Gap Analysis for Integrated Atmospheric ECV CLImate Monitoring

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

D5.9: “Final version of the Virtual Observatory User Guide and Implementation Description”

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Executive summary

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

A key outcome the GAIA-CLIM project is the provision of a Virtual Observatory (VO) facility that consists of 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 all include case studies of traceable uncertainty estimates for the measurements and / or a characterisation of space-time mismatch and scale-smoothing uncertainties. The main intended 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). Satellite radiance comparison 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 uncertainty-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 guidance to the VO and how to get user support following the end of the GAIA-CLIM project.

Contents

1 Introduction

1.1 Background

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

The GAIA-CLIM project aimed 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.

These satellites need to be fully characterised if the data from them is to be used with confidence for climate applications. One aspect (but by no means the only) of such a sustained characterisation can be achieved via comparison to high-quality well-characterised non-satellite measurement series.

However, access to the non-satellite 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 satellite products cannot generally be compared directly with non-satellite data without considerable effort. To address this, GAIA-CLIM set out with the aim of providing a unified platform for co-located measurements, with built-in uncertainty propagation and statistics tools for both Level-1 and Level-2 products, making it a potentially unique and powerful set of tools and approaches for users.

The Virtual Observatory[1] (VO) is the primary external showcase of what the GAIA-CLIM project has achieved, 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 comprehensive data discovery tool, not limited to the observational data ingested into the VO. This data discovery portal permits users to explore almost all ongoing atmospheric measurements by high quality measurement infrastructures. It is important to stress that the VO constitutes a demonstrator facility and is not, at this time, operational.

1.2 Purpose and scope

This document is prepared to help users from R&D, Copernicus services, academia, satellite agencies, and the general public to use the current functionalities and data available in the VO. This version of the User Guide represents the status of the VO at the end of the project in February 2018.

This User Guide provides an overview of the major functionalities and controls in the VO, usage limitations, and access point guidance to the VO, as well as how to get user support. Specific examples for usage are available online in a series of YouTube video tutorials[2] that can be launched via the Graphical User Interface by clicking on *Info and Tutorials*. These on-line tutorials supplement the guidance provided in this document.

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[1] The GAIA-CLIM Virtual Observatory is accessible under: http://gaia-clim.vo.eumetsat.int/vo

[2] The VO tutorials are available under: http://gaia-clim.vo.eumetsat.int/vo/#/tutorials

1.3 Structure of the document

The VO User Guide is structured into 6 sections and a number of annexes to help the user to navigate into the VO, to explore the available data, 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;
- 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;
- Annex C presents a list of data accessible from the VO;
- Annex D provides an overview about the known caveats on the metrological and co-location uncertainties and information on the data sources and Intellectual Property Rights (IPR) to be respected.

2 Virtual Observatory

2.1 Overview

The VO enables users to discover, select, interrogate, extract, visualise and analyse satellite to non-satellite data comparisons including examples of how to handle relevant uncertainties for such a comparison. Currently, the VO considers comparisons for the following ECV products:

- Temperature and humidity profiles represented in brightness temperature space,
- Ozone total columns, and
- 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 as far as available, the smoothing uncertainties (random and systematic), and the co-location mismatch uncertainty due to atmospheric variability, depending on the distance in time and space between the compared measurements that form a co-located observation pair. Such mismatch uncertainties between satellite and non-satellite observations have been described in detail in other GAIA-CLIM documentation as listed in Annex B.

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: emission, absorption of solar (or lunar) light 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.

Traditionally, in satellite to non-satellite data comparisons, geophysical (Level-2) 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.

For these reasons satellite data are preferably analysed in radiance space, which is required, for example, to ensure the continuity of a data record when one satellite is being replaced with a newer one (see the FIDUCEO project[3] 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 GCOS ECVs[4]. 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 in addition. Thus, the VO also shows Level-2 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 “GRUAN processor” converts the pressure, temperature, and 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) to simulate 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 the future to include further satellite radiances arising from further ECVs and ECV combinations.

2.2 VO design

The VO has been designed and developed as a traditional client-server application (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 versatile allowing easy addition of new data of various types to the

[3] www.fiduceo.eu

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

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.

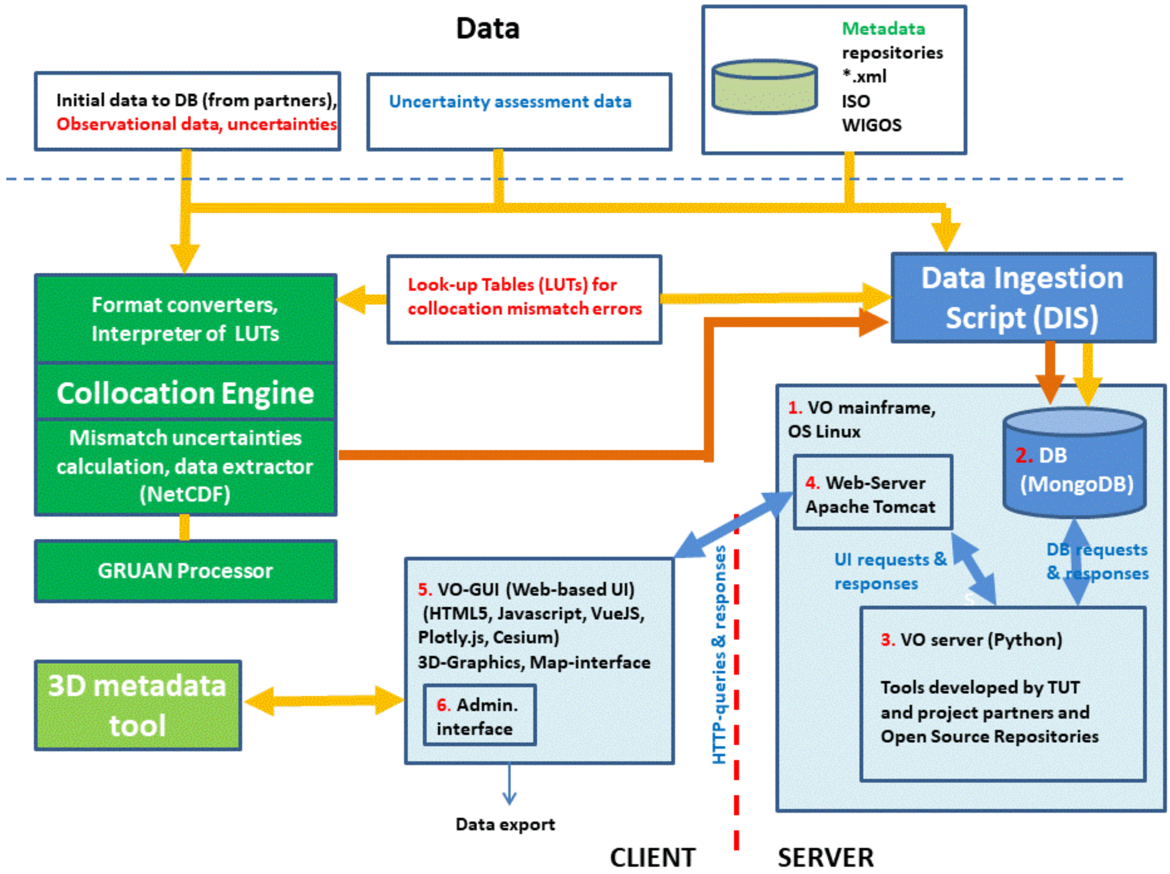


Figure 1: Architecture of the VO, consisting of the front end (client) and back end (server)

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 VO

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. Annex C presents an overview of data accessible from the VO database.

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

- Temperature and humidity profiles represented by simulated radiances as seen by a satellite instrument;
- Ozone total columns;
- Aerosols optical depth.

The VO database consists of metadata in the VO's internal metadata format, which has been derived from the metadata contained in 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 could be added in subsequent developments post-project completion.

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

3.1 Data co-locations for the VO

For practical reasons, the VO has been designed to work with pre-co-located data. Co-locations are made offline, prior to data ingestion into the VO. The offline co-location process maximises the number of co-locations. The user can alter the co-location criteria by varying the permitted spatial and temporal match criteria to arrive at the best co-location set-up for the user's application. Two co-location methods are used: one for the simulated radiances represented as brightness temperatures and ozone total columns and another for aerosol optical depth as covered in the next two sub-sections.

3.1.1 Co-location between radiances, ozone and reference observations

As the non-satellite fiducial reference observations used in GAIA-CLIM are very sparse, a completely different approach for finding co-locations is used here, where the value of each reference observation is maximised. Reference observations are organised as single data-files (hereafter files) per observation. For each observation, the effective latitude and longitude of the sampled air mass is calculated. In case of a radiosonde, this is the location when passing the 300hPa pressure level. For FTIR instruments this is the latitude, longitude, and altitude of the volume mixing ratio of the targeted trace gas weighted along the line of sight. For a satellite instrument, this is the latitude and longitude of the observation taken over ground.

Satellite data is typically organised to contain about 100 minutes of observation time per data file, which contains observations from one complete revolution around the earth. Firstly, all satellite observation files on record that match the observation day of any candidate reference observation plus one swath path before or after midnight are identified, if the reference observation falls within 5 hours of midnight. Then for each reference observation all potentially matching satellite observation files are searched for. For each pair of files, one output file is created if at least one valid co-location is found. Occasionally, this can result in two output files per reference observation if data in more than one satellite orbit fulfil the temporal co-location criteria.

To find the actual co-locations, the user-defined maximum distance is considered for a co-location (e.g., 500 km) in terms of a square box in degrees of latitude and longitude. A pointer is placed onto each of the satellite latitude and longitude data sets, which are then incremented synchronously to find out if the satellite observation is within the latitude and longitude box of the reference observation. This procedure is continued until the end of the data record is reached. If the latitude and longitude pair falls within the box, the actual distance in kilometres from the reference location is calculated. If the latitude and longitude pair is within the maximum distance of the co-location, it is checked if the value of the observation (brightness temperature, total ozone quantity, etc.) is valid and if the observation times fall within the maximum time difference the user has selected for the co-locations. If both conditions hold, the given co-location is further considered. Each new co-location is stored in an array sorted by co-location distances. If a threshold of 128 candidate co-locations between a satellite and a single non-satellite measurement is reached, only those co-locations are kept that have better matches than the currently poorest match, and the poorest match is discarded. This makes sure that for each reference observation we keep at most the 128 closest co-locations in time and space of a satellite instrument.

After creating the initial list of co-locations, which only stores the index of the monitored data set along with the corresponding latitudes, longitudes, acquisition times, and co-location distances, all quality criteria including cloud screening for satellite measurements are analysed for the co-location candidates found and all compromised observations are removed.

A simple but effective drift correction is added for balloon-borne instruments. If present, the effective (i.e., drift corrected) distance is calculated in addition to the static co-location distance from the radiosonde location at 300hPa. The details of the drift correction for balloon-borne instruments like radiosondes have already been described in detail in the GAIA-CLIM Deliverable 3.7. In case of drift-corrected data, the list of co-locations is re-ordered by effective distance.

Where applicable, clouds are detected in the satellite data (e.g., for HIRS brightness temperature products) as well as the smoothing biases and uncertainties for the reference and monitored instruments from the corresponding Look Up Tables (LUT) and the co-location mismatch uncertainty from the corresponding LUT. Thereafter all co-located data including all the metadata from both observations is written into the output file in the netCDF-format. In addition to the main measurand, like brightness temperature or ozone total column amounts, additional parameters matching the co-located observations are extracted and stored into the output file, such as uncertainties related to the measurand, averaging kernels, co-location matrices, integration times, layering schemes, a-priori profiles, solar zenith angles, solar azimuth angles, partial columns, mean values of 3x3 and 5x5 pixels, and the corresponding standard deviations. With the help of a list of the names of the data sets of interests, it can be specified very easily which additional parameters are finally stored into the output file for the identified co-located observations.

3.1.2 Co-location between aerosol and reference observations

The principle of this co-location is to identify all AATSR overpasses that fall in the vicinity (defined by a given radius around the site) of the location of an AERONET instrument that performed at least one observation within a given time window around the overpass time. For each co-location, one unique average value of satellite and reference Aerosol Optical Depth (AOD) is provided.

Because of the high frequency of AERONET AOD observations (typically 15 minutes), there are usually several observations within the chosen time window for each co-location. Similarly, because of the AATSR Aerosol Dual View algorithm product spatial sampling (10 x 10 km), there are usually several

AATSR pixels surrounding each AERONET measurement site. The presence of clouds can lower the number of co-location observations.

All satellite AOD retrievals and uncertainties matching the spatial co-location criterion (i.e., within the given radius around the AERONET site) are spatially averaged. Similarly, all AERONET observations matching the temporal co-location criterion (a given time interval around the satellite overpass time) are temporally averaged. This method to co-locate satellite and ground-based observations is described in detail in Bréon et al. (2011).

The standard deviation of all AATSR and AERONET samples is derived by computing the average AOD. The standard deviation represents the precision of the respective observations (e.g., due to spatial and temporal variability).

The spatiotemporal co-location criteria chosen are +/- 30 minutes around the AATSR overpass time and within a radius of 25 km around each AERONET site. These criteria are based on the study with various thresholds for space and time windows performed by Virtanen et al. (2018). The criteria can be adjusted by the VO user.

4 Working with the VO

4.1 Access to the VO

The VO can be accessed online under: http://gaia-clim.vo.eumetsat.int/vo that brings the user to the welcome page of the VO (Figure 2).

Figure 2. VO welcome page

When clicking on either “Data Selection” or anywhere on the big VO image, the user is taken to the main data selection page (Figure 3).

Figure 3 Data page

The data selection page has the main menu on the top, data selector pane on the left and plot area on the right. Before the user has clicked "Send data request", the plot area shows all possible sites, start and end dates and number of data sets available for each site for the current selections including the co-location criteria. When the user changes the selections on the left, the VO updates the table on the right immediately.

The purpose of the main menu is to enable the user to switch between "Data selection", "Info and Tutorials" and "Metadata". The procedure for data selection is described in Section 4.3. "Info and 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.

4.2 The 3D-metadata viewer

The mapping of geographical capabilities is described in detail in the GAIA-CLIM project deliverable D1.9[5]. The 3D-visualization tool is accessible from the main menu of the VO.

The meta data viewer covers non-satellite observation 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 Principal Investigators and data managers.

The main menu for exploring the metadata is represented in Figure 4 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

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

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.

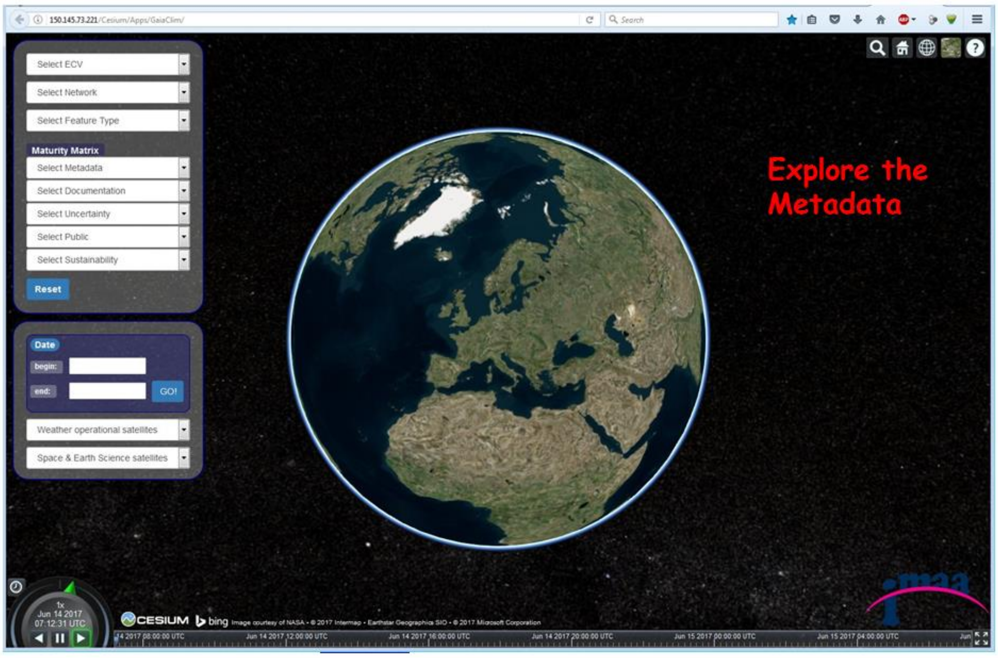


Figure 4: The main menu for exploring the metadata

Figure 5 shows an example 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)[6]. The search can be further refined by choosing a network such as GRUAN as shown in Figure 6.

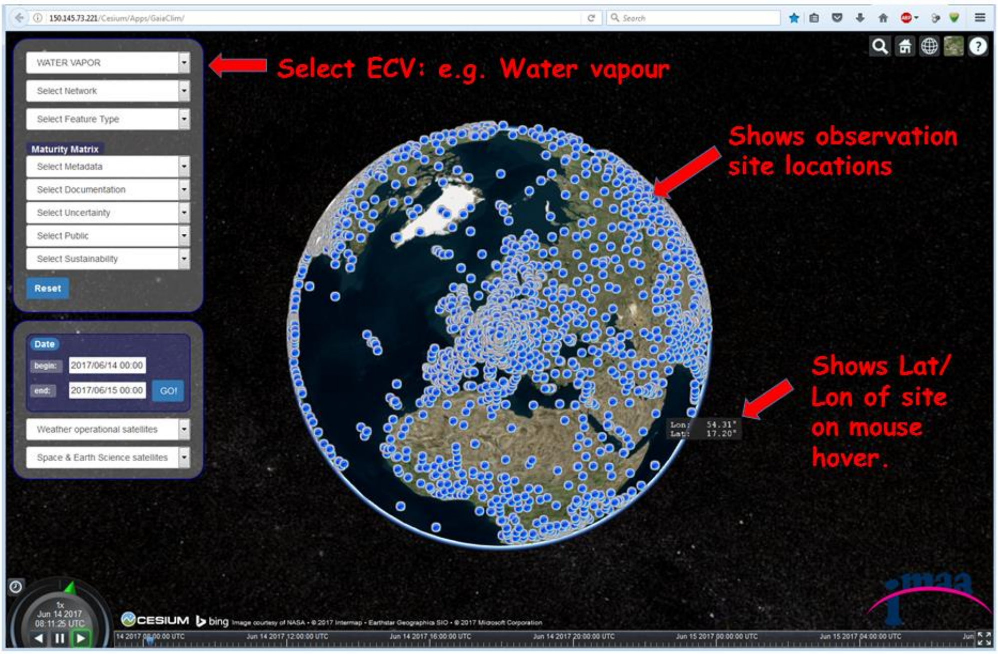


Figure 5: Selecting ECVs.

[6] The Global Observing System for Climate: Implementation Needs. (GCOS-200): https://unfccc.int/files/science/workstreams/systematic_observation/application/pdf/gcos_ip_10oct2016.pdf .

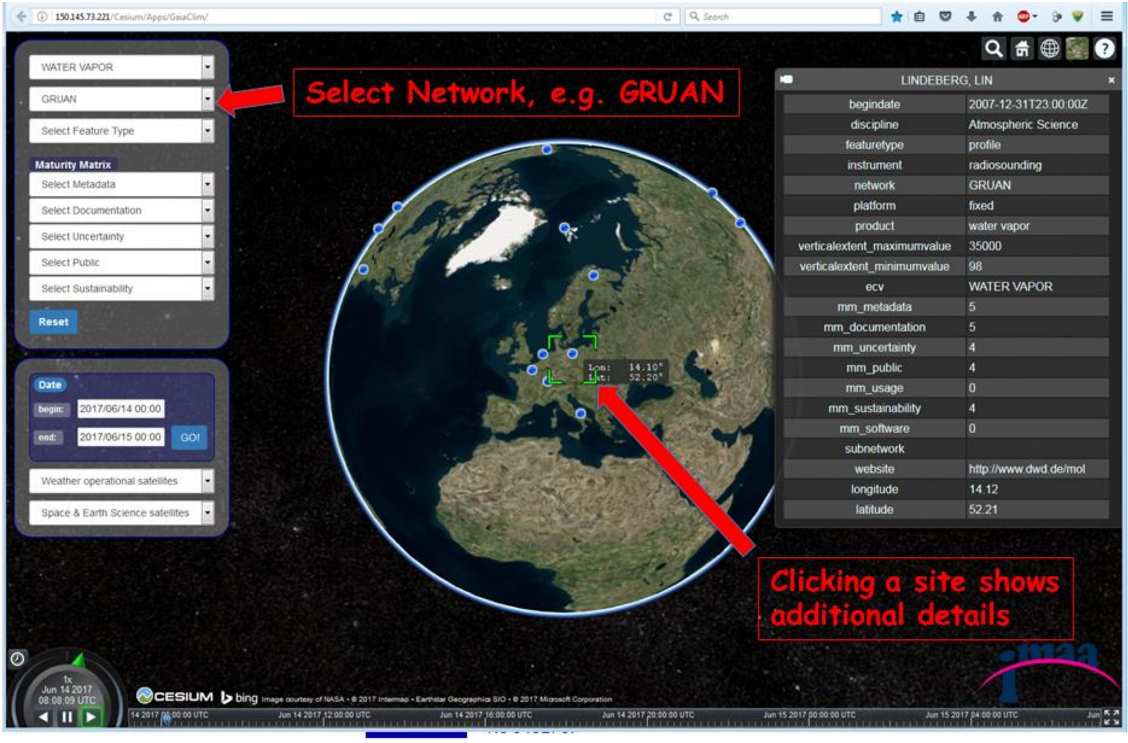


Figure 6: Selecting a reference network

In a next step, the user can explore which satellite observations could potentially be co-located to the chosen reference network by selecting a satellite platform and instrument. The metadata viewer shows the satellite overpass on top of the map, which allows the user to get an overview of at what times of the day each station of the reference network may have a co-location of observations available, depending on choices of space and time coincidence tolerances for the match-ups. Figure 7 shows as an example the overpass for the HIRS instrument aboard the EUMETSAT Metop-A satellite and Figure 8 shows a selection of the ozone observations with the GOME-2 instrument aboard the EUMETSAT Metop-B satellite. In Figure 8 also additional information on quantifiable performance measures for the ground-based network is displayed. Information on the process leading to categorisations for the performance can be found in Thorne et al. (2017)[7].

[7] 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.

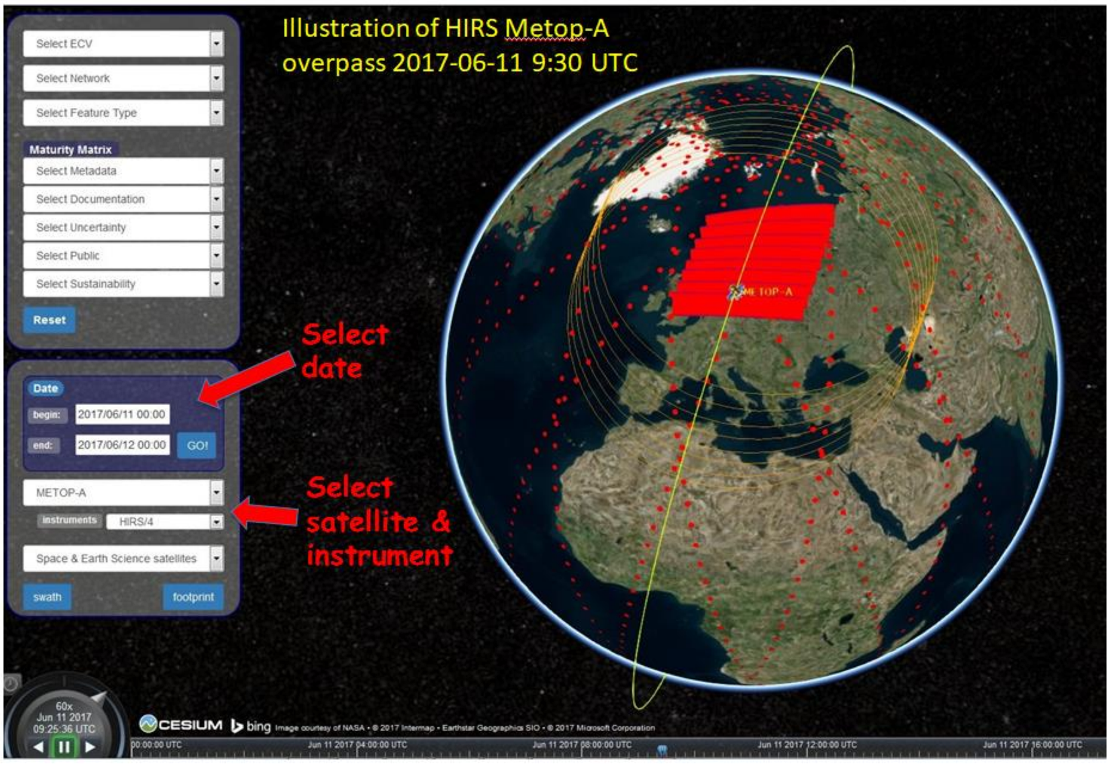


Figure 7: Animation of satellite overpasses

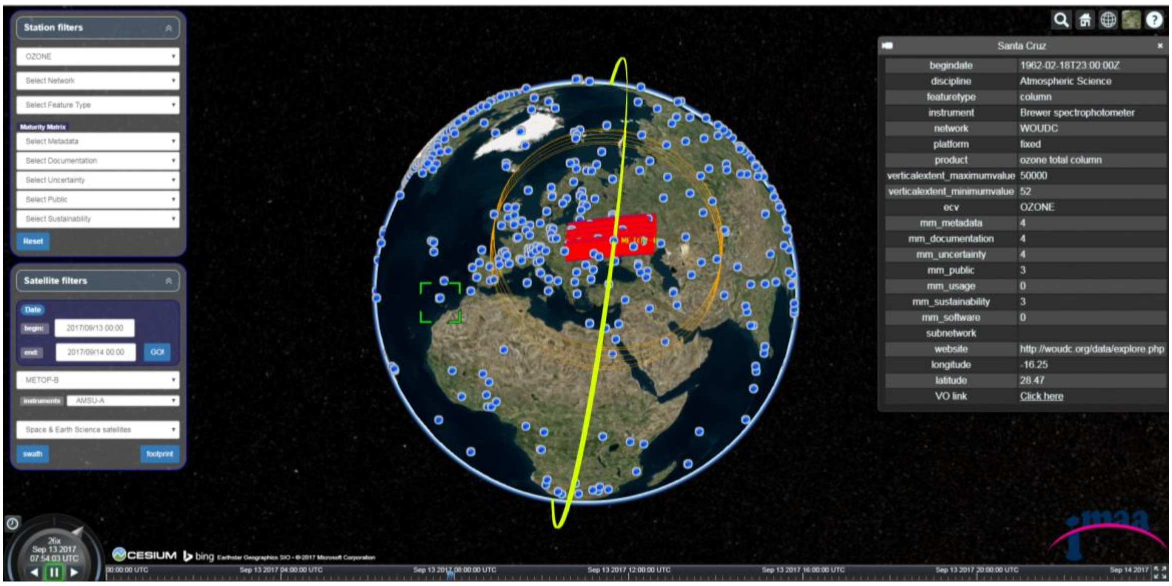


Figure 8: Locations of ozone-network stations performing columnar and profiler ozone observations and the orbit and position of the GOME-2 instrument on the Metop-B satellite.

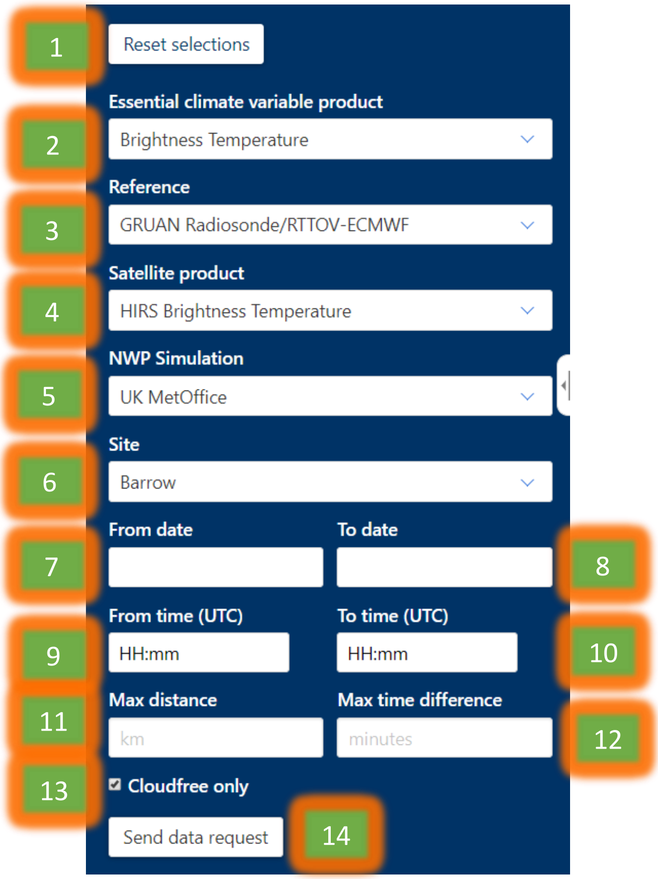


Figure 9. Data selection tool of the VO

4.3 Graphical control system

The GUI of the VO's data selection tool is represented in Figure 9. Graphical control elements of the tool consist of the following options for filtering the data:

1. Reset selections – the user can reset the values of all selections to the initial (default) values;
2. ECV product – the user can choose between three different variables: humidity and temperature represented in brightness temperature space, aerosol optical depth and ozone. The choice made determines the options the user then has for the remaining fields, as well as the types of data that are subsequently presented by the GUI;
3. Reference – here the user can choose between the available reference data for the chosen variables (for example, *GRUAN Radiosonde* for *brightness temperature*, etc.).
4. Satellite product – the user can choose between the available satellite products that match the chosen variable (for example, *HIRS Brightness Temperature* for the HIRS instrument brightness temperature).
5. NWP Simulation – this choice is only valid for the brightness temperature co-locations and selects the NWP model that is used to complement the radiosonde profile above its maximum height and adjusts to the model surface estimates. The user can choose between two available NWP models, *UK MetOffice* and *ECMWF*, respectively;
6. Site – this dropdown menu is populated with all the available sites according to the choices 1-4 the user has made (for example, *Barrow*);

7. 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. The number of available co-locations is updated automatically;
8. 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. The number of available co-locations is updated automatically;
9. 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. The number of available co-locations is updated automatically;
10. 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, The number of available co-locations is updated automatically;
11. Max distance – here the user may enter the maximum permitted distance in kilometers between the observation location of the reference data and satellite observation location, as provided by the database. Only co-locations with distances below or at the given value are considered. If no number is entered, all co-locations consistent with other choices are considered;
12. Max time difference –the user may enter the maximum permitted time difference in minutes between the observation location of the reference data and satellite observation, as provided by the database. Only co-locations with time differences below or at the given value are used. If no number is entered, all co-locations consistent with other choices are considered;
13. Cloud free only – this checkbox is used for choosing cloud-free data only. For those variables where cloud cover is not recorded, this checkbox cannot be used. By default only cloud-free scenes are selected;
14. 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. If no data meets the user specified request, an empty set is returned.

Until the final data request is made, a table showing all available sites, start and end dates and number of observations for each site are displayed in a table on the right. The table is updated dynamically when the user changes any of the selections.

Figure 10 shows the choices of the VO GUI for calculating statistics and data filtering. The part of the GUI represented in Figure 10 consists of the following elements:

15. As a default a time series plot for the selected data is displayed to the right of the data selection panel. For comparison of GRUAN radiosondes to HIRS brightness temperatures the user can in addition click on an individual co-location to display the statistics for all satellite channels for that co-location;
16. The *Show Time Series* button. When an individual co-location for GRUAN comparisons is displayed, this button switches back to the Time Series plot;
17. The *Filter* field above the list of co-locations can be used to further narrow down the set of co-locations, e.g., by choosing a specific time to sort morning and evening satellite overpasses. The list will update itself accordingly to easier select individual co-locations, but the time series plot on the right always contains the originally selected data.

Figure 10 Data sets list

When the user clicks *Send data request*, the plot area opens on the right after the VO has requested and downloaded the requested data from the server. A rotating spinner informs the user that the data is requested and currently being read from the server (Figure 11).

While selecting the variable *Aerosol Optical Depth*, the GUI limits the number of available sites in the listing on the right pane (by default, showing only those having 50+ co-locations available). To see all sites, the user can activate the *Show all sites* option in a checkbox below the selected sites.

This checkbox is activated for the Aerosol Optical Depth only.

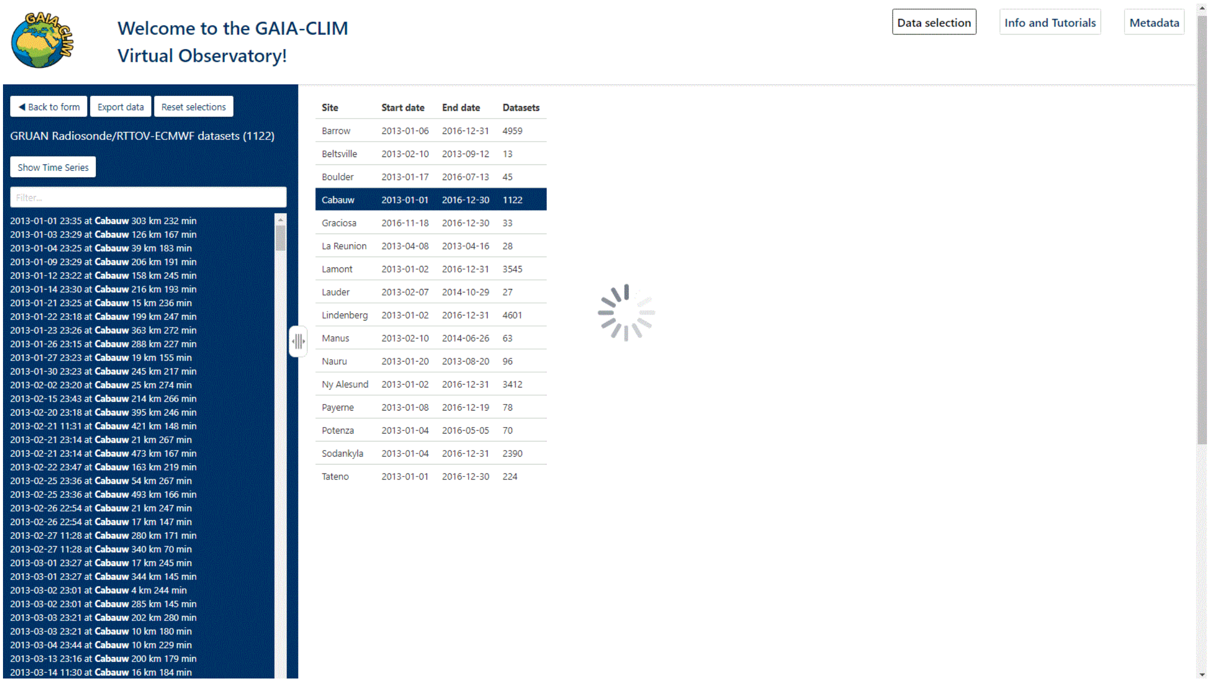


Figure 11 Data loading from the server

Depending on how much or what data the user has requested, the time that it takes for it to load is typically very short. However, if the user has a weak internet connection it may take considerable time or the request may even get a time out. In such cases, the user is advised to reload the page and change the selection parameters.

When the data are successfully loaded, two plots are displayed on the right (Figure 12) – The variable on the left and the differences from the reference on the right. By default, the GUI shows automatically a time series of the variable.

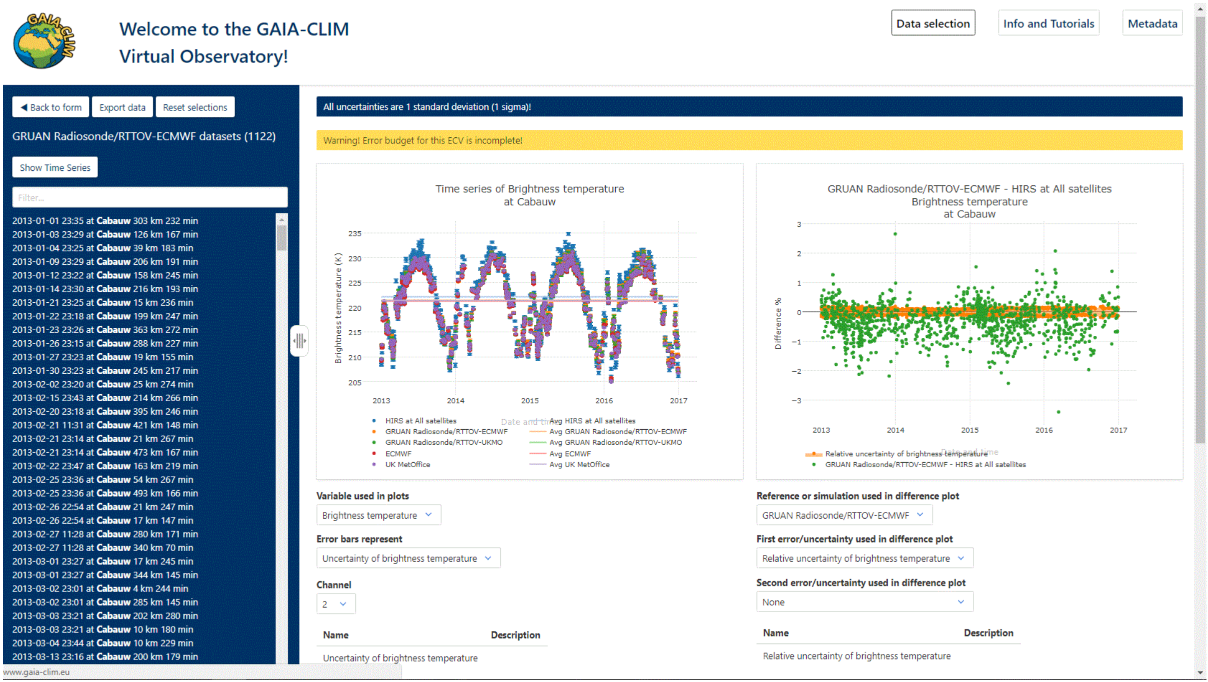


Figure 12 Data plots for HIRS BT time series and differences with a reference at Cabauw

As explained previously for multi-channel satellite data at Level 1, the user can click on any co-location or observation in the list and retrieve additional data to see a plot corresponding to the chosen co-location/observation. For Level 2 data clicking on a co-location data set has no effect.

For the co-located data at Level 1, the user can compare values for reference, satellite and NWP model simulated data. Also, where possible, the uncertainties for the observations are plotted. Below the plots, the user can use drop-down menus to choose between different variables and statistics that are available to be displayed.

There are the following additional buttons above the list of available co-locations / observations, which are presented in Figure 13:

1. Back to form – This choice takes the user back to the initial GUI page.
2. Export data – This choice allows the user to download the selected data, as CF compliant netcdf files, by querying the original files from the database;
3. Reset selections – This choice allows the user to reset all selections and return to the initial GUI page.

Figure 13 Additional buttons

4.4 Exemplified Data Selection Process

This section demonstrates the functions explained above on the example of the comparison of GRUAN radiosonde data to Level 1 HIRS radiances. Selecting the data to be displayed and analysed by the VO occurs by taking the steps presented below:

4.4.1 Step 1: Select a variable

Choose the variable brightness temperature.

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) complemented with NWP model data for parts of the atmospheric column where the radiosonde does not provide measurements.

4.4.3 Step 3: Select a satellite product

From the list of satellite products choose one of the two HIRS brightness temperature options. The HIRS brightness temperature originates from observations 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, the VO focuses 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 high impacts of clouds in the field of view). More information about the HIRS instrument can be found at the EUMETSAT website[8].

[8] www.eumetsat.int/website/home/Satellites/CurrentSatellites/Metop/MetopDesign/HIRS/index.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.

4.4.5 Step 5: Select a reference site

All available reference sites for the current selections are listed in the drop-down list. The list of available reference sites can also be investigated in the 3D metadata tool described in 4.2.

4.4.6 Step 6: Select a date or UTC time limits

Use this for example to consider specific periods in time (plots sometimes get overloaded if time series got too long). Or use the UTC time limits to distinguish between morning and afternoon orbits of the satellite. The table on the right is updated “on the fly”, so the user can adjust the time limits accordingly.

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

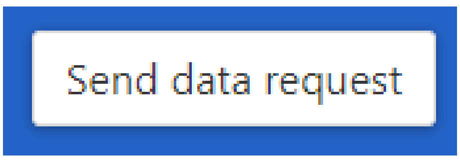
4.4.7 Step 7: Select the maximum distance and time difference

The default co-location criteria are 500 kilometres and 3 hours. Use this window for narrowing down the co-locations to higher spatial and / or temporal proximity. Note that more relaxed criteria are not possible to select.

4.4.8 Step 8: Select “Cloud Free”

The cloud detection for HIRS 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 as all simulations for GRUAN radiosondes are only done for cloud free cases.

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 data for the example above. The user is recommended to watch the on-line video tutorials for a better overview about available choices of the variables and their visualisation (by clicking *Info and Tutorials* in the main menu).

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

- Variable = Brightness Temperature
- Reference Measurement = GRUAN radiosondes
- Satellite product = HIRS Brightness Temperature
- NWP model = ECMWF or UKMO
- Period = 2013-2016

Tip: The user can visualise the results for one co-location or statistics/time-series for all co-locations.

By default, after hitting the *Send data request* button the GUI displays time series of a chosen ECV in plot windows according to the date/time criteria given – i.e., plotting the aggregate statistics (Figure 14 for an example of comparison of brightness temperatures between GRUAN radiosondes, HIRS and NWP fields from the UK MetOffice at Cabauw).

When the user clicks on any of the single co-locations (in case of multi-channel satellite Level 1 data only) listed on the left pane, the GUI plots the results for this specific co-location. Average values over all sets of co-locations are displayed on the left and the corresponding differences from a reference are displayed on the right, as is exemplified by Figure 15.

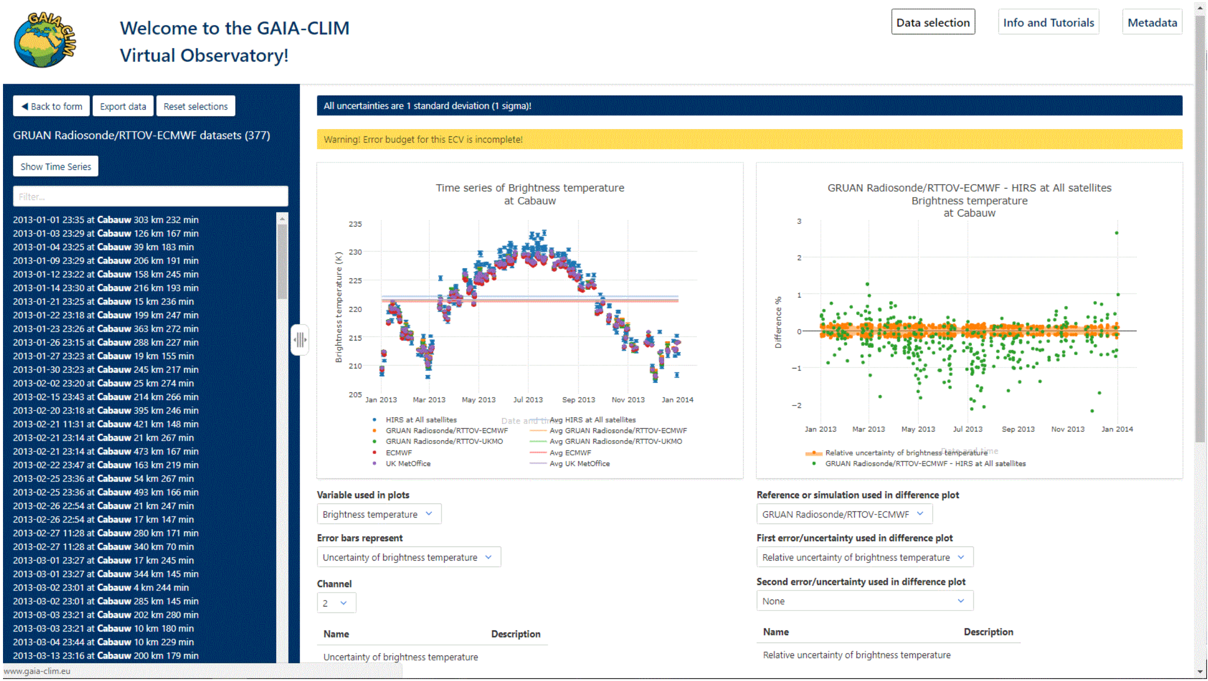


Figure 14: Example of comparison of brightness temperatures using co-located data.

For this multi-channel Level 1 data example, when a measurand for co-location data is plotted, the user may compare co-located HIRS brightness temperatures (represented by blue in Figure 15 with two independent RTTOV simulations using as input atmospheric profiles from either GRUAN radiosondes (orange and green in Figure 15) or NWP fields (red and violet in Figure 15).

On the left plot the number of plotted variables depends on the co-locations available. Currently the VO has four different co-location pairs in its database:

1) GRUAN/UK MetOffice - HIRS
2) GRUAN/ECMWF - HIRS
3) UK MetOffice - HIRS
4) ECMWF – HIRS

Figure 15: Example of comparison of brightness temperatures between GRUAN radiosondes, HIRS, and NWP fields from the UK MetOffice and ECMWF at Cabauw

For example, by selecting GRUAN/UK MetOffice, the GUI searches for all available co-locations between GRUAN/UK MetOffice and HIRS for a selected station. If the VO finds additional co-locations between GRUAN/ECMWF - HIRS, UK MetOffice - HIRS or ECMWF - HIRS with the same timestamp, these are also displayed. If not, we see values only for GRUAN/UK MetOffice and HIRS. Please keep in mind that the number of co-locations for each pair above is different. Therefore, sometimes only values for the selected reference and HIRS are displayed.

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 uncertainty 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. These functions are available for all plots that the VO displays.

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 CF-compliant NetCDF-format. There is one NetCDF file for each set of co-locations, which has been zipped into several compressed files.

5 Limitations

The current version of the VO is a demonstrator, which has been designed and implemented as a proof-of-concept prototype. 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.

General Limitations

- The VO is verified as working with the Chrome, Firefox and Safari browsers. The VO is currently not compatible with Internet Explorer.
- The VO will be transferred to its final server destination at EUMETSAT one to two months after the project due to needed security reviews that shall only be done for the final version. Until then it is running in a development environment that is not optimised for huge number of visitors at the same time. It therefore cannot be excluded that the server has temporal outages or is showing slow response;
- The download speed for the data export function may drop while the user tries to export a “too large dataset”. It is suggested that the number of co-locations displayed on the data list requested should not exceed 150.

Metadata and metadata viewer:

- The metadata database, used in the 3D-metadata tool, is currently not synchronised with the VO database. Due to a rather loose coupling of these two VO components, the “VO link” in the 3D metadata tool will direct the user to the VO main page, but it does not automatically fill the data selection directly for the reference site specified in the 3D-metadata tool.

Caveats and Traceability

- Annex D contains specific information on the level of measurement system understanding, co-location understanding completeness, and general issues in the computation of uncertainties and links to original data sources and the IPR to be respected;
- The GUI is supported with dedicated controls that provide user access to this additional information and any exported data file contains a dedicated subdirectory *disclaimer* to inform the user about all known caveats and restrictions, given as pdf-documents.

6 Access and support

The user can access the online VO platform at http://gaia-clim.vo.eumetsat.int/vo

Note: please, copy and paste this link to your browser (remember the browser limitations a section above).

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 16.

The VO is supported with **video tutorials accessible by clicking *Info and Tutorials*** tab in the GUI main menu, where the user can get more information and practical tips for using the VO.

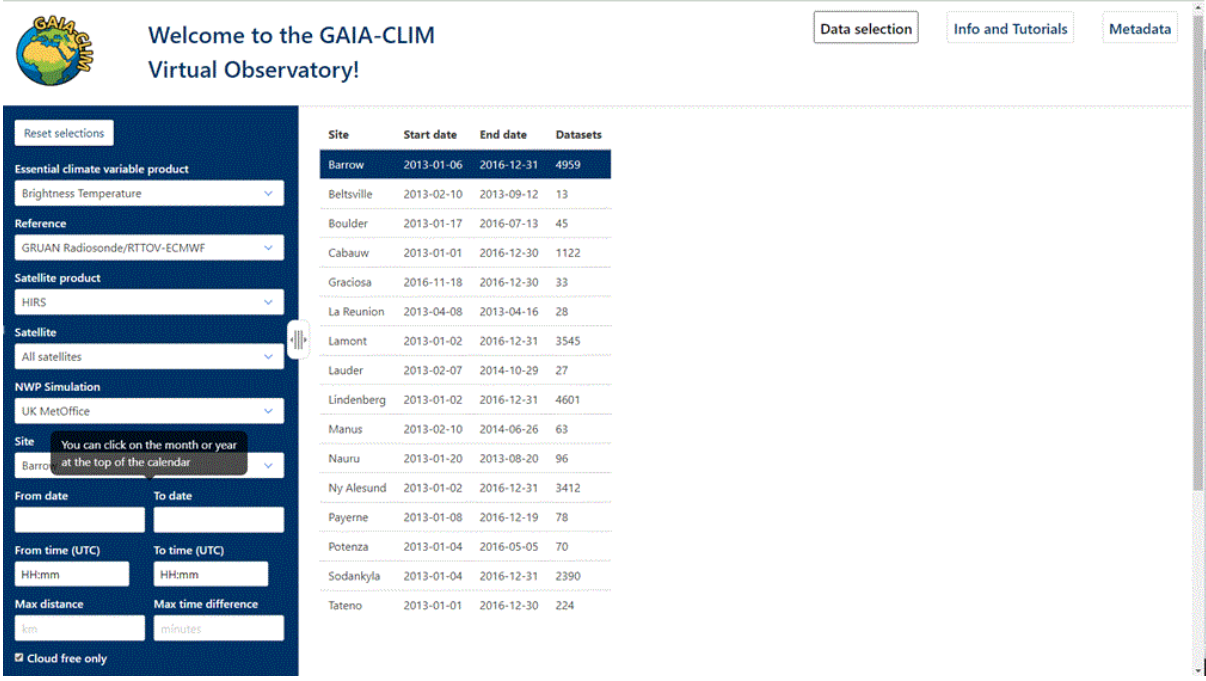


Figure 16: Example of pop-up help window.

Annex A Acronyms

AATSR	Advanced Along Track Scanning Radiometer
AATSR_ADV	A dataset processed with ADV retrieval algorithm for AATSR
ADV	Aerosol Dual View
AERONET	Aerosol Robotic NETwork
AOD	Aerosol Optical Depth
BT	Brightness Temperature
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 Reference Upper-Air Network
GUI	Graphic User Interface
HIRS	EUMETSAT High-resolution Infrared Radiation Sounder
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

Annex B Further Reading

Scientific articles

Bréon, F. M., Vermeulen, A., and Descloitres, J., An evaluation of satellite aerosol products against sunphotometer measurements, Remote Sens. Environ., 2011

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

Virtanen, T. H., Kolmonen, P., Sogacheva, L., Rodríguez, E., Saponaro, G., and de Leeuw, G.: Collocation Mismatch Uncertainties in Satellite Aerosol Retrieval Validation, Atmos. Meas. Tech., https://doi.org/10.5194/amt-2017-420, in review, 2018.

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 available in the VO

Table C.1. Data accessible from the VO.

ECV / Type	Method	From	To	No of co-locations	No of stations
Brightness temperature / Co-location	ECMWF vs HIRS on Metop-A	01.01.2013	31.12.2016	33 096	16
Brightness temperature / Co-location	UK MetOffice vs HIRS on Metop-A	01.01.2013	31.12.2016	51 816	17
Brightness temperature / Co-location	GRUAN Processor (ECMWF) vs HIRS on Metop-A	01.01.2013	31.12.2016	33 038	16
Brightness temperature / Co-location	GRUAN Processor (UK MetOffice) vs HIRS on Metop-A	01.01.2013	31.12.2016	51 674	17
Brightness temperature / Co-location	ECMWF vs HIRS on Metop-B	01.01.2013	31.12.2016	21 432	16
Brightness temperature / Co-location	UK MetOffice vs HIRS on Metop-B	01.01.2013	31.12.2016	21 720	17
Brightness temperature / Co-location	GRUAN Processor (ECMWF) vs HIRS on Metop-B	01.01.2013	31.12.2016	21 411	16
Brightness temperature / Co-location	GRUAN Processor (UK MetOffice) vs HIRS on Metop-B	01.01.2013	31.12.2016	21 689	17
Brightness temperature / Co-location	ECMWF vs HIRS on NOAA19	01.01.2013	31.12.2016	5 716	16
Brightness temperature / Co-location	UK MetOffice vs HIRS on NOAA19	01.01.2013	31.12.2016	23 540	17
Brightness temperature / Co-location	GRUAN Processor (ECMWF) vs HIRS on NOAA19	01.01.2013	31.12.2016	5 708	16
Brightness temperature / Co-location	GRUAN Processor (UK MetOffice) vs HIRS on NOAA19	01.01.2013	31.12.2016	23 497	17
Aerosol optical depth / Co-location	AERONET Sunphotometer vs AATSR on Envisat	01.07.2002	08.04.2012	30 086	527
Ozone / Co-location	NDACC DOAS vs GOME-2	23.01.2007	30.09.2017	12 710	2
Ozone / Co-location	NDACC FTIR vs GOME-2	29.01.2007	21.09.2017	17 409	10

Annex D Credits, Caveats and Traceability

D.1 AERONET Lidar Aerosol Optical Depth (AOD) vs Envisat AATSR

D.1.1 Measurement system understanding

This product was not assessed within the GAIA CLIM project. No Product Traceability and Uncertainty (PTU) document currently exists. Sufficient evidence has not been provided to assess the reference quality status (fully traceable with well characterized uncertainties) of this product from a metrological viewpoint.

Since AERONET, however, imposes a clear standardization of instrumentation, a fully automated measurement protocol, prescribed calibration, real time data reception and centralised processing, and given that a new improved version (Version 3) of the AERONET data has just been released, a full re-assessment of its maturity status is advisable. Typically, the total quantified uncertainty in aerosol optical depth from a newly calibrated field instrument under cloud free conditions is expected to be <±0.01 for wavelengths >440 nm and <±0.02 for shorter wavelengths. These uncertainties are used within the Virtual Observatory, but we stress they lack fiducial reference quality traceability and may be substantially mis-specified.

D.1.2 Co-location understanding completeness

Caveats:

Co-location mismatch uncertainty is derived from measured AOD variability within the co-location window. This is known to be affected not only by the variability of the true AOD but also by (scene-dependent) retrieval uncertainties. As such, it may include measurement uncertainty and will then be an overestimate of the actual co-location mismatch uncertainty.

Reference material:

- Virtanen, T. H., Kolmonen, P., Sogacheva, L., Rodríguez, E., Saponaro, G., and de Leeuw, G.: Collocation Mismatch Uncertainties in Satellite Aerosol Retrieval Validation, Atmos. Meas. Tech., https://doi.org/10.5194/amt-2017-420, 2018.
- Measurement mismatch studies and their impact on data comparisons (GAIA-CLIM deliverable D3.4): http://www.gaia-clim.eu/system/files/document/D3.4%20Paper%20reporting%20on%20measurement%20mismatch%20studies%20and%20their%20impact%20on%20data%20comparison_1.pdf

D.1.3 Data sources and IPR

Official documents can be found on the AERONET NASA – Goddard Space Flight Center (NASA-GSFC) website: https://aeronet.gsfc.nasa.gov/.

D.2 NDACC DOAS Ozone total column vs EUMETSAT AC SAF GOME2 on Metop-A and B

D.2.1 Measurement system understanding

The uncertainty assessment for the UV-vis DOAS ozone product is given in the Product Traceability and Uncertainty (PTU) document: http://www.gaia-clim.eu/system/files/document/ptu_ndacc_uv-vis_totalcolumnozone_final.pdf.

Construction of the PTU document highlighted a number of effects that had not been considered and others that, although estimated in their native units, have not been propagated through the fitting and retrieval processes to the geophysical product. A fully traceable assessment of the overall uncertainty would require element uncertainties on a common (geophysical product) unit base. It is difficult to assess the relative magnitude or make a robust assessment of the overall uncertainty at a range of temporal and spatial averaging requirements. Given the level of the caveats applied, from a metrological viewpoint, this product does not constitute a reference quality measurement series at this time. Users should be aware that the uncertainties while comprehensive are not necessarily complete and lack full traceability at this time.

D.2.2 Co-location understanding completeness

Caveats:

- Estimated uncertainties are of a climatological nature and may not account for extreme events.
- No systematic error estimate for the sampling mismatch is available at the moment. However, it is known to be significantly smaller than the random component in most cases (Verhoelst et al., 2015).
- Uncertainty components are added quadratically, assuming no correlations. Correlations may exist when satellite and ground-based viewing geometries are aligned, in which case the reported uncertainties are too small.

  Reference material:

- Verhoelst, T., Granville, J., Hendrick, F., Köhler, U., Lerot, C., Pommereau, J.-P., Redondas, A., Van Roozendael, M., and Lambert, J.-C.: Metrology of ground-based satellite validation: co-location mismatch and smoothing issues of total ozone comparisons, Atmos. Meas. Tech., 8, 5039-5062, https://doi.org/10.5194/amt-8-5039-2015, 2015.
- Measurement mismatch studies and their impact on data comparisons (GAIA-CLIM deliverable D3.4): http://www.gaia-clim.eu/system/files/document/D3.4%20Paper%20reporting%20on%20measurement%20mismatch%20studies%20and%20their%20impact%20on%20data%20comparison_1.pdf

- Library of (1) smoothing/sampling error estimates for key atmospheric composition measurement systems, and (2) smoothing sampling error estimates for key data comparisons (GAIA-CLIM deliverable D3.6): http://www.gaia-clim.eu/document/library-1-smoothingsampling-error-estimates-key-atmospheric-composition-measurement-systems, including information sheets at: ftp://ftp-ae.oma.be/dist/GAIA-CLIM/D3_6/Ozone/BIRA/ (anonymous ftp)

D.2.3 Data sources and IPR

Information on data formats and protocols is available from the NDACC website: http://www.ndsc.ncep.noaa.gov/ and more instrument-specific information can be found on the NDACC UV-vis working group website: http://ndacc-uvvis-wg.aeronomie.be/

D.3 NDACC FTIR Ozone total column vs EUMETSAT AC SAF GOME2 on Metop-A and Metop-B

D.3.1 Measurement system understanding

The uncertainty assessment for the NDACC FTIR ozone product is given in the Product Traceability and Uncertainty (PTU) document:

http://www.gaia-clim.eu/system/files/document/ptu_ftir-ndacc_o3.pdf.

Construction of the PTU document highlighted insufficient knowledge of the uncertainties of the spectroscopic parameters, and the propagation of these uncertainties through the lineshape model and optimal estimation procedures. Also, some uncertainty components that are currently assumed to be negligible would need to be checked in order to provide a set of fully traceable reference FTIR data products. Given the level of the caveats applied, from a metrological viewpoint, this product does not constitute a reference quality measurement series at this time. Users should be aware that the uncertainties while comprehensive are not necessarily complete and lack full traceability at this time.

D.3.2 Co-location understanding completeness

Caveats:

- Estimated uncertainties are of a climatological nature and may not account for extreme events.
- No systematic component estimate for the sampling mismatch is available at the moment. However, it is known to be significantly smaller than the random component in most cases (Verhoelst et al., 2015).
- Uncertainty components are added quadratically, assuming no correlations. Correlations may exist when satellite and ground-based viewing geometries are aligned, in which case the reported uncertainties are too small.

Reference material:

- Verhoelst, T., Granville, J., Hendrick, F., Köhler, U., Lerot, C., Pommereau, J.-P., Redondas, A., Van Roozendael, M., and Lambert, J.-C.: Metrology of ground-based satellite validation: co-location mismatch and smoothing issues of total ozone comparisons, Atmos. Meas. Tech., 8, 5039-5062, https://doi.org/10.5194/amt-8-5039-2015, 2015.
- Measurement mismatch studies and their impact on data comparisons (GAIA-CLIM deliverable D3.4): http://www.gaia-clim.eu/system/files/document/D3.4%20Paper%20reporting%20on%20measurement%20mismatch%20studies%20and%20their%20impact%20on%20data%20comparison_1.pdf
- Library of (1) smoothing/sampling error estimates for key atmospheric composition measurement systems, and (2) smoothing sampling error estimates for key data

comparisons (GAIA-CLIM deliverable D3.6): http://www.gaia-clim.eu/document/library-1-smoothingsampling-error-estimates-key-atmospheric-composition-measurement-systems, including information sheets at: ftp://ftp-ae.oma.be/dist/GAIA-CLIM/D3_6/Ozone/BIRA/ (anonymous ftp).

D.3.3 Data sources and IPR

Information on data formats and protocols is available from the NDACC website: http://www.ndsc.ncep.noaa.gov/ and more instrument-specific information can be found on the NDACC infrared working group website: https://www2.acom.ucar.edu/irwg.

D.4 GRUAN radiosondes simulated Brightness Temperature (BT) vs HIRS/4 data from Metop-A, B and NOAA-19 satellites

D.4.1 Measurement system understanding

The uncertainty assessment for the GRUAN temperature and humidity profile products is given in the respective Product Traceability and Uncertainty (PTU) documents:

http://www.gaia-clim.eu/system/files/document/gruan_ptu_1.pdf

http://www.gaia-clim.eu/system/files/document/gruan_ptu_2.pdf

The additional GRUAN Processor steps required to convert to the TOA BT has not been assessed. Construction of the PTU document highlighted the 'black-box' nature of the Vaisala radiation correction is the main unknown. A number of minor effects that had not been considered to date exist, but are assumed small. With these caveats applied, the profile data is valid to serve the data from a metrological viewpoint as constituting a reference quality measurement series.

D.4.2 Co-location understanding completeness

Caveats:

While co-location mismatch uncertainties were estimated for temperature and humidity profile comparisons, these have not (yet) been propagated to brightness temperature space. Consequently, the Virtual Observatory at this point does not provide co-location mismatch uncertainties for brightness temperatures.

Reference material:

- Measurement mismatch studies and their impact on data comparisons (GAIA-CLIM deliverable D3.4): http://www.gaia-clim.eu/system/files/document/D3.4%20Paper%20reporting%20on%20measurement%20mismatch%20studies%20and%20their%20impact%20on%20data%20comparison_1.pdf

D.4.3 Other uncertainty issues

- The 'GRUAN Processor' converts GRUAN relative humidity in specific humidity. The conversion uses the Hyland and Wexler (1983) formulation and coefficients. The uncertainty associated with this conversion is unknown.
- The calculation of top-of-atmosphere (TOA) brightness temperature requires information at the surface and above the balloon ceiling:

    - Some surface information (surface pressure, temperature, and humidity) are available in GRUAN metadata but without associated uncertainty.
    - The skin temperature is calculated as follows:

      $$Tskin = Tsurf + \Delta T$$

      where Tsurf is GRUAN surface temperature from the metadata and ΔT the difference between the NWP model skin and surface temperature. The model skin and surface temperature uncertainties are unknown.

    - 10m U and V wind from NWP model fields are used above ocean to calculate the surface emissivity (only apply to GRUAN sites based on small islands: REU, MAN, GRA, NAU, NYA, TEN). The associated uncertainty is unknown.
    - The NWP model sea-ice threshold is used for the calculation of surface emissivity. The associated uncertainty is unknown.
    - Above the balloon ceiling, NWP model fields are used to top-up GRUAN profiles and calculate TOA BT. The associated uncertainty is unknown, but the covariance can be estimated out of an ensemble of profiles.

  These caveats are negligible at frequencies sensitive to mid-tropospheric and upper-tropospheric-lower stratospheric temperature, and mid-tropospheric humidity. Thus, the VO only contains a subset of temperature and humidity channels from the HIRS instrument excluding channels that contain strong emission signals from Earth and cloud surfaces;

- Although the GRUAN processor has the capability to simulate any viewing angle, only nadir simulations have been provided to the Virtual Observatory. This represents an addition source of uncertainty if the satellite viewing angle to which GRUAN profiles are compared to is different from nadir.
- All radiative transfer calculations are done assuming clear-sky conditions, i.e. ignoring the scattering effect. It is recommended to make sure that both the sonde environment and the satellite field of view are clear when compared.

D.4.4 Data sources and IPR

The GRUAN website provides all information about the data, data handling and data products: https://www.gruan.org/

The GRUAN Processor post-processed outputs (monthly averaged profiles per GRUAN station) are publicly available on a demonstrator webpage hosted by NWP SAF:
https://www.nwpsaf.eu/GProc_test/ins.shtml