

GAIA-CLIM Report / Deliverable D3.7

Gap Analysis for Integrated Atmospheric ECV CLimate Monitoring:

Final version of tools for quantification of co-location mismatch and smoothing uncertainties and associated documentation for integration in the virtual observatory that reflects any subsequent updates arising as a result of a. feedback from WP5 and b. any subsequent finessing in tasks T3.1 and 3.2



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Executive summary

GAIA-CLIM, a H2020 project funded by the European Commission, aims to support Europe's Earth Observation programme Copernicus by assessing and improving the fitness-for-purpose of sub-orbital (ground- and balloon-based) reference measurements in the validation of observational data sets from satellites. In particular, the project aims at improved traceability and characterization of uncertainty of the individual sub-orbital measurement (systems) and of the comparison with satellite data.

A key issue in the geophysical validation of satellite data sets with respect to sub-orbital reference measurements is the interpretation of their differences in terms of known, quantified uncertainties. This aspect includes not only the measurement uncertainties associated with the individual measurements, but also the additional (e.g. comparison) uncertainties that appear when comparing different perceptions of the inhomogeneous and variable atmosphere, that is, when comparing data sets characterized with different sampling and smoothing properties, both in space and time. The investigation of uncertainties in comparisons of data sets in spacetime has been the main topic of GAIA-CLIM Work Package 3 (WP3) and results on that have been published in deliverable D3.4 (Fassò et al., 2017).

To translate these developments and results into a practical, usable resource for Copernicus Climate Change Services (C3S) users, two avenues were foreseen within GAIA-CLIM: (1) an integration of (derived) tools into the Virtual Observatory (VO), where they serve to estimate smoothing, sampling, and co-location uncertainties for the data ingested into the VO and for the satellite-ground co-locations performed by that system, and (2) publication of libraries (i.e., guiding material and data files) of such uncertainties for key ground-based measurement systems and for key comparisons. The former avenue constitutes the material for deliverable D3.5 and its update, D3.7, while the latter was the topic of deliverable D3.6.

The current document describes the progress made in the VO tool development since the status presented in D3.5. The library of IASI-GRUAN (T and q) space-and-time co-location uncertainties (UniBG/CNR) is used by the VO as a direct result published in D3.6. All in all, it gives two final tools for implementation in the VO (ozone Look-up Tables (LUTs) were delivered and partly implemented already in D3.5).

The scope and life-time of the libraries delivered as the result of work done in frames of WP3 is actually much broader than the GAIA-CLIM project and its VO as it is targeting C3S. In the limited time-frame, only parts of it can be implemented in the VO.

1. Introduction

The work in WP3 started with a description of the concepts of co-location mismatch in D3.2. Thereafter, the concepts were elaborated further and applied to several case studies in D3.4. The results published in D3.6 translate these developments and results into a practical, usable resource

for C3S users, in parallel with and contributing to an integration of (derived) tools into the GAIA-CLIM VO, where they serve to estimate smoothing, sampling and co-location uncertainties for the data ingested into the VO and for the satellite-ground co-locations performed by that system.

This deliverable D3.7 gives an overview of how the results obtained in WP3 have been embedded in the VO. It is an update of deliverable D3.5, which already described a beta set of tools, documenting subsequent development of improved/new Look-Up Tables and their integration in the VO. The VO developed within WP5 enables end-users to explore, interrogate, extract and analyse co-locations between satellite data and high-quality reference and baseline network data. The tools developed in the frame of WP3 have been integrated into the VO, particularly

1. the ozone co-location mismatch LUTs and
2. the temperature and humidity co-location mismatch LUTs.

“Integration into the VO” means developing additional software for reading/interpreting the LUTs, extracting and/or interpolating the mismatch uncertainties and writing the results into the files of co-located data.

The VO follows a Client-Server architecture that has been described in detail in the deliverables D5.3, D5.4 and D5.5, and is visualized in Figure 1.

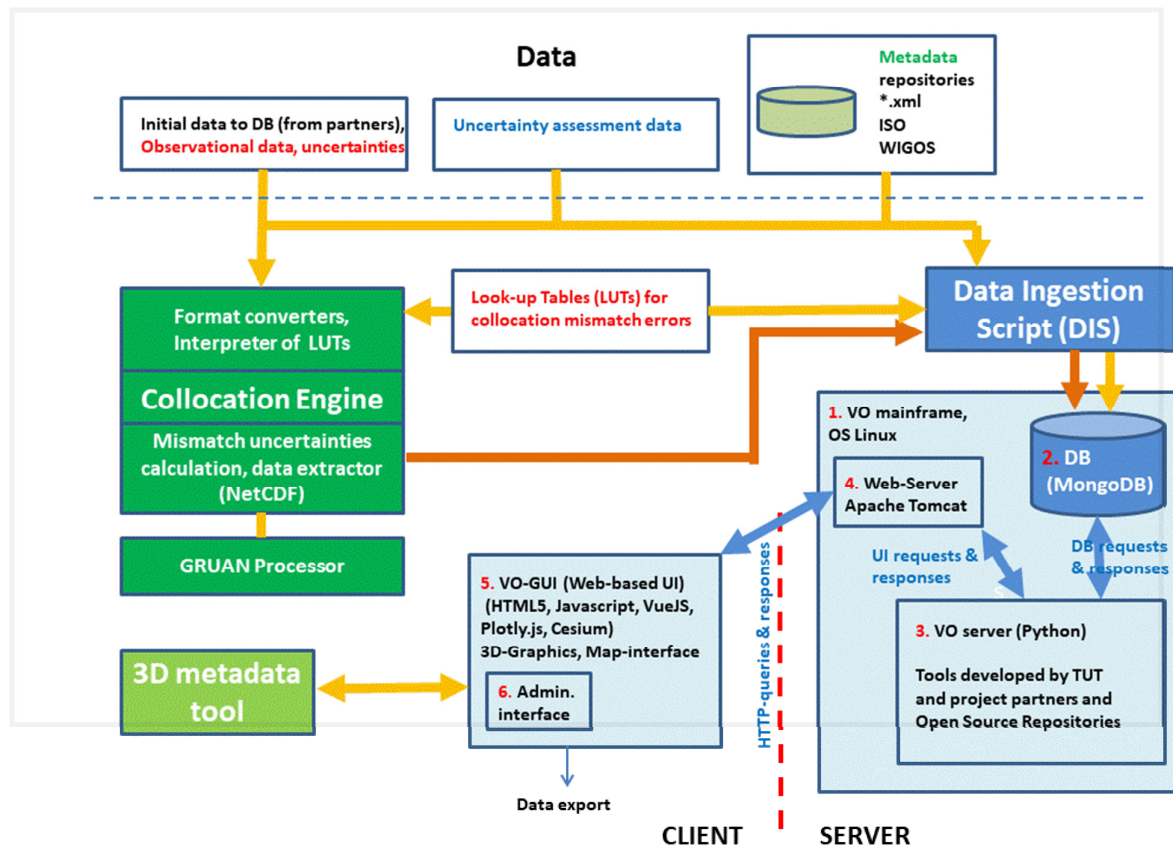


Figure 1: The VO architecture

The functionalities provided by the VO for data management and processing include finding the co-locations, presenting the measurement uncertainties and calculating additional uncertainties due to spatio-temporal mismatch and smoothing errors. The operations dealing with uncertainties arising from mismatch effects are based on the research results originating from WP3.

The calculation of individual unique spatio-temporal mismatch effects and the related data processing is often rather complicated and requires a lot of computing power. The most cost-effective way for the VO to calculate co-location uncertainties is therefore achieved by using LUTs based on the climatological behaviour of a large set of pre-computed co-location uncertainties. Within the VO, the only required operation is then the extraction from -or interpolation within- the LUTs for a given measurement (pair).

Although the LUTs do not by themselves constitute a traditional software tool, they are considered as tools or core-components of any script or module used by the VO for visualization of uncertainties originating from co-location mismatch and smoothing errors. Actually, the LUTs have become inseparable parts of both the Collocation Engine (developed by EUMETSAT on the basis of the STAMP software) and of the Data Ingestion Script (DIS, developed by TUT), illustrated later in Fig. 2. However, in the present version of the VO the DIS does not yet apply LUT's directly. Instead, it uses the LUT's output as extracted by the Collocation Engine. The DIS has been modified to ingest these co-location mismatch and smoothing errors and to store this information according to the needs of GUI for plotting.

Finally, all the tools or technical means (including particular LUTs) developed in frames of WP3 and WP5 as components of the VO and the VO GUI, the data coming from different sources and partners (delivered off-line but ingested into the VO database), the VO Server, its GUI and the MongoDB are all installed at -and hosted by- EUMETSAT server(s).

2. Developments since D3.5

It was indicated in D3.5 (the beta set of tools) that the VO's development status (as of April 2017) did not allow working with co-located data. This has changed. A pragmatic solution has been accepted - working with pre-located data only (limited to the experimental data ingested into the VO database). A related restriction mentioned in D3.5 was that the VO was not foreseen to allow the user to refine co-location criteria. This has been changed as well. The latest versions of the VO GUI allow users to set co-location criteria with only one limitation: the criteria set by a user must stay below the default upper bounds (6 h and 500 km), which results from the fact that this VO prototype (or in fact its database) contains pre-located data only (co-locations found by the Collocation Engine). Subsequently, the user can only squeeze the spatiotemporal co-location criteria, i.e., choosing a subset of all available co-locations for certain ECVs chosen from the database (depicted with an asterisk in Fig. 2). After the user's session is ended, this user-targeted temporary data set disappears (however, it is possible to extract these data into the user's own working environment for further analysis with his/her own tools).

Usage instructions for the VO and GUI with all available options can be found in the VO User Guide (a section of deliverable D5.5).

2.1. Architecture of the VO

The data flow is described in Figure 2. The data for the VO is delivered off-line by different data providers. The observational data is always accompanied by relevant uncertainties. Uncertainties from smoothing errors and co-location mismatch are delivered in the form of pre-computed LUTs. While in deliverable D3.5 (which is describing the tools for quantification and smoothing of uncertainties) the need for a specialized tool/module was foreseen for the implementation of the LUTs (a co-location module and a LUT interpreter), finally, there was no need for such independent module. Instead, the implementation of the LUTs is realised by an enhancement of the functionalities of the Collocation Engine and Data Ingestion Script (DIS), as depicted in Fig. 2.

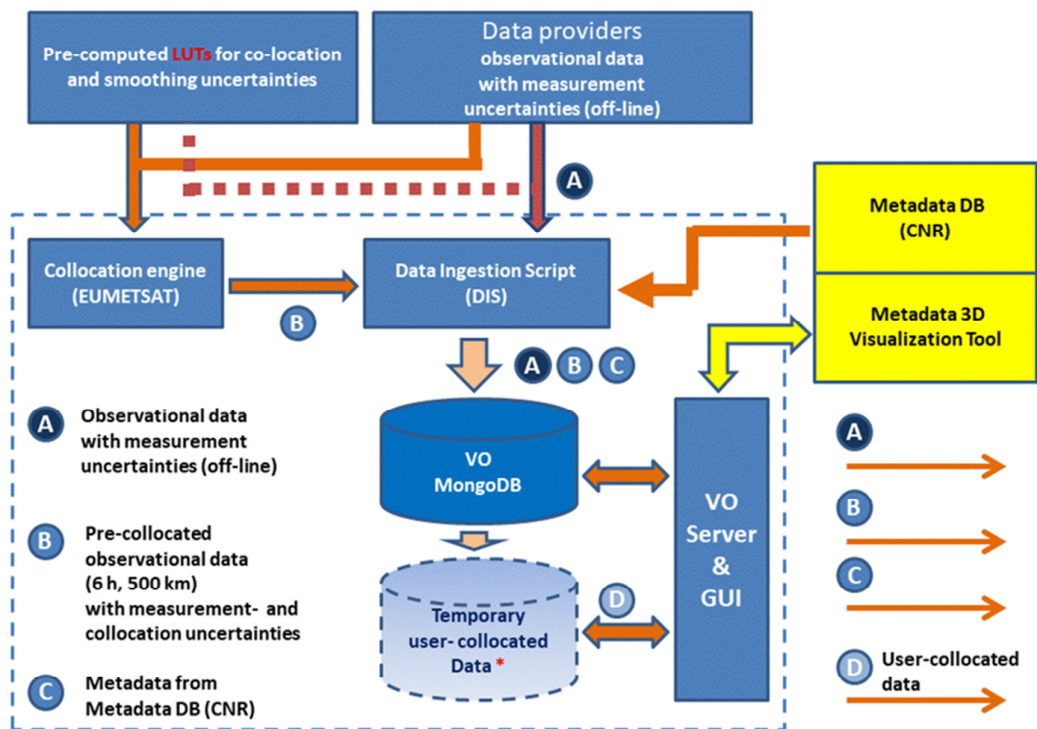


Figure 2: Data flow with uncertainty information in the VO, delivered by data providers.

At the very early stage of the project, it was planned that the DIS would only have the role of data harmonisation and ingestion to the VO database. During the evolution of the project, the calculation of uncertainties from smoothing errors and co-location mismatch was added (i.e., implementation of LUTs) to the desired functionalities.

After the status documented in D3.5, however, the functionalities of the DIS and the Collocation Engine have been revised. Implementation of LUTs in the DIS was put on hold and replaced with adding these functionalities to the Collocation Engine. This solution avoids functional redundancy of these two modules. The Collocation Engine will find the co-locations from the observations available,

calculates the uncertainties by using the LUTs (delivered in D3.5 and D3.6) and compiles NetCDF files of collocated data. These NetCDF files are used as input for the DIS.

The implementation of LUTs in the Collocation Engine follows from the project team's decision to use only pre-collocated data in this prototype version of the VO. As a result, the DIS works only for data harmonisation and ingestion.

The VO Server allows creating new temporary sets of user-co-located observations with appropriate smoothing and co-location uncertainties.

2.2. Integration of WP3 LUTs into the VO

At the time of writing D3.5, LUTs were ready only for ozone, as such serving as pilot examples for the project partners to develop similar LUTs for other ECVs. Since then, the partners have accepted the paradigm of using LUTs and have started to develop their own pre-computed look-up tables following the examples of ozone.

Creating LUTs for all ECVs will make it relatively easy to expand the capabilities of the VO to work with a wide range of co-located observations with appropriate estimation of uncertainties without adding significant computing load to the VO Server.

The ozone LUTs were already developed for D3.5 and only minor improvements are reported in the next section. New in this deliverable are the LUTs for IASI-GRUAN temperature and humidity comparisons. These are built on work done and published in deliverable D3.6.

3. Observing System of Systems Simulator for Multi-mission Synergies Exploration look-up tables for total ozone column

No major modifications have been made to the OSSSMOSE-based LUTs for total ozone column smoothing and co-location uncertainty estimates w.r.t. the versions already presented in D3.5.

The following LUTs were constructed:

1. Smoothing uncertainties for UV-Vis zenith scattered-light differential optical absorption spectroscopy (ZSL-DOAS) measurements (see Section A.1.1 of D3.5),
2. Smoothing uncertainties for direct-sun UV-Vis measurements (Brewers and Dobsons, see Section A.1.2 of D3.5),
3. Smoothing uncertainties for UV-Vis nadir backscatter measurements (e.g. GOME/ERS-2 and GOME-2 on MetOp-A/B, see Section A.1.3 of D3.5)
4. Co-location mismatch uncertainties for various spatial and temporal co-location constraints (see Section A.2 of D3.5)

The only change w.r.t. D3.5 concerns the co-location mismatch uncertainties LUTs (#4 in the above list): the version constructed for D3.5 reported uncertainties for co-locations up to a certain time-space constraint, assuming a set of randomly distributed co-locations within those criteria (dr within $[0, dr_max]$, dt within $[-dt_max, +dt_max]$). As such, they were applicable to the statistics of a set of differences, obtained under the specified criteria. After further development of the VO, it became clear that integration was more straightforward if the LUT could be applied to a single pair of co-located measurements. A new version was therefore constructed which contains the co-location uncertainty at a specific (dr, dt) combination, and this for the following values for dr and dt :

- $dr \in [0.1, 0.5, 1.0, 3.0, 5.0, 10.0]$ in great-circle degrees
- $dt \in [0.1, 0.3, 1.0, 3.0, 10.0, 23.0]$ in hours

A screen shot of the contents of one of the 12 (one for each month) new files is shown in Figure 3.

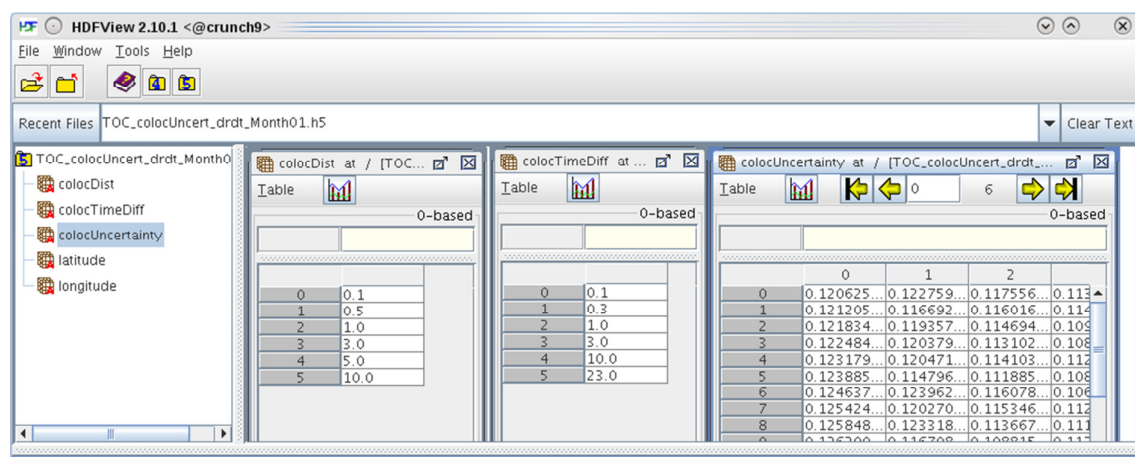


Figure 3: Screen shot of the file contents for the new LUTs for total O_3 co-location mismatch uncertainties, now providing uncertainties at a given (dr, dt) combination (i.e. applicable to a single pair), rather than for a set of pairs randomly distributed up to the criteria (the previous version, reported on in D3.5).

4. Tools for comparing Infrared Atmospheric Sounding Interferometer (IASI) with radiosonde observations

Two main outputs are offered to the end users through the VO regarding the considered study area of Central Europe (CEU) as described in D3.4:

1. Vertical smoothing uncertainty. This is the component of the total co-location mismatch uncertainty due to vertical smoothing. It should be displayed as a profile for each IASI-GRUAN co-location considered. Vertical smoothing are provided as a pre-computed LUT with the entries for pressure, latitude, longitude, season, and day or night, and it can be attached to the observational data for each co-location. Note that vertical smoothing is computed by averaging over CEU and does not depend on the co-location distance.
2. Harmonized co-location uncertainty adjusted for differences in vertical smoothing. Spatiotemporal mismatch uncertainty has been estimated for temperature and humidity as a function of air distance and delay at pressure levels available for IASI. This uncertainty will

be given as a LUT with the entries for pressure, season, day or night, horizontal distance, and time distance (i.e., delay). The LUT of this kind enables the user to easily find this “harmonized co-location uncertainty adjusted for differences in vertical smoothing”.

For the given values of the entries, the harmonized co-location uncertainty has to be considered as an average over CEU. This uncertainty is provided to the VO as a pre-computed stand-alone table. This information can be displayed by the VO either as a 3D-plot or as a contour plot. All these outputs for IASI-GRUAN comparisons developed and provided by WP3 will be used as inputs for the VO, which are uploaded offline onto the VO.

More details are available in D3.6.

5. Further developments

Not all libraries described in D3.6 are actually LUTs – i.e., for calculating mismatch uncertainties. Some libraries cannot be considered “tools”, which help to calculate uncertainties, for instance these libraries already provide uncertainty for specific pre-located measurements.

NPL has offered libraries (in Excel and NetCDF) for radiosonde T and q temporal mismatch uncertainties. These are not implemented in the VO yet, but work is continued to include them later.

Similarly, FMI has delivered a data set of dedicated GRUAN-processed RS92 launches for co-location with IASI. According to D3.6, these data do not present co-location uncertainties but rather a data set of dedicated radiosonde launches (measuring temperature, humidity and occasionally ozone), timed to coincide with IASI/MetOp overpasses, in order to avoid the temporal co-location errors altogether. The launches took place well before the GAIA-CLIM project, but they have now been GRUAN-processed to make them truly reference quality.

This data set is not available in the current version of the VO. Work is continued to include it later. In order to find co-locations and prepare the data for ingestion, we also need to process GRUAN and IASI files with the Collocation Engine.

6. The Collocation Engine (STAMP)

In the H2020 project FIDUCEO (as described in the project deliverable D4.8), one of the tasks for EUMETSAT has been to create co-locations of HIRS data with IASI and AIRS data. EUMETSAT’s in-house Space Time Angle Matchup Procedure (STAMP) co-location tool (A. Lattanzio, 2015a,b), which was originally designed to generate co-locations between measurements from geo-stationary satellites and polar orbiting satellites, has been adapted to create co-locations between measurements of polar orbiting satellites.

It has been the most practical way to create a suitable Collocation Engine for the VO of GAIA-CLIM by modifying and expanding the functionalities of the same tool for finding co-locations with non-

satellite reference observations. The modifications comprise adding necessary data format conversions, adaption of different LUTs (as delivered within the frame of D3.6) for calculating mismatch uncertainties, addition of drift correction for radiosonde observations (see below), determination of per pixel cloud parameters (see below) and the creation of files of collocated observations in NetCDF that include all error and uncertainty information, cloud information and inclusion of up to 48 pixels matching the co-location criteria sorted by effective distance. The choice of keeping a maximum of 48 pixels is a fair compromise of collecting all valid collocation pixels and runtime-memory considerations. The vast majority of collocations have fewer than 48 valid matching pixels.

The working of STAMP is illustrated in Figure 4. STAMP reads in a configuration script that provides the location and type of reference and monitored data set, the collocation criteria, grid sizes, etc. It then reads the geo-location of the reference measurement(s) and searches for any matching monitored observation within a grid cell around the reference measurement. Next, it checks the respective acquisition times and keeps only those collocations that are within the user-defined time window. Then, it checks the observation geometry followed by a check of all data-quality flags that may eliminate further co-location candidates. For the remaining matching satellite pixels, the cloud flags are calculated, if not already provided, and the smoothing and co-location mismatch errors are being read from the LUTs. Finally, all valid data is written into a netCDF output file.

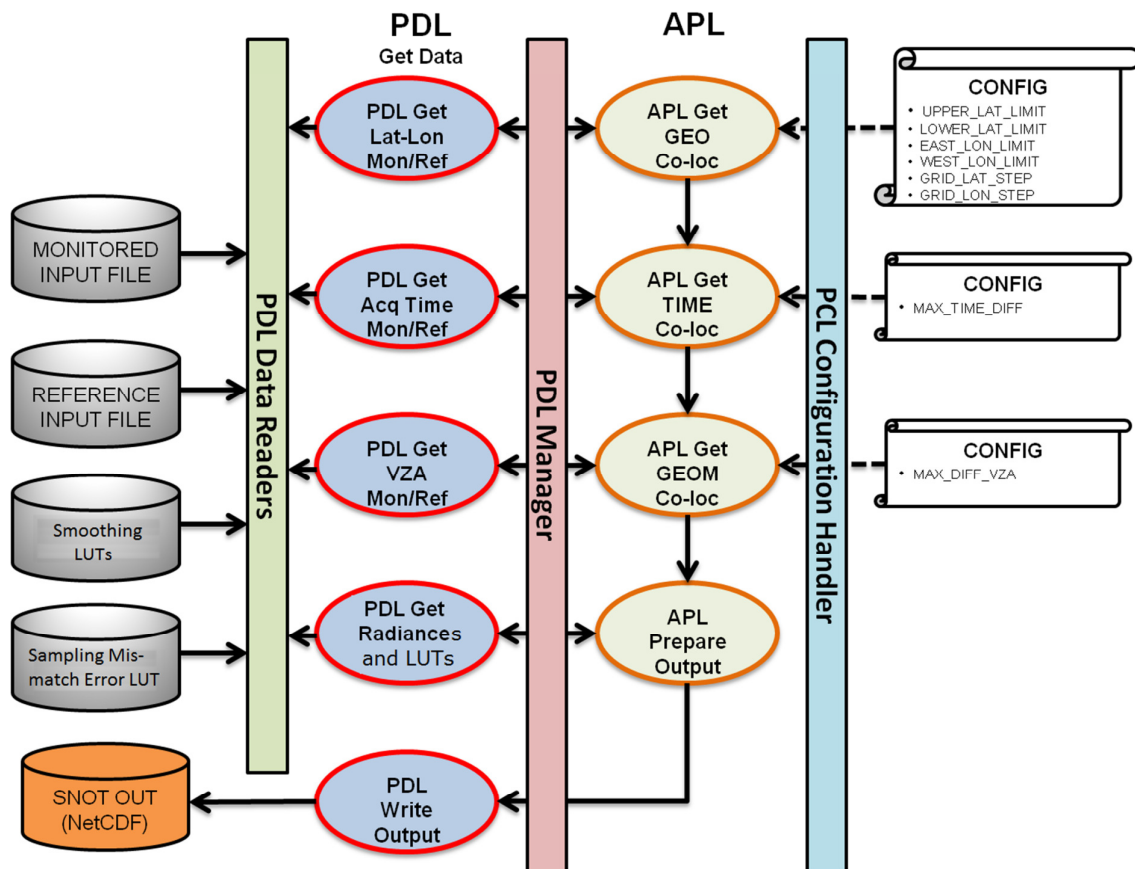


Figure 4: Flow diagram of the Collocation Engine STAMP.

Most observations are either fairly fast (typically a few seconds for satellite imagers) or at a fixed ground location such that only a single data acquisition location pair needs to be considered for the determination of the co-location. However, radiosondes are a notable exception. They take on the order of 1 to 2 hours, sometimes even more, to reach ceiling altitude and they drift with a velocity close to the local wind speeds.

A simple, yet quite effective drift correction has been built into the collocation engine. An analysis of existing Level-1 radiosonde data that used the launch site co-ordinates showed the best agreement with satellite data taken approx. 30 min after the radiosonde launch, which corresponded to an altitude of the GRUAN sonde of about 300 hPa. This is to be expected given typical ascent rates and the location of the bulk of the water vapour in terms of altitude. Hence, instead of the site location, the location of the sonde when it crosses the 300 hPa layer is used to find the nearest collocations amongst the satellite observations. Additionally, the resulting differences in latitude/longitude from the sonde drift are used to derive an airmass-motion vector. The latter is used to estimate the movement of the airmass sampled by the satellite to account for the time difference between the 2 observations of sonde and satellite. This provides an “effective distance” as illustrated in Figure 5.

- Sonde Drift: $\Delta T = T_1(300\text{hPa}) - T_0(1000\text{hPa})$ (approx. 30min) $\Rightarrow \Delta\text{Lat}, \Delta\text{Lon}$
- The best agreement between GRUAN sondes and HIRS BT is found for satellite observations made at $(T_1, \text{Lat}_1, \text{Lon}_1)$. In a first order approximation, we assume that airmasses near the sonde are moving with a speed vector of $\Delta\text{Lat}/\Delta T$ and $\Delta\text{Lon}/\Delta T$.
- Hence with $T_{\text{diff}} = T_1 - T_s$, an airmass sampled by satellite at $(T_s, \text{Lat}_s, \text{Lon}_s)$ is approx. found at $(T_1, \text{Lat}_{\text{Seff}} = \text{Lat}_s + T_{\text{diff}} * \Delta\text{Lat}/\Delta T, \text{Lon}_{\text{Seff}} = \text{Lon}_s + T_{\text{diff}} * \Delta\text{Lon}/\Delta T)$ from which we calculate the effective distance $D_{\text{eff}} = (\text{Lat}_1 - \text{Lat}_{\text{Seff}}, \text{Lon}_1 - \text{Lon}_{\text{Seff}})$ [km].

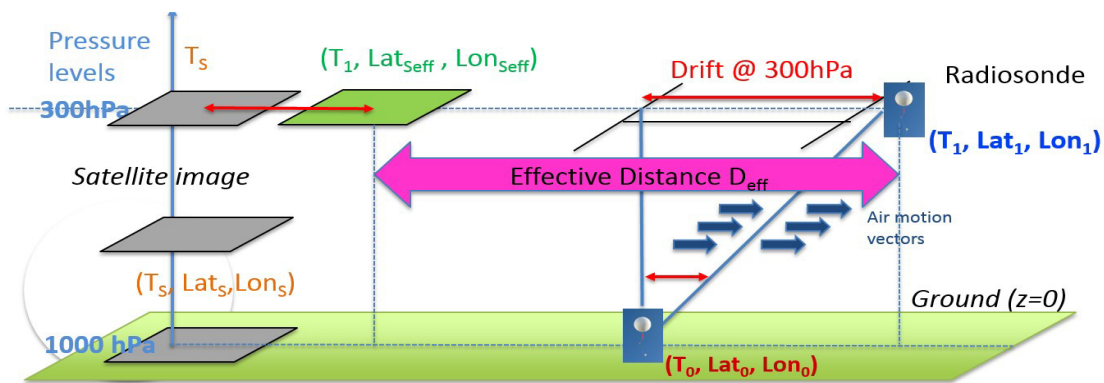


Figure 5: Illustration of a co-location with a radiosonde.

For most of the measurement types, it is important to know whether conditions were clear sky or not. GOME2 data (ozone) provides appropriate cloud information. However, HIRS-4 data products

(water vapour) do not provide any explicit cloud information. Therefore, cloud information is derived following 2 approaches: The water vapour sensitive channels 11 and 12 are not sensitive to low clouds and the method for high clouds by Shi et al., 2013, is implemented and stored with the channel 11 data. From scatter plots we found that a slightly modified criterion after Shi et al., with a cut-off value for the brightness temperature in channel 8 of $BT > 260K$ as opposed to $235K$, results in more “cloud-free” observations without compromising the quality of the cloud flag. This modified high clouds flag is stored with Channel 12 data. All remaining channels are affected by low clouds and the more conservative criterion after Kottayil et al., 2011, is implemented and stored with all channels except for 11 and 12 described above.

The Collocation Engine processes one reference observation at a time and creates one netCDF file per co-location that is then ingested into the MongoDB by the ingestion script. A 2.5 by 2.5 degrees area around the effective reference observation location is searched for any valid satellite pixels fulfilling the co-location criteria. For ingestion, these criteria are a maximal distance of 500 km and 6 hours, which the user may narrow in the VO. Up to 48 collocated pixels, including the nearest pixels, are being kept and sorted by effective distance. The cloud information is derived, as well as the smoothing and co-location mismatch error, for each collocated pixel being stored. The output netCDF file then contains collocated data for one reference observation and all its matching satellite observations from up to 48 pixels with all data listed for each matching pixel, individually. In the case of brightness temperature, 3x3 pixels and 5x5 pixels mean values around the matching pixel in addition to the actual pixel values are being provided, as well as their respective 1-standard-deviations.

7. Practical implementation of LUTs in the Collocation Engine

In D3.5, “the beta-set of tools”, a cost-effective method was proposed to avoid having to integrate numerically demanding models and software for quantifying uncertainties from smoothing errors and co-location mismatch. The adopted approach uses pre-computed LUTs. In D3.5, only LUTs for total ozone column smoothing and co-location uncertainties were described. Since delivering D3.5, the WP3 partners have continued working on characterising co-location-related uncertainties, and LUTs are now also available for temperature and humidity co-location mismatch.

From practical considerations, it has been found most effective to implement usage of LUTs not as an independent software tool (expectation in D3.5), but as an enhancement of the functionalities of the Collocation Engine and DIS. As a result, the usage of LUTs (computing uncertainties for smoothing errors and co-location mismatch) is realized as a step of data pre-processing in the VO.

It has been found that changes in LUT values are quite small in latitude and longitude from one grid-point to another. Therefore, the collocation tool STAMP only picks the nearest latitude/longitude coordinates in any LUT. However, a bilinear interpolation is used for picking the most adequate mismatch error value from the LUTs for distance and time difference of any collocated pixel. Also, no attempt is being made to interpolate in time between 2-monthly mean LUT files for the co-location mismatch error.

8. Conclusions

Within the GAIA-CLIM project, specifically in WP3, several methods for the quantification of smoothing and sampling issues and uncertainties from co-location mismatch have been developed and published in deliverables D3.2 and D3.4. The outcomes of D3.5 and D3.6 have facilitated the integration of WP3 results into the VO, as described in this deliverable D3.7. These tools (developed in the frame of the VO) serve to estimate smoothing, sampling and co-location uncertainties for the data ingested into the VO database for the satellite-ground co-locations. Implementation of these libraries has been the main task for transferring the WP3 results into the VO.

The tools developed in the frame of WP3 have been integrated into the VO, particularly

1. the ozone co-location mismatch LUTs and
2. the temperature and humidity co-location mismatch LUTs.

The integration has been part of software development for the Collocation Engine, including software for data conversion, interpretation of the LUTs and calculation of smoothing, sampling and co-location uncertainties.

The project's timeframe does not allow implementation of all what is developed in WP3 by the end of the project, but just a part of it. Not all tables delivered in D3.6 can be used for calculation of mismatch uncertainties, but they can be considered as tables of pre-co-located data with relevant pre-computed uncertainties (e.g., co-locations for aerosols). Before integrating (i.e., reading and applying) these libraries, which are originally in different format, for other ECVs than total ozone column, an effort has still to be made by means of writing method-specific scripts.

These achievements (i.e., publishing co-location-related uncertainty values or their retrieval methods for all ECVs accessible by the VO) have been starting points for additional software developments in WP5.

Additional work must continue on the:

- Library of radiosonde T and q temporal mismatch uncertainties (NPL)
- Library of AOD spatial and temporal mismatch uncertainties (FMI)
- Data set of dedicated GRUAN-processed RS92 launches for co-location with IASI (FMI)

Each step in the development chain needs its time, as also for evolving from concepts (D3.2) to tests and case-studies (D3.4) up to final libraries offering tables and instructions how to use these results in practical implementations (D3.6). The time left within GAIA-CLIM is too short to implement all what has been made available in D3.6. Though everything can be seen (from WP3 perspective) finished and delivered for implementation, the fact is that each library needs additional work to adapt them working with one software application (the VO).

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Acronyms

AATSR	Advanced Along Track Scanning Radiometer
AERONET	Aerosol Robotic Network
AOD	Aerosol Optical Depth
CALIOP	Cloud-Aerosol Lidar with Orthogonal Polarization
CALIPSO	Cloud-Aerosol Lidar and Infrared Pathfinder Satellite Observations
CEU	Central Europe
DIS	Data Ingestion Script
EARLINET	European Aerosol Research Lidar NETwork
ECV	Essential Climate Variable
GRUAN	Global climate observing system Reference Upper-Air Network
GUI	Graphical User Interface
IASI	Infrared Atmospheric Sounding Interferometer
LIDAR	Light Detection And Ranging
LUT	Look-Up Table
OSSSMOSE	Observing System of Systems Simulator for Multi-mission Synergies Exploration
RAOB	RAdiosonde OBservations
TOC	Total Ozone Column
VO	Virtual ObservatoryAOD Aerosol Optical Depth
CALIOP	Cloud-Aerosol Lidar with Orthogonal Polarization
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