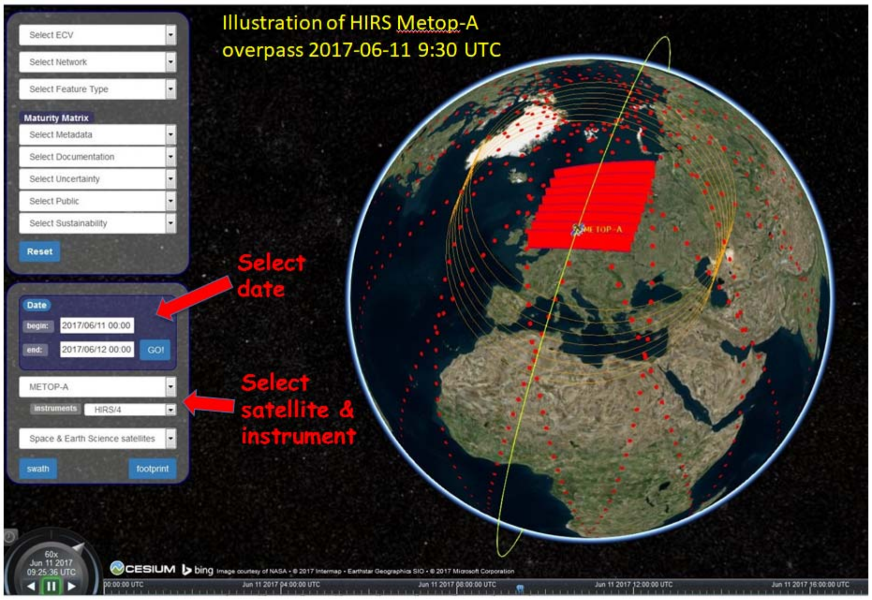


Figure 6: Animation of satellite overpasses

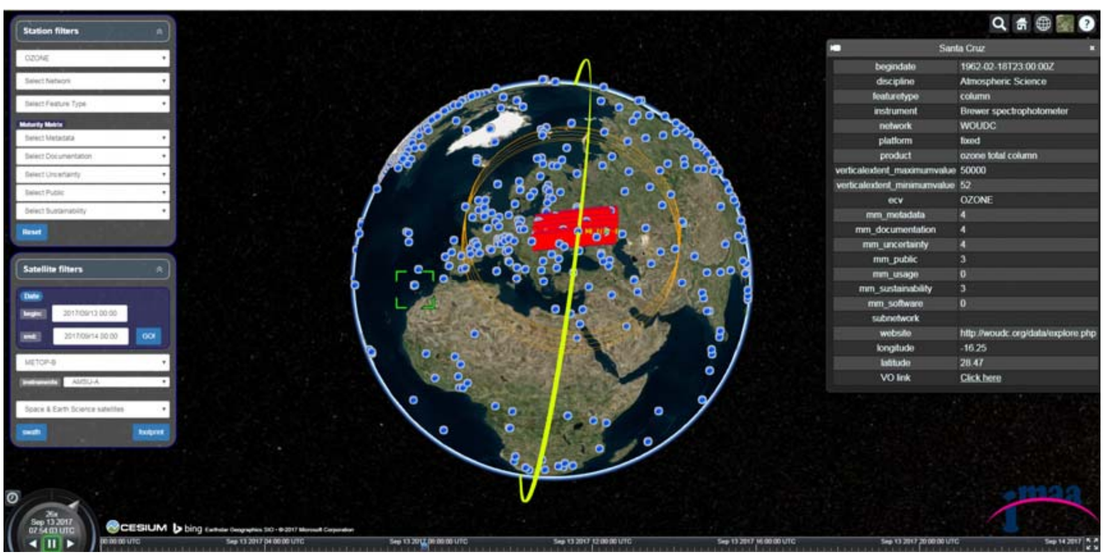


Figure 7: Locations of ozone-network stations performing columnar and profiler ozone measurements and the orbit and position of the GOME-2 instrument on the Metop-B satellite.

---

5 Thorne, P. W., Madonna, F., Schulz, J., Oakley, T., Ingleby, B., Rosoldi, M., Tramutola, E., Arola, A., Buschmann, M., Mikalsen, A. C., Davy, R., Voces, C., Kreher, K., De Maziere, M., and Pappalardo, G.: Making better sense of the mosaic of environmental measurement networks: a system-of-systems approach and quantitative assessment, Geosci. Instrum. Method. Data Syst., 6, 453-472, https://doi.org/10.5194/gi-6-453-2017, 2017.

4.3 Graphical Control System

The GUI of the VO's data selection tool is represented in Figure 8. Graphical control elements of the tool consist of the following options for filtering the data:

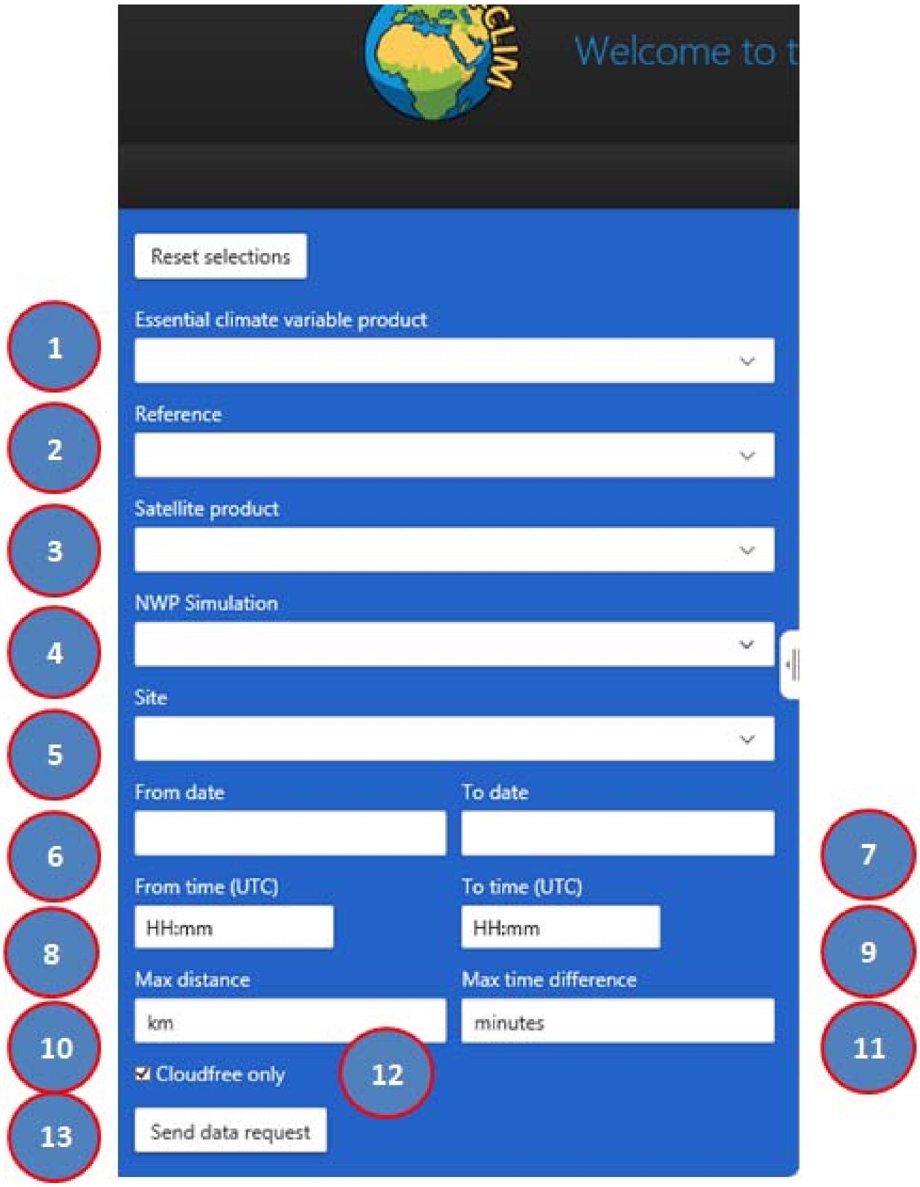


Figure 8. Data selection tool of the VO

1. ECV product – the user can choose between four different ECVs: Humidity, Temperature, Aerosol and Ozone. The profiles determine the options the user has for the remaining choices, as well as the types of data that are subsequently presented by the GUI.
2. Reference – here the user can choose between the available reference networks for the chosen profile (for example, "GRUAN Radiosonde" for temperature or humidity).
3. Satellite product – the user can choose between the available satellite products that match the chosen profile (for example, "HIRS Brightness Temperature" for humidity).

4. NWP Simulation – the user can choose between the available simulations for the chosen profile (for example, "UK MetOffice").
5. Site – this dropdown menu is populated with all the available sites according to the choices 1-4 the user has made (for example, "Barrow").
6. From date – the user can choose (using a built-in calendar) the start date for the data query. When the choice for the start date is left empty, the selected date range has no lower limit.
7. To date – the user can choose (using a built-in calendar) the end date for the data query. When the choice for the end date is left empty, the selected date range has no upper limit.
8. From time (UTC) – the user can enter the minimum time of day for all the observations queried. The time should be presented in the format "HH:mm", where "HH" denotes the hours in the 24-hour system and "mm" denotes the minutes.
9. To time (UTC) – the user can enter the maximum time of day for all the observations queried. The time should be presented in the format "HH:mm", where "HH" denotes the hours in the 24-hour system and "mm" denotes the minutes.
10. Max distance – here the user may enter, for co-location data, the maximum permitted distance in kilometers between the observation location of the reference data and satellite observation location, as has been given in the database. Only co-locations with distances below or at the given value are considered. If no number is entered, all co-locations compliant with other choices are considered.
11. Max time difference –the user may enter, for co-location data, the maximum permitted time difference in minutes between the observation location of the reference data and satellite observation, as given in the database. Only co-locations with time differences below or at the given value are used. If no number is entered, all co-locations compliant with other choices are considered.
12. Cloud free only – this checkbox is used for choosing only cloud-free data for some profiles. Data is considered as cloud free if the lowest channel is marked as cloud free in the data. For the profiles where cloud cover is not recorded, this checkbox cannot be used.
13. Send data request – when the user clicks this button, the GUI sends a data request to the database. The data request returns a list of datasets corresponding to the user's choices. The request also returns time-series data from all the datasets in the list and plots the time-series data as is shown in Figure . If no data meets the user specified request, an empty set is returned. In subsequent releases users will be guided by a table showing the availability of data in the VO to avoid empty set requests.

Figure 9 shows the choices of the VO GUI for calculating statistics and data filtering. The part of the GUI represented in Figure 9 consists of the following graphical elements:

14. The "Calculate Statistics" button.
15. The choice for data filtering. On the right, the GUI displays the time series plot of all the co-locations/observations in the list.
16. When the filter above the list is used, the list will update itself accordingly, but the plot on the right does not change.

The user can click on any co-location or observation in the list and retrieve additional data and sees a plot corresponding to the chosen co-location/observation.

In case of co-location data, the user can compare values for reference, satellite and simulation data. Also, where possible, the uncertainties for the measurements are given on the same plot.

Below the plots, the user can use drop-down menus to choose between different variables and statistics that are available to be shown on the plot. In the case of retrieving data with multiple channels, there is another dropdown menu enabling the user to choose the desired channel or certain channels that may be displayed concurrently for the given co-location / observation.

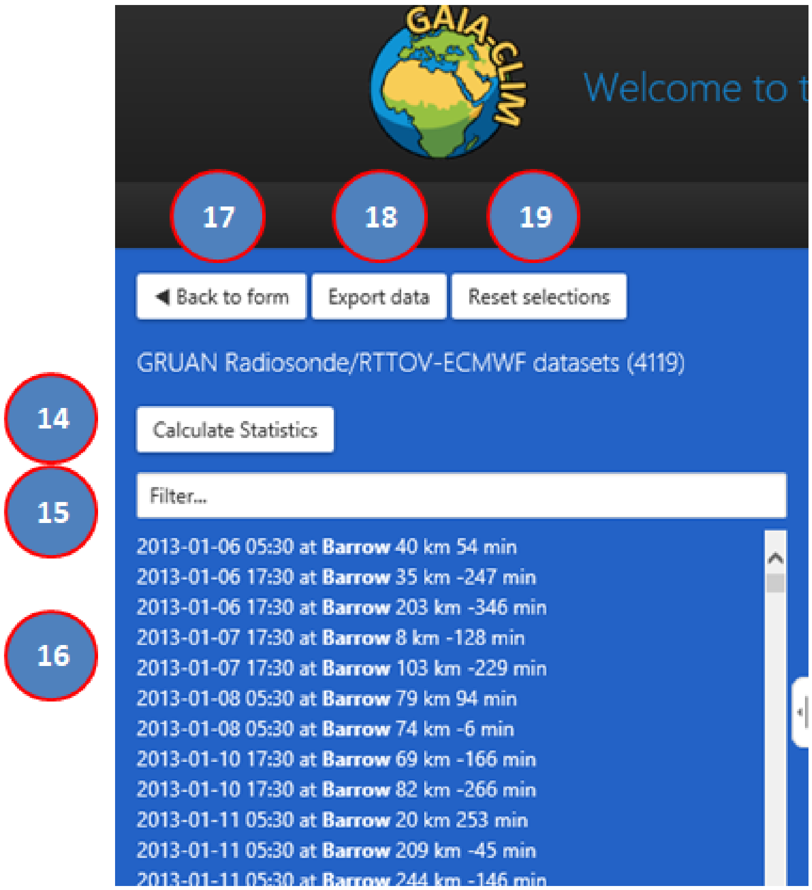


Figure 9. Calculating statistics and data filtering

There are the following additional buttons above the list of available co-locations / observations, which are also represented in 9:

17. Back to form – This choice takes the user back to the initial GUI page.
18. Export data – This choice allows the user to download the chosen data by querying the original files from the database.
19. Reset selections – This choice allows the user to reset all selections and return to the initial GUI page.

4.4 Exemplified Data Selection Process

This section gives a brief overview of the data selection process along with an overview of the data that has been ingested into the VO as of September 2017 and that is available to the users. A list of ingested data is described in detail in Appendix B. Selecting the data to be displayed and analysed by the VO occurs by taking the steps presented below:

4.4.1 Step 1: Select an ECV

The user of the VO can currently choose between the following key ECVs: temperature, humidity, ozone (total column and profiles) and aerosols.

Note 1: Currently, the brightness temperature can only be shown when the ECV "Humidity" has been chosen.

Note 2: Ozone and aerosol data are not available and a search will return empty.

4.4.2 Step 2: Select reference data

The following sets of high-quality reference data are available for the user to perform comparative studies:

- GRUAN Radiosonde/+ECMWF or GRUAN Radiosonde/+UKMO are **temperature and humidity** profiles measured from the Global Climate Observing System (GCOS) Reference Upper-Air Network (GRUAN, www.gruan.org).

4.4.3 Step 3: Select a satellite product

The VO considers Level-1 brightness temperature and Level-2 retrievals of ECV observations. Both Level-1 and Level-2 products consist of data that is co-locationed with the reference data that is chosen at Step 2. Further details of the co-location methodology will be made available with the final VO version. The user may refer to Appendix B to access the list of ingested data. From the list of satellite products presently displayed on the VO website, the user may select the HIRS brightness temperature. The HIRS brightness temperature originates from measurements of the High-resolution Infrared Radiation Sounder (HIRS) aboard the polar-orbiting EUMETSAT Metop-A and B and NOAA-19 satellites. Among their 20 channels, it has been decided to focus on three temperature sounding channels (2, 3 and 4) and on two humidity sounding channels (11 and 12). Other channels have been rejected for many reasons (e.g., influence by the surface emission and the clouds). More information about the HIRS instrument can be found at the websites of EUMETSAT (www.eumetsat.int/website/home/Satellites/CurrentSatellites/Metop/MetopDesign/HIRS/index.html) and NASA (https://poes.gsfc.nasa.gov/hirs4.html).

4.4.4 Step 4: Select a NWP simulation

This data is considering simulated brightness temperatures by both the UK MetOffice and ECMWF NWP systems. Atmospheric profiles are extracted from the model field (short range forecast) at the closest location to the reference site chosen at Step 5. Thereafter, the radiative transfer model RTTOV is used to simulate the brightness temperature at the instrument channels. NWP simulations co-located with the brightness temperature are available for HIRS channels for most GRUAN sites.

4.4.5 Step 5: Select a reference site

The list of available reference sites can be found by the 3D metadata tool described in Appendix A or on respective database websites.

4.4.6 Step 6: Select a date or UTC time limits

The user is recommended to check the availability of the data from Appendix C. Only a small subset of data is available for the current prototype version of the VO. If the user does not select any date or time limits, the VO will start to search through all the data in the VO database, which can be very time-consuming.

Tip: Move with the cursor to the date/time field and click to open the date/time tabs and scrolling in them for making your selections.

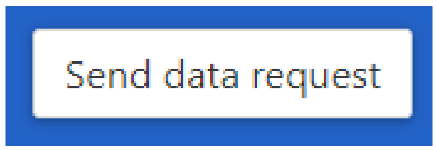
4.4.7 Step 7: Select the maximum distance and time difference

This selection is concerned with the co-located data. The user can define the acceptable limit in space and time between the reference database and the satellite pixel. If the user does not select any distance or time difference, the VO will use the respective default values 500 kilometres and 3 hours. The user can provide numerical co-location criteria which are lower than the default values.

4.4.8 Step 8: Select "Cloud Free"

The cloud detection relies on the approach put forward by Kottayil et al. (2012). First, a target area of 50 kilometres within a time window of 2 hours is defined around any available reference sites. Each pixel included in the target area is subjected to a series of cloud detection tests on brightness temperature differences. HIRS channels 8, 18 and 19 are used for this task. In using the VO, it is recommended to switch on the "Cloud Free" selection.

4.4.9 Step 9: Everything is ready and the data request can be sent by clicking the "Send data request" button:



4.5 Plotting and data export

This section describes plotting and exporting humidity and temperature ECVs, plotting and comparing co-located brightness temperature data, calculating statistics and exporting data.

For the humidity and temperature ECV product, the user can plot profiles of various observations from GRUAN radiosondes as well as information related to uncertainties, instrument drift and several other statistics. An example is presented in Figure 10. In the example, uncertainties of observations are plotted on the horizontal axis. The user can visualise uncertainties in relation to the altitude, pressure or time plotted on the vertical axis. The user may switch from one profile to another from the list on the left (blue panel) or using the link below the plot. The following data is available for comparison and plotting:

- ECV = Temperature and Humidity
- Reference = GRUAN radiosondes
- Period = individual days in 2013, 2015 and 2016 (cf. Appendix C)

Tip: The choice "Satellite product" must be set to "None" to display single profiles from GRUAN radiosondes

For comparison and plotting of co-located brightness temperature data, the following data is available:

- ECV = Brightness Temperature belongs to Humidity
- Reference = GRUAN radiosondes
- Satellite product = HIRS Brightness Temperature
- NWP = ECMWF and UKMO
- Period = 2013

<u>Tip</u>: The user can visualize the results for one co-location or statistics/time-series for all co-locations. A site for visualising should be selected according to this potential.

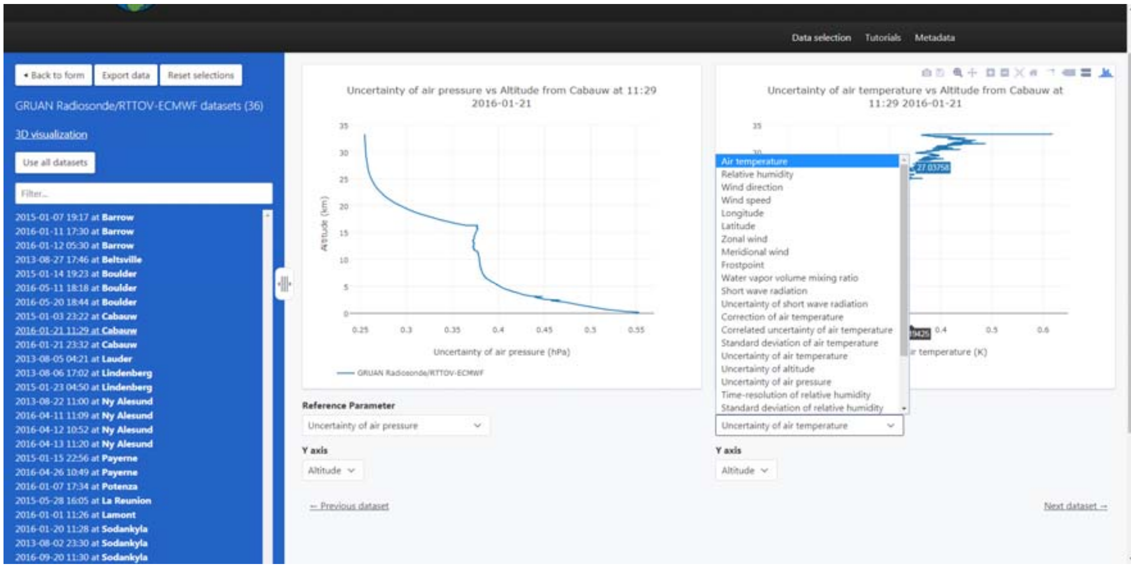


Figure 10: Example of plotting and analysing single profiles from GRUAN radiosondes

An example of comparison of brightness temperatures between GRUAN radiosondes, HIRS and NWP fields from the UK MetOffice at Ny Alesund is presented in Figure 11. In the example depicted in Figure 11, when any of the sets of co-locations presented on the left is chosen, two plots for the chosen set of co-locations are displayed on the right. By default, some measurand is plotted in the left plot window and the difference between the values of the reference data and satellite data for that measurand is plotted in the right plot window. When a measurand for co-location data is plotted, the user may compare co-located HIRS brightness temperatures (represented by orange in Figure 11 with two independent RTTOV simulations using as input atmospheric profiles from either GRUAN radiosondes (blue in Figure 11) or NWP fields (green in Figure 11).

On either plot, bars can be plotted representing total uncertainties of the HIRS brightness temperature. Measurement uncertainties related to the sets of co-located data in brightness temperature space can be added as error bars in the left window. The list of the sets of co-locations represented on the left may be minimised to improve the visibility of plots. The button between the list and the plot windows can be used to open and close the list area.

In addition, there is a row of icons on top of each plot window, which becomes visible when hovering the mouse indicator over the window. From left to right, these icons allow the user of the VO to:

- download the plot as a ".png"-file;
- save and edit the plot using the "plot.ly" cloud environment;
- zoom in on a selected area by clicking and dragging to select the area;
- pan around the zoomed-in plot;
- zoom in and out without selecting an area;
- use full scale for plotting;
- reset axis back to default values;
- toggle spike lines (shown when hovering over the graph);
- change what data is displayed during hovering.

Additionally, the user can switch between full-scale and default zoomed-in scale by double-clicking on the plot window.

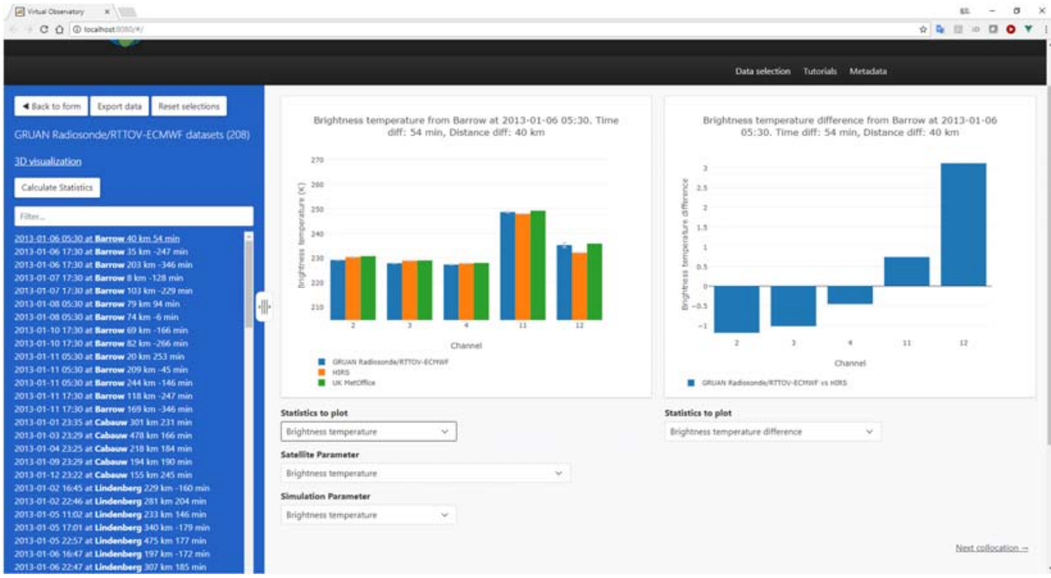


Figure 11: Example of comparison of brightness temperatures between GRUAN radiosondes, HIRS, and NWP field from the UK MetOffice at Ny Alesund

When the user clicks on the "Calculate Statistics" button, the aggregate statistics for all the sets of co-locations in the list is displayed. In the current version of the VO, statistics can be plotted to compare HIRS brightness temperatures. By default, average values over all sets of co-locations are displayed on the left and the corresponding time series are displayed on the right, as is exemplified by Figure 12. In each plot window, averages, standard deviations or time series can be displayed.

When the user clicks on the "Export Data" button, the selected co-location data are exported. This allows the user to download a full set of co-located data that matches the selection criteria. The data is exported in its original NetCDF-format. There is one NetCDF file for each set of co-locations, which has been zipped into several compressed files. However, the user of the VO should be aware that if the number of selected sets of co-locations is high, the request for export may take several minutes to process and may result in very large data files to be downloaded. Therefore, it is recommended to limit the initial selections performed on the selection page. The current version of the VO allows data export for all co-location data in brightness temperature space.

5 Limitations

The current version of the VO is a demonstrator, which has been designed and implemented as a proof-of-concept prototype. Further development is ongoing and shall be complete at the end of the project. Therefore, only samples of data have been ingested into the VO to demonstrate the future potential of this unified platform for accessing and using co-located observations.

Within the current list of ECVs, the VO will enable the user to undertake comparisons between satellite and non-satellite data for solely four ECVs – temperature, humidity, ozone and aerosol – as well as for some satellite instruments simulated radiances. Currently implemented are temperature and humidity and simulated HIRS brightness temperatures. For the latter, the focus is on a subset of

temperature and humidity channels from the HIRS instrument as the forward simulations using the GRUAN processor has limitations for channels that contain strong emission signals from the surface.

The GUI is not fully developed. The user needs to be aware that not all selections for data filtering work as expected.

The VO has also not yet been transferred to its final server destination and is running in a development environment that is not optimised for huge number of visitors. It therefore cannot be excluded that the server has temporal outages or is showing slow response.

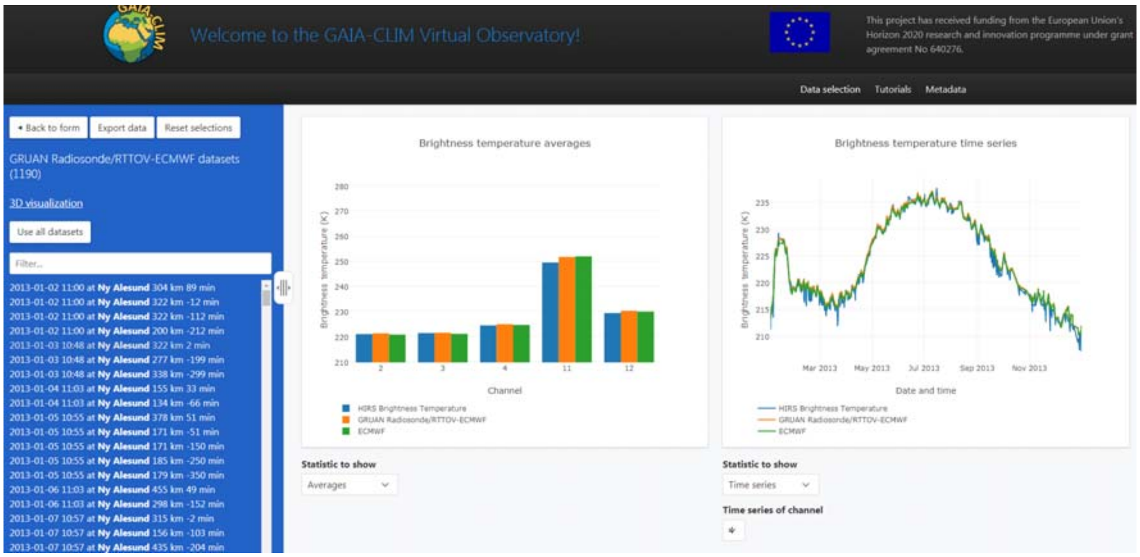


Figure 12: Example of comparison of brightness temperatures using co-locationed data.

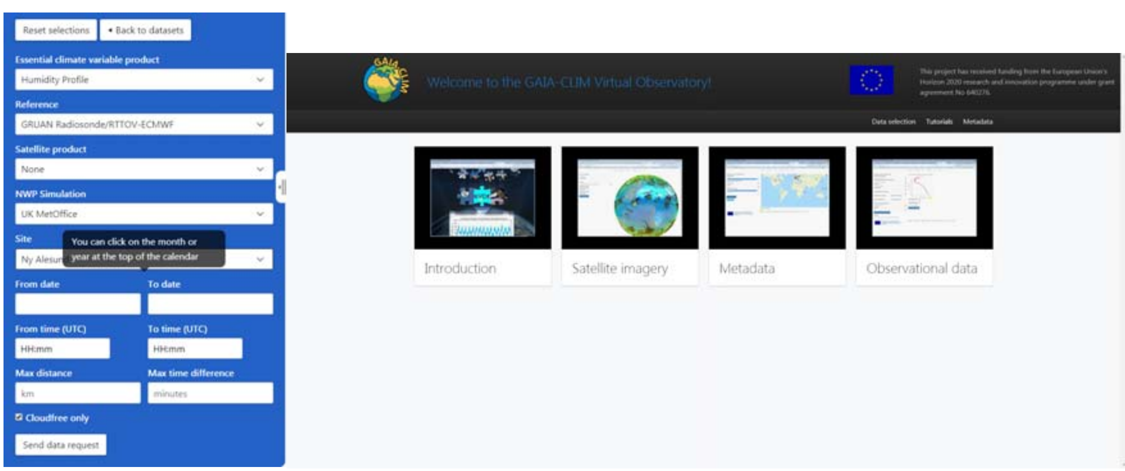


Figure 13: Example of pop-up help window on the left and links to the video tutorials on the right.

6 Access and Support

The user can access the online VO platform at **http://193.40.13.83/vo/#/**

Note: please, copy and paste this link to your browser. The VO is working with the Chrome, Firefox and Safari browsers. At the time of writing of this deliverable, the VO is not compatible with Internet Explorer, yet.

The GUI will be migrated to the EUMETSAT server "gaia-clim.vo.eumetsat.int" as soon as we receive the authorization from EUMETSAT.

Some pop-up help windows are displayed on the GUI for the user to get more information about the functionalities of the GUI. An example is displayed on the left panel represented in Figure 13. Figure 13 also shows that YouTube video tutorial are available on the GUI. They will be updated on a regular basis along with the development of the VO.

Annex A Acronyms

AERONET	AErosol RObotic NETwork
AE	Ångström exponent
AOD	Aerosol Optical Depth
BT	Brightness Temperature
CCI-CF	Climate Change Initiative - Climate and Forecasting
DIS	Data Ingestion Script
DOAS	Differential Optical Absorption Spectroscopy
ECV	Essential Climate Variable
FTIR	Fourier-transform infrared spectroscopy
GAIA-CLIM	Gap Analysis for Integrated Atmospheric ECV CLImate Monitoring
GCOS	Global Climate Observing System
GRUAN	GCOS The Reference Upper-Air Network
GUI	Graphic User Interface
HIRS	EUMETSAT High-resolution Infrared Radiation Sounder
ITT	manufacturer of HIRS - ITT Exelis in Fort Wayne, Indiana, US
JSON	Java Script Object Notation
LIDAR	LIght Detection And Ranging
LUT	Look Up Table
NASA	National Aeronautics and Space Administration
NDACC	Network for the Detection of Atmospheric Composition Change
NOAA	National Oceanic and Atmospheric Administration
NWP	Numerical Weather Prediction
RTTOV	Radiative Transfer for TOVS (TIROS Operational Vertical Sounder)
SAF	EUMETSAT Satellite Application Facility
TCCON	Total Carbon Column Observing Network
VO	Virtual Observatory
WIGOS	WMO Integrated Global Observing System

Annex B Further Reading

Scientific articles

Carminati F., F., W. Bell, S. Migliorini, S. Newman and A. Smith, An introduction to the GRUAN processor, Satellite Applications Tech Memo 46n, January 15, 2016

Dirksen R. J., M. Sommer, F. J. Immler, D.F. Hurst, R. Kivi, and H. Vömel,“Reference quality upper-air measurements: GRUAN data processing for the Vaisala RS92 radiosonde”, Atmos. Meas. Tech., 7, 4463–4490, 2014, www.atmos-meas-tech.net/7/4463/2014/, doi:10.5194/amt-7-4463-2014

Holben, B. N. et al.: AERONET—A Federated Instrument Network and Data Archive for Aerosol Characterization, Remote Sensing of Environment, 66, 1 – 16, 1998.

Immler F. J., J. Dykema, T. Gardiner, D. N. Whiteman, P. W. Thorne, and H. Vömel, “Reference Quality Upper-Air Measurements: guidance for developing GRUAN data products”, Atmos. Meas. Tech., 3, 1217–1231, 2010, www.atmos-meas-tech.net/3/1217/2010/, doi:10.5194/amt-3-1217-2010

Kottayil A., S.A. Buehler, V.O .John, L.M. Miloshevich, M. Milz, G. Holl, “On the importance of Vaisala RS92 radiosonde humidity corrections for a better agreement between measured and modeled satellite radiances” J. Atmos. and Oceanic Technology, 29 (2), 248-259, 2012 (This document includes the description of the cloud detection method used in HIRS.)

Schneider M., P. M. Romero, F. Hase, T. Blumenstock, E. Cuevas, and R. Ramos, “Continuous quality assessment of atmospheric water vapour measurement techniques: FTIR, Cimel, MFRSR, GPS, and Vaisala RS92”, Atmos. Meas. Tech., 3, 323–338, 2010, www.atmos-meas-tech.net/3/323/2010

Technical notes

EUM/OPS/DOC/17/896561 (Red Hat Enterprise Linux V7.2 Virtual Machine for the USC Climate Services group, Software Release Note V1.2)

The data-format description for HIRS4 Level 1c radiance product (created with AAPP): NWPSAF-MF-UD-003_Formats

Space Time Angle Match-up Procedure (STAMP): EUMETSAT Software Release Note (EUM/OPS/DOC/14/771241)

Space Time Angle Match-up Procedure (STAMP): EUMETSAT Design and User Manual document (EUM/OPS/DOC/13/724358)

The AC-SAF product user manuals for satellite ozone products available at http://acsaf.org/pums.html, such as the SAF/AC/DLR/PUM/01 document “GOME-2 Total Columns of Ozone, NO_2, BrO, HCHO, SO_2, H_2O, OClO and Cloud Properties”

Product User Manual NTO OTO DR GDP48_Jun_2017 and O3MSAF/KNMI/PUM/001 “NRT and Offline Vertical Ozone Profile and Tropospheric Ozone Column Products” product user manual Product User Manual NOP NHP OOP OHP O3Tropo Jul 2015.

GRUAN Technical Documents, available at http://www.dwd.de/EN/research/international_programme/gruan/docs.html, in particular TD 4, “Brief Description of the RS92 GRUAN Data Product”

Other GAIA-CLIM deliverables are accessible at: http://www.gaia-clim.eu/page/deliverables

GAIA-CLIM Guidance note, "Guide to Uncertainty in Measurement & its Nomenclature, Version 3.0", Paul Green & Tom Gardiner (NPL), 18/May/2017

GAIA-CLIM WP1-D1.8: “Beta version of a 3D tool for the online visualization of existing measurements”, 14-September-2016

GAIA-CLIM WP1-D1.9 “Final version of a 3D tool for the online visualization of existing measurements”, 31-August-2017

GAIA-CLIM WP3-D3.5 “Beta set of tools for quantification of co-location mismatch and smoothing uncertainties and associated documentation for integration in the development of the virtual observatory”, 30-April-2017

GAIA-CLIM WP5-D5.4 “Graphical User Interface”, 11-September-2017

Annex C List of data ingested into the VO

Table C.1. Data availability for temperature and humidity profiles

Type	Method	From	To	No of measurements / pairs	No of stations
Co-location	GRUAN Processor (Radiosonde) vs HIRS	06.01.2013	30.12.2013	16 774	9
Co-location	GRUAN Processor (ECMWF model) vs HIRS	06.01.2013	30.12.2013	9 892	9
Co-location	GRUAN Processor (UK MetOffice model) vs HIRS	06.01.2013	30.12.2013	9 612	9
Single-profile	GRUAN Processor (Radiosonde)	01.01.2011	31.12.2014	4 941	1
Single-profile	GRUAN Processor (UK MetOffice)	01.01.2011	31.12.2014	4 941	1
Single-profile	GRUAN Radiosonde	01.08.2013	05.08.2016	36	13

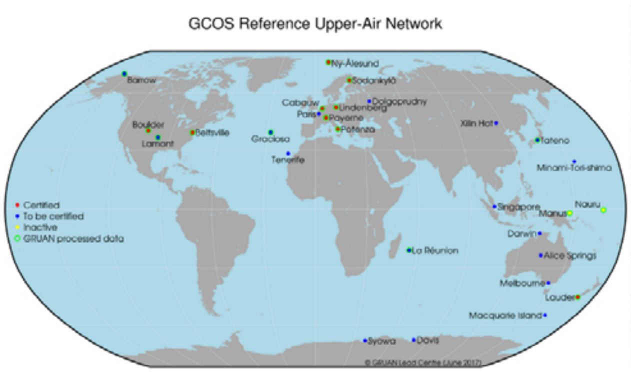
Annex D Reference Data Source

D.1 GRUAN reference humidity and temperature profiles

Observations from all 15 fully operational sites of the Global Climate Observing System (GCOS) Reference Upper-Air Network (GRUAN) have been ingested into the VO.

The goal of GRUAN is to provide the scientific community with comprehensive information about the climate system, involving a wide range of atmospheric and oceanic processes. GRUAN is expected to provide long-term, highly accurate observations of atmospheric profiles, complemented by ground-based state-of-the-art instrumentation to constrain and calibrate data from spatially more comprehensive global observing systems, including satellites and current radiosonde networks.

GRUAN is envisioned a network of 30–40 high-quality long-term upper-air observation stations that have been built on existing observational networks. Among the 25 stations listed in Figure D.1, the data that is currently certified as compliant with the GRUAN standards is the data originating from Vaisala-RS92 radiosondes. A subset of this data has been ingested into the VO. The GRUAN data processing for the RS92 radiosonde has been developed to meet the criteria of reference observations as described by Immler et al. (2010) and Dirksen et al. (2014).



Code	Name	Latitude	Longitude	Altitude	WMO No.	Status
ALC	Alice Springs, Australia	-23.70°	133.87°	546 m	94326	to be certified
BAR	Barrow, AK, USA	71.32°	-156.61°	8 m	70027	to be certified
BEL	Beltsville, MD, USA	39.05°	-76.88°	53 m		certified
BOU	Boulder, CO, USA	39.95°	-105.20°	1743 m	72471	certified
CAB	Cabauw, Netherlands	51.97°	4.92°	1 m	06260	certified
DAR	Darwin, Australia	-12.43°	130.89°	30 m	94120	to be certified
DVS	Davis, Australia	-68.58°	77.97°	18 m	89571	to be certified
DLG	Dolgoprudny, Russia	55.75°	37.62°	185 m	27612	to be certified
LAU	Lauder, New Zealand	-45.05°	169.68°	370 m	93817	certified
LIN	Lindenberg, Germany	52.21°	14.12°	98 m	10393	certified
MAQ	Macquarie Island, Australia	-54.62°	158.85°	6 m	94998	to be certified
MAN	Manus, Papua New Guinea	-2.06°	147.42°	6 m		inactive
MEL	Melbourne, Australia	-37.81°	144.98°	113 m	94866	to be certified
NAU	Nauru, Nauru	-0.52°	166.92°	7 m		inactive
NYA	Ny-Ålesund, Norway	78.92°	11.92°	5 m	01004	certified
PAY	Payerne, Switzerland	46.81°	6.95°	491 m	06610	certified
POT	Potenza, Italy	40.60°	15.72°	720 m		certified
REU	La Réunion, France	-21.08°	55.383°	2200 m		to be certified
SGP	Lamont, OK, USA	36.60°	-97.49°	320 m	74646	to be certified
SIR	Paris, France	48.7°	2.2°	156 m	07151	to be certified
SNG	Singapore, Singapore	1.30°	103.80°	21 m	48698	to be certified
SOD	Sodankylä, Finland	67.37°	26.63°	179 m	02836	certified
TAT	Tateno, Japan	36.06°	140.13°	25 m	47646	to be certified
TEN	Tenerife, Spain	28.32°	-16.38°	115 m	60018	to be certified
XIL	Xilin Hot, China	43.95°	116.12°	1013 m	54102	to be certified

Figure D.1: GRUAN station map, location and status as of September 2017 (www.gruan.org)

The following parameters have been ingested into the VO:

- Atmospheric parameters: air temperature, relative humidity, wind direction, wind speed, zonal wind, meridional wind, frost point, water vapour mixing ratio, short wave radiation.
- Location: longitude, latitude.
- Uncertainties: air temperature, altitude, air pressure, wind speed and wind direction, short-wave radiation.
- Corrections: air temperature, relative humidity, radiosonde drift.
- Correlated uncertainties: air temperature, relative humidity.
- Standard deviation: air temperature, relative humidity.
- Time resolution: relative humidity

The GRUAN data product has full metrological certification being of reference quality.