GAIA-CLIM deliverable D5.3

Gap Analysis for Integrated Atmospheric ECV CLImate Monitoring

WP5: Creation of a "virtual observatory" visualization and data access facility

D5.3: "Technological platform for collocation database".

A Horizon 2020 project;

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GAIA-CLIM deliverable D5.3

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[1] Introduction

The objectives of this work package are:

- Creation of a collocation database for satellite and reference measurements including NWP model-based (re)analyses.
- Creation of data interrogation and visualization tools building upon existing European and global infrastructure capabilities.
- Evaluation of the resulting Virtual Observatory to demonstrate its utility for scientific/statistical analysis of respective observations, performance characteristics and the monitoring of instrument and product behaviour over time.
- Provision of a transition roadmap for the Virtual Observatory (including outputs from WP1 through WP4) from research to operational status enabling operational use in Copernicus services.

The main deliverable of WP5 is the Virtual Observatory (VO) facility which will enable users to carry out comparisons of satellite data products to non-satellite reference-quality data. A range of visualisation and analysis tools are to be developed to enable users to explore, analyse, and interact with the data provided within the VO. The Virtual Observatory is built to showcase potential methods by which the underlying scientific advances in WPs 1 through 4 can be made available to a larger user community. It is built in such a way that it could subsequently become an operational service, e.g., as part of the Copernicus services. However, the implementation supported within the GAIA-CLIM project remit shall only serve as a proof-of-concept for an operational VO facility.

Work Package 5 partners are EUMETSAT (lead), Tallinn University of Technology (TUT), and ICARE (University of Lille) with in kind contributions from NOAA in particular with respect to radiosonde processing concepts and data serving. In addition, substantial contributions have been made by many other GAIA-CLIM project partners in the form of software, actual GAIA-CLIM deliverables as well as discussion and support. Work Package 5 integrates and serves the data and products developed in the underlying work packages. Noteworthy contributions from underlying work packages are:

- the metadata database and the CESIUM visualisation tool (WP1 lead CNR),
- error traceability diagrams, measurement system questionnaires, and reference product readiness (WP2 lead BKS),
- Look-up tables for collocation mismatch and smoothing errors derived with OSSSMOSE (WP3 lead BIRA-IASB), and
- the GRUAN processor (WP4 lead UK MetOffice).

[2] Outline of Deliverable 5.3

The “Virtual Observatory” visualization and data access facility, or VO for short, is essentially a functional piece of software with an underlying database which is accessible through the internet. Therefore, this document is only a short description explaining where to find and how to access this online deliverable and putting it into context of other relevant deliverables of the project.

The VO distinguishes itself from existing web portals serving EO data with respect to:

- The traceability of the uncertainties throughout the processing, that is to say that the reporting of uncertainties is complete and each component can be traced back to metrological standards. Further, the collocations include a comprehensive uncertainty budget, i.e. both measurement and collocation uncertainties;
- Comparison of reference data with satellite observations at both level 1 (realised using Radiative Transfer forward modelling) and level 2;
- The provision of a standardised framework that allows users to compare any two observational products that participate, meaning that several independent reference data sets can be compared to data products originating from multiple satellite sensors and/or algorithms for any chosen ECV.

In addition to this short description four video tutorials have been created that explain in detail the present functionality of the VO and should enable a user to reproduce the examples shown and to create queries of his or her own.

The URL of a live demonstration of the VO and the aforementioned video tutorials are listed in Appendix A.

[3] Design of the Virtual Observatory (VO)

The technical design of the VO is based on user requirements derived from the user survey and two user workshops. The user survey confirmed many assumptions made in the proposal, in particular core functionalities such as comparison of data sets, radiative transfer capability, selection tools for data and data formats. A new requirement from the survey is the usage for comparison of reference measurements with climate model data, which will not be implemented within GAIA-CLIM, due to resource limitations, but will be kept as a potential extension towards a climate service usage of the VO in Copernicus.

The technical design specification of the VO has been finalised and the different elements are being implemented. Figure 1 represents the architecture of the VO, consisting of a front end (client) and the back end (server). The co-location data base and the repository of tools belong to the back end, whereas the Graphical User Interface activities (developed under Task 5.2) belong to the front end.

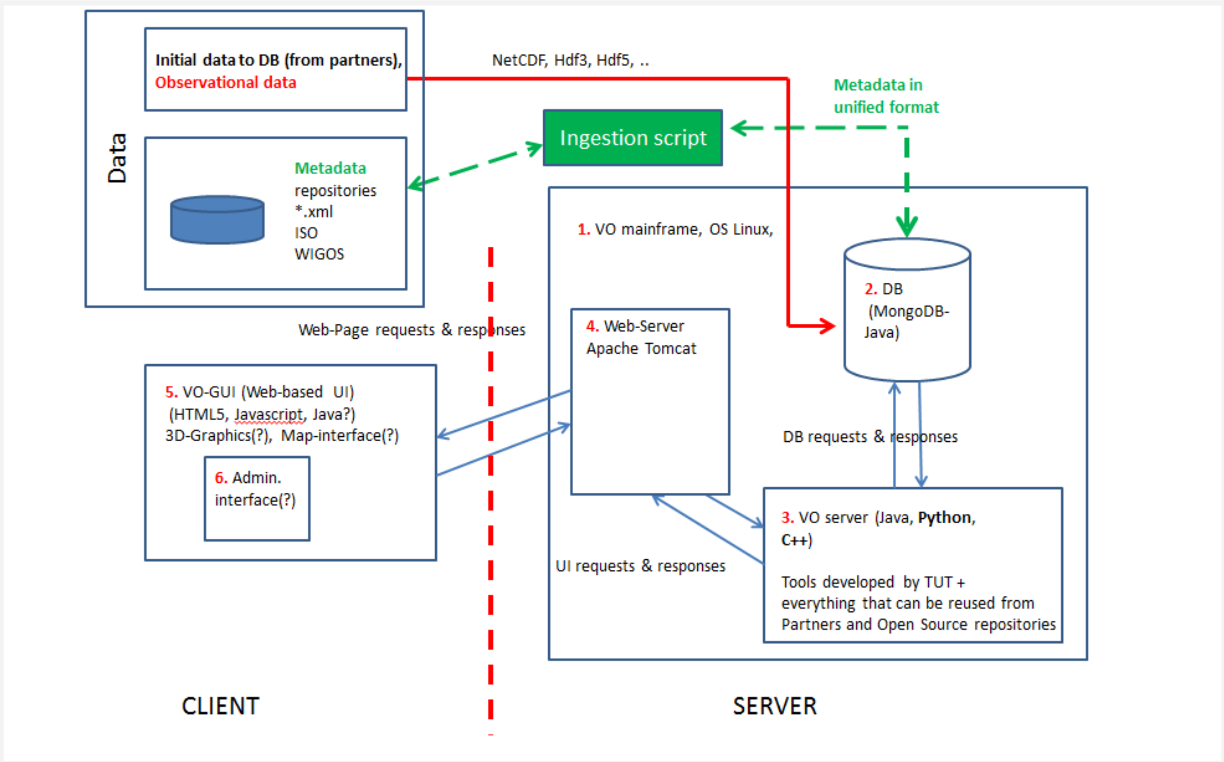

Figure 1: Sketch of the VO architecture – Client (as VO GUI), Server with DB, Web-Server and Server Software supporting the VO and GUI functionalities

The deliverable D5.3 is largely based on Tasks 5.1 and 5.2. The collocation database for satellite and reference measurements is created in Task 5.1 while Task 5.2 creates the graphical user interface and online tools.

Task 5.1 was mostly concerned with the creation of a co-location database of reference quality non-satellite measurements and satellite measurements. The central database has been implemented as a modern object-oriented non-SQL database and the choice has been the open source product MongoDB (mongodb.org). MongoDB was chosen over traditional databases like MySQL, PostgreSQL or OracleDB, because the object oriented approach does not require defining the layout of the database in advance, and the layout and data structure can thus be modified as needed in future in an extendable and seamless manner without the need to convert existing records to the new format each time. This object oriented approach is of great advantage as not all required fields are known at this stage of the project and we anticipate that different future observational data will have slightly different needs, and hence these anticipated changes in data structures will not cause problems. Besides, MongoDB is a mature product with the biggest user base (68 million) amongst the non-SQL type databases, does not entail any licensing costs, is scalable, and works seamlessly across all major operating systems.

The collocation software for the VO benefits from existing tools, (e.g. the EUMETSAT Space Time Angle Matchup Procedure (STAMP) software for co-locations and NOAA NPROVS software suite) and web-based data extraction and visualisation tools (ICARE, http://www.icare.univ-lille1.fr/extract/). It will expand the capabilities of STAMP from satellite-

satellite to satellite-non-satellite measurement comparison, and it will provide more refined data selection tools (e.g. the size of the time window and the radius for a co-location as well as selected metadata and combined measurement uncertainty criteria) in addition to more advanced products, as all combined uncertainty information is included.

Data Base Population Status

The development server for creating the GUI specified in Appendix A holds only small samples of the metadata and of the observational data. The full metadata database is currently held on an internal server at CNR with no public access and the same is true for the observational and collocation database (EUMETSAT/TUT) where ingestion is still at an early stage.

Sample observational data has been ingested into the VO database and been provided to partners at TUT who are implementing the GUI and data visualisation capabilities. These include water vapour profiles from GRUAN radiosondes matching Level 1 and 2 satellite data where the latter has been produced using the GRUAN processor delivered by WP4. In addition, sample ozone observations from NDACC DOAS and FTIR have been ingested into the VO data base.

ICARE has consolidated satellite aerosol data set provision and support including data access tools in anticipation of their future inclusion into the VO database. Although aerosol data sets are not among the pilot data sets being explored during the construction of the VO software, the objective is to include aerosol data sets during 2017.

Feed-back from 2nd user workshop

At the second user workshop in Brussels in November 2016 a preview version of the VO was presented. A lot of useful feedback was collected from users at this opportunity in the form of a wish-list that we converted into a to-do list with specific technical action items. A copy of this document is given in Appendix B and provides important guidance in further GUI development and bug-fixing.

Graphical User Interface (GUI)

The subtask of creating the GUI is lead by TUT with contributions from EUMETSAT, ICARE, NOAA, BIRA, and USTL. A snapshot of the current status of the ongoing task of creating the graphical user interface and user tools which form the front end of the VO can be seen in the live version of the development server and in the video tutorials. The GUI is subject of the next deliverable (D5.4) of work package 5.

A roadmap exists for the further development of the GUI that incorporates the feedback from the 2nd user workshop (see Appendix B for details). Valuable feedback is also expected from the outreach programme that is replacing the 3rd user workshop. However, some flexibility does exist in the roadmap and some decisions have been deferred to a later stage so we can continue to involve the users, but for some questions, more functionality needs to be in place before we and the users can take some of the remaining decisions.

[4] Synergies with our EU sister projects FIDUCEO and QA4ECV

Possible bilateral synergies between GAIA-CLIM, FIDUCEO and QA4ECV projects were discussed with a focus on the web delivery, data streams, data bases, GUI, GUI functionality, data formats, naming conventions, error visualisation and related topics. WP5 key strategists discussed with Thomas Block from Brockmann Consult (FIDUCEO) during the joint GAIA-CLIM FIDUCEO Meeting on the 2nd of February 2017 and with Sander Niejmeier from stcorp.nl (QA4ECV) during the QA4ECV GA on the 22nd of February 2017.

Synergy with QA4ECV

Where possible, synergies aspects between QA4ECV and GAIA-CLIM have been identified and close collaborations was agreed:

- Both projects are agreed on using netCDF as the principal data format for observational data as well as for any derived products;
- Both projects follow the principle of using user requirements as the driver for what is implemented and how;
- QA4ECV has developed a harmonised naming convention system implemented as netCDF fields that GAIA-CLIM is happy to adopt;
- QA4ECV uses an abstraction layer of “vertical dimension” to avoid early individual handling of pressure and altitude schemes. This is an elegant approach and GAIA-CLIM wants to adopt this;
- QA4ECV has standard tools for unit conversions (e.g. from ozone number density, or volume mixing ratio to concentrations etc) that GAIA-CLIM is happy to implement in the same way;
- A lot of mundane but important tools like interpolation of vertical profiles onto a common grid (altitude levels, pressure levels, different vertical resolutions etc) are handled through the BEAT/HARP and file IO through the BEAT/CODA packages within QA4ECV (http://www.stcorp.nl/beat/). GAIA-CLIM had been exploring this route independently (see demonstration given with BEAT/VISAN at the 2nd user workshop) and GAIA-CLIM feels encouraged to further embark on that road. However, unlike

QA4ECV,GAIA-CLIM is offering more control over interpolation schemes to the user, which will make GAIA-CLIM interface different, but not the underlying interpolation algorithm. It is also noteworthy that stcorp.nl is the author of the BEAT packages and GAIA-CLIM may get better support through this informal collaboration.

- We aim to have full interoperability of product files.

The two projects developed different data handling systems. QA4ECV processes big amounts of data that are all processed in one agreed way and it leaves very little control to the user on selection, processing and filtering criteria, which is very different to the GAIA-CLIM position. GAIA-CLIM searches through huge satellite data archives to match high-quality reference quality observations. However, unlike QA4ECV, the latter are comparatively small in number, which is why we put the search results into a database together with comprehensive NWP auxiliary data and then offer to the user very high control over the exact nature of collocation criteria and post-processing according to user specifications. Working file-based as opposed to database-oriented is a natural choice for QA4ECV and it would be highly impractical if not worthless to use a database. Also, given the fact that both projects have only one year left, there is insufficient time and resources left to look for a common solution for both projects in this fundamentally different approach.

Synergy with FIDUCEO

The common FIDUCEO GAIA-CLIM day in February 2017 further solidified the already existing good collaboration between the two projects clearly setting out goals. In particular, the scientific question of water vapour uncertainty budget closure has raised much interest in both projects at EUMETSAT.

On the level of the VO and its backend, the collaboration details may be less well known. Common functionality between FIDUCEO and GAIA-CLIM are:

- Same database system: Mongo DB
- Same satellite data archive
- Same access tools
- Same underlying Linux system that was custom built by GAIA-CLIM.
- Same software for identifying collocations (STAMP).
- Principal data format for derived data sets is netCDF.

During the meeting with Thomas Block from FIDUCEO, discussion about data collocation took place. FIDUCEO is using a very efficient algorithms for faster collocation matching that is based on the google-s2 library that essentially converts all latitude/longitude floating value pairs into an integer based lookup table that uses much less resource and thus is much faster. Although the speed of STAMP has not been an issue for GAIA-CLIM so far this collocation tool may be checked out nonetheless.

FIDUCEO is not planning on any data visualisation, so there is no synergy for the VO GUI. However, given the interoperability of the backend and the close collaboration on the water vapour uncertainty budget closure, results from FIDUCEO would be extremely easy to make available through the VO platform should one wish to do so in the future.

[5] Summary and recommendations

A Technological platform for the collocation database has been created and delivered in agreement with the plans set out in the GAIA-CLIM project plan. We have a well designed and well implemented backend. The metadata database from WP1, which originally had been thought of as a stand-alone product, has been fully integrated into the VO. This eliminates potential inconsistencies between observational data and corresponding metadata and presents to the user in a one-stop-shop experience thus excelling the original project plans. This has only been possible through the excellent collaboration with WP1 who did most of the hard work on this feature.

All basic functionality promised for this deliverable has been delivered and the interactive GUI and is usable. 2D-plots are implemented for a number of different reference products. Video tutorials have been produced that fully guide new users. However, we will have to keep up a fast pace to get a lot more functionality, in particular around collocated data sets, into place before the submission of D5.4.

We plan to update the GAIA-CLIM community regularly on VO progress and invite them and previous test users to try new features and provide feedback on their experiences so GAIA-CLIM VO developers can use this information to continue building the best possible VO for our users within the given resources. We also expect the outreach programme that is replacing the 3rd user workshop to provide important feedback that will improve the usability and relevance of the VO and also helps to create D5.8 (Transition roadmap for the VO) that will take up all feedback. Also, GAIA-CLIM will keep close contacts with the FIDUCEO and QA4ECV projects to support a comprehensive as possible transition of results from FP7 and H2020 research projects into Copernicus Services.

Glossary

BEAT	Basic ENVISAT Atmospheric Toolbox
CESIUM	Cross-platform virtual globe for dynamic-data visualisation in the space and defense industries
CODA	Common Data Access toolbox
DOAS	Differential Optical Absorption Spectroscopy
ECV	Environmental Climate Variable
EO	Earth Observation
FIDUCEO	Fidelity and Uncertainty in climate data records from Earth Observations
FTIR	Fourier Transform Infrared Spectroscopy
GRUAN	GCOS Reference Upper-Air Network
GUI	Graphical User Interface
ISO	International Standard Office
NetCDF	Network Common Data Form
NDACC	Network for Detection of Atmospheric Composition Change
NPROVS	NOAA Products Validation System
QA4ECV	Quality Assurance for Essential Climate Variables
STAMP	Space Time Angle Match-up Procedure
VO	The Virtual Observatory of GAIA-CLIM
WMO	World Meteorological Organization

APPENDIX A: The Virtual Observatory and Tutorials on the internet

The development server is presently located on a small server at TUT:

http://193.40.13.83/vo/main.html

After clicking on the central puzzle piece labelled "VO" one enters the interactive area of the VO:

http://193.40.13.83/vo/index.html

https://youtu.be/Qt4edW3A8hc GAIA-CLIM.eu tutorial part 1: Introduction

Tutorial part 1 (Introduction): The Virtual Observatory of the GAIA-CLIM project
http://www.gaia-clim.eu

https://youtu.be/VwJCzelAKuI GAIA-CLIM.eu tutorial part 2: Satellite imagery

Tutorial part 2 (Satellite Imagery): The Virtual Observatory of the GAIA-CLIM project
http://www.gaia-clim.eu

https://youtu.be/OeshL9IVTKc GAIA-CLIM.eu tutorial part 3: Metadata

Tutorial part 3 (Metadata): The Virtual Observatory of the GAIA-CLIM project
http://www.gaia-clim.eu

https://youtu.be/MKj0Y00KqMY GAIA-CLIM.eu tutorial part 4: Observational Data

Tutorial part 4 (observational data): The Virtual Observatory of the GAIA-CLIM project
http://www.gaia-clim.eu

Tags: Earth Observation, Climate Monitoring, Satellite Validation, Meteorology, GAIA-CLIM

APPENDIX B: Action items resulting from 2nd user workshop

At the 2nd user workshop in Brussels in November 2016 an early preview version of the VO was presented. A lot of useful feed-back was collected and converted into a to-do list with specific technical action items. A copy of this document is given here.

Table B1: VO action items – details. keys: *A) Priority:* 1=high, 2=normal, 3=low *B) People:* AM=Arndt Meier, HK=Hannes Keernik, NL=Neeme Loorits, NN=to be decided later, tut=TUT to decide on a TUT staff including the new staff planned *C) When ready*: months since the start of the project.

Item	Priority	Task	Difficulty	Owner/ assignee	When ready	Status / comment
1	1	Collocation algorithm working for ingestion	a little more work	AM	22	implemented, currently being tested
2	1	ingestion of selected collocated data sets (GRUAN sondes plus one ozone set)	normal	AM+HK	23	
3	1	Adding NWP fields to collocated data sets - including access to/data transfer from NWP data centers	a little more work	AM	23	
4	1	In the data selection area when in observational data mode, "Data Selection and management area" the first selection should be the "ECV - Essential climate variable" - here we list Aerosols, water vapour/humidity, temperature, Brightness temperature, ozone for a start - perhaps in alphabetical order.	normal		22	fixed
5	1	The second selector should be the "Reference Network/Observational Platform" where we have GRUAN radiosondes, Processed GRUAN radiosondes (BT),	normal		22	fixed

		EARLINET Aerosol LIDAR, NDACC FTIR, NDACC ECC ozone sondes, NDACC uvvis/DOAS, EUBREWNWT Brewer, NDACC Dobson/Brewer for a start.				
6	1	3rd selection area "Include/show model data" tickboxes for "UK MetOffice NWP", "ECMWF NWP" (others may follow later)	normal	depends on items 2 & 3	22	
7	1	4th selection - dynamic list with tick boxes "Satellite sensor" according to separate table on Sheet 2. The ECV is always the same as in the first drop box (by definition), so here goes the name of the instrument or derived product, e.g. IASI/MetopA or GEWEX analysis etc. However, for now this is a dummy field until you get collocation data from me.	normal	depends on items 2 & 3	22	
8	1	5th selection area - dynamic list with tick boxes: "Location Reference Instrument" to be queried from database; would result in "Lindenberg" (and soon many more) for radiosondes.	normal	??	22	
9	2	5th selection area: Start time / End time	easy		22	fixed
10	3	we will possibly dream up more like "pool latitude bands"	normal	??	26	
11	1	review the page layout, in particular when plotting observational data	normal		22	it is better than before. I would make the selection area for the

						observational data (to the left) about 25% less wide giving the extra space to the plotting.
12	1	default y-axis: altitude in [m]. Selectable alternative: pressure in [hPa] (==mbar)	normal		22	not fixed, when plotting ECC ozone sonde, default is pressure on y-axis but should be altitude in m.
13	1	show the total number of observational data records that match each selection (level) - see NORS server for illustration http://nors-server.aeronomie.be/report/	a little more work	something done	22	fixed
14	1	Drop-down boxes/Selections should only list those alternatives that make sense in the context and as a result of selection choices already made. E.g. a radiosonde does not have extinction coefficients. Perhaps Hannes to guide Inna? Questions to Arndt?	a little more work	?i think i have it done	23	partly fixed, may need some refining
15	1	When choosing a new parameter the output lists should be flushed/refreshed	easy		22	fixed
16	1	Reset button to reset all selections and clear all data records	easy		22	fixed
17	1!!	Currently it is not possible to plot Brightness Temperature (e.g. from gruan processed sonde or NWP model) versus Channel. (Not meaningful to plot against altitude or pressure)	easy		22	I still cannot BT is not a vertical profile, it is not plotted against altitude or pressure but channel
18	1	For NDACC ozone sondes I	easy		22	Partly fixed, I can

		was able to print a temperature profile and corresponding uncertainties. However, I was not able to plot ozone concentrations correctly. Besides, there is no 2nd drawing area for e.g. uncertainty profiles.				now plot ozone concentration vs. pressure, but not versus altitude. 2nd drawing area still missing.
19	1	plotting the gruan processed radiosonde Brightness Temperature versus channels. Note that this should be a bar graph, not a line graph, with channel as the x-axis.	normal	there are no Channels in the tabase	22	
20	2	For EARLINET Lidar I was able to plot an extinction coefficient profile (see attachment). Very good. A backscatter plot is created, but there is no curve / data visible in the plot.	normal	yeah, because for backscatter no data in database	22	
21	2	Metadata map projections: The selection of an area is cumbersome - even reducing the shapes to just one could be acceptable to make this really sleek.	normal	do not understand what is wrong	24	
22	3	If displaying multiple networks on a map they should have different colours	easy	randomized markers of 4 colours	24	fixed
23	2	Multiple choice of networks, stations and parameters should be possible	normal	ok in metadata	24	fixed
24	3	Locations belonging to more than one network should display all available metadata and have a kind of 'super site' or mulitple colours	normal	randomized markers of 4 colours	24	

25	3	conversion of volume mixing ratios into concentrations and vice versa (e.g. for ozone and other trace gases, requires pressure and temperature profile) or between relative and specific humidity and water vapour volume mixing ratios.	a little more work		24	
26	2	show the maturity matrix for selected network or site (when requsted by user)	easy	??	23	
27	2	plotting of time series - for scalars like total columns (not profile data)	a little more work		23	
28	2	plotting of time series - scroll and/or animate through a stack of profile data	a little more work		23	
29	2	Collocation criteria: Distance (editable number field in units of km, default 200)	normal		23	
30	2	Collocation criteria: Time difference (editable number field in units of minutes, default 120)	normal		23	
31	2	world map: the zooming out should not go further than 'one earth map', at the moment still 2 x the Earth can appear	easy		22	fixed
32	2	When going to the entry page of the VO (see screenshot) the background image is often bigger than the area in the browser. We do need a scroll bar in that case. Or if we want to go fancy, scale it down to fit the available area (with some lower	easy		22	

		limit perhaps).				
33	2	Pressure when used in plotting should be shown in hPa instead of mbar or other no matter what the input	easy		27	fixed
34	3	User should be able to save the search result and to reload at later session	normal		27	
35	3	Optional export of selected observational data, initially as netCdf.	normal		24	
36	2	hdf5 export of observational data	normal		26	
37	3	visualisation of averaging kernels for FTIR & TCCON profiles	complex		27	
38	3	3d visualisation of sampling footprints	very complex		29	
39	3	in the graph menu: user selection of line thickness and line colour for the graphs	normal		24	
40	3	in the graph menu: Radiobutton for: show corresponding or chosen errors as - envelope - errorbars - none	normal		24	
41	3	Display of uncertainty can be done in extra plot as now or as envelop on profiles. Small uncertainties may become hardly visible in the envelope case. A zoom function would help with that	normal		29	
42	3	in the graph menu: drop down list for type-of-error: - total - statistical - systematic - followed by a list of all other errors related to the data shown	normal		24	

43	3	in the graph menu: selection of colour bar code in case colour represents a value (e.g. when plotting total amounts of ozone on a map using colour to show the amount of ozone)	normal		24	
44	3	Collocation criteria: Transport Corrected Distance (editable number field in units of km, default 200) - put in in grey, to be activated once Arndt has the formulae for it	complex		26	
45	3	Collocation criteria: uncertainty based, k values less than x (editable number field, unitless, default 2) - put in in grey, to be activated once Arndt has the formulae for it	complex		26	
46	3	Profile graphics could include a small map to see where the station is	normal		29	
47	3	location of metadata blips off by 5 deg. Latitude (at times) when moving the map	easy			
48	2	When plotting 'obs.Data' => 'Satellite Image' it can take a long time to load and display the image. The user needs to get an indication whether a data record was found and is being loaded or whether 'no data' was found. Perhaps a display field near the 'reguest data' button is needed, flashing slowly, saying either 'no matching data found' or 'data found. loading...' that stops flashing and is being	easy		25	

		reset to an empty field as soon as the user either starts editing any of the selection criteria fields or when the image has finished loading.				
49	3	When plotting 'obs.Data' => 'Satellite Image' and specifying a "Region of interest" results in no data being plotted at all / nothing happens after hitting "Request data". Perhaps this functionality has not been implemented yet and this feature being a placeholder only ...?	normal		30	
50	2	When plotting 'obs.Data' => 'Satellite Image' and specifying a "Region of interest", the available entry fields should change to "Latitude (North positive)", "Height in degrees", "Longitude (West positive)", "Width (in degrees).	easy		27	