

The Virtual Observatory of GAIA-CLIM

General Assembly, Reading, UK, Feb 2017

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Verhoelst



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 640276.

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Overview

- Progress and achievements in Reporting Period
 - Inputs to the GAID
 - Development of the Virtual Observatory
- Objective of the VO
- Implementation of the VO
- Status of the VO
- Outlook



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WP5 Input to the GAID

- Second input provided for the third version of the GAID contains 10 gaps;
- A number of gaps associated with WP5 identified in version 2 of the GAID have been retired and/or rationalised (governance gaps have been moved out, overlaps to other WPs removed and some gaps have been summarised into one).
- Ongoing work in the project and further consultation with C3S has led to 3 new gaps addressing:
 - the need for an online radiative transfer capability;
 - the need for a more systematic and similar characterisation of uncertainty of the reference measurements;
 - the need for operational provision of reference measurements for operational VO.



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WP5 Input to the GAID

- Latest round of gap questionnaires have been perceived as overly complicated with some questions going beyond what could reasonably be expected to be answered by the gap owner alone.
- Consequently only gaps G5.05, G5.07 and G5.10 have been completed with remaining gaps being partially ready



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WP 5 Tasks and Deliverables

Nr.	WP5 Tasks	Y1	Y2	Y3
T5.1	Co-location database for satellite and reference measurements	1 2 3 4	1 2 3 4	1 2
T5.2	Graphical user interface and tools	1 2 3 4	1 2 3 4	1 2
T5.3	Evaluation of Virtual Observatory			1 2 3 4
T5.4	Transition roadmap from research to operations			3 4

Nr.	Deliverables	Y1	Y2	Y3
D5.1	Initial input from WP5 to the gap analysis and impacts document	4		
D5.2	Review of and input to Gap Analysis and impacts document aspects relevant to WP5		16	
D5.3	Technological platform for collocation database		24	
D5.4	Graphical user Interface			30
D5.5	Virtual Observatory Product User Guide and Implementation Description			30
D5.6	Final review of and update to the GAID from the perspective of WP5			34
D5.7	Report on the evaluation of the Virtual Observatory			36
D5.8	Transition roadmap for the Virtual Observatory (Report)			36



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WP 5 Tasks and Deliverables

Deliverable due 2017-02-28

D5.3 Technological platform for collocation database

We need to clarify with WP7 and with the EU representative (Monica) the format of how this should be delivered.

Is this a copy of the server as a virtual machine on a usb stick? A short report with some screenshots ? Complemented with a live-demo (e.g. via webex)? Or something else?



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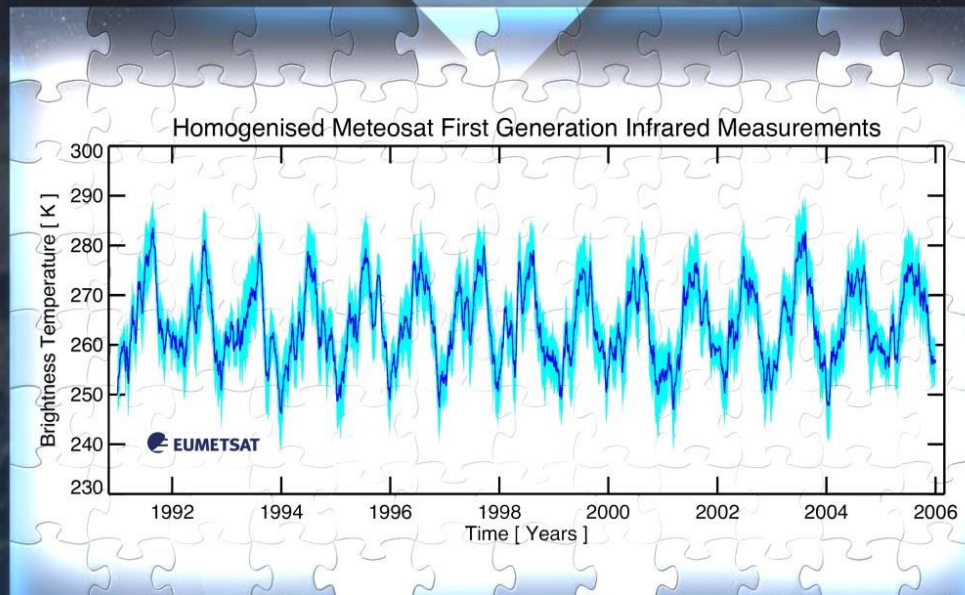
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And now over to the Virtual Observatory...



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Objective

- Unearth potential of and enhance exploitation of ground-based reference data for satellite sensor and product validation through organising access to data and comparison results;
- Integrate ground-based and in-situ reference data with existing satellite-satellite comparisons and observation feedback from NWP models and reanalysis;
- Increase awareness among users of satellite and non satellite data on the concept of traceable uncertainty estimates;
- Provide a facility that can support Copernicus Services to analyse product quality in a sustainable routine mode.



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Implementation

- The VO consists of an object-oriented modern data base (MongoDB) that holds selected earth observations.
- It provides the functionality to select, explore, visualise, compare, analyse and export selected pairs of climate data sets.
- Data sets that have been identified by WP2 as being of “reference quality” are ingested into the VO.
- Each data record is matched with one (or several) co-located satellite observation using fairly generous co-location criteria. These are stored as observation pairs in the data base.
- Users may select subsets according to their own, typically stricter, co-location criteria based on distance, time difference and dynamic quality criteria (e.g. combined measurement uncertainties).



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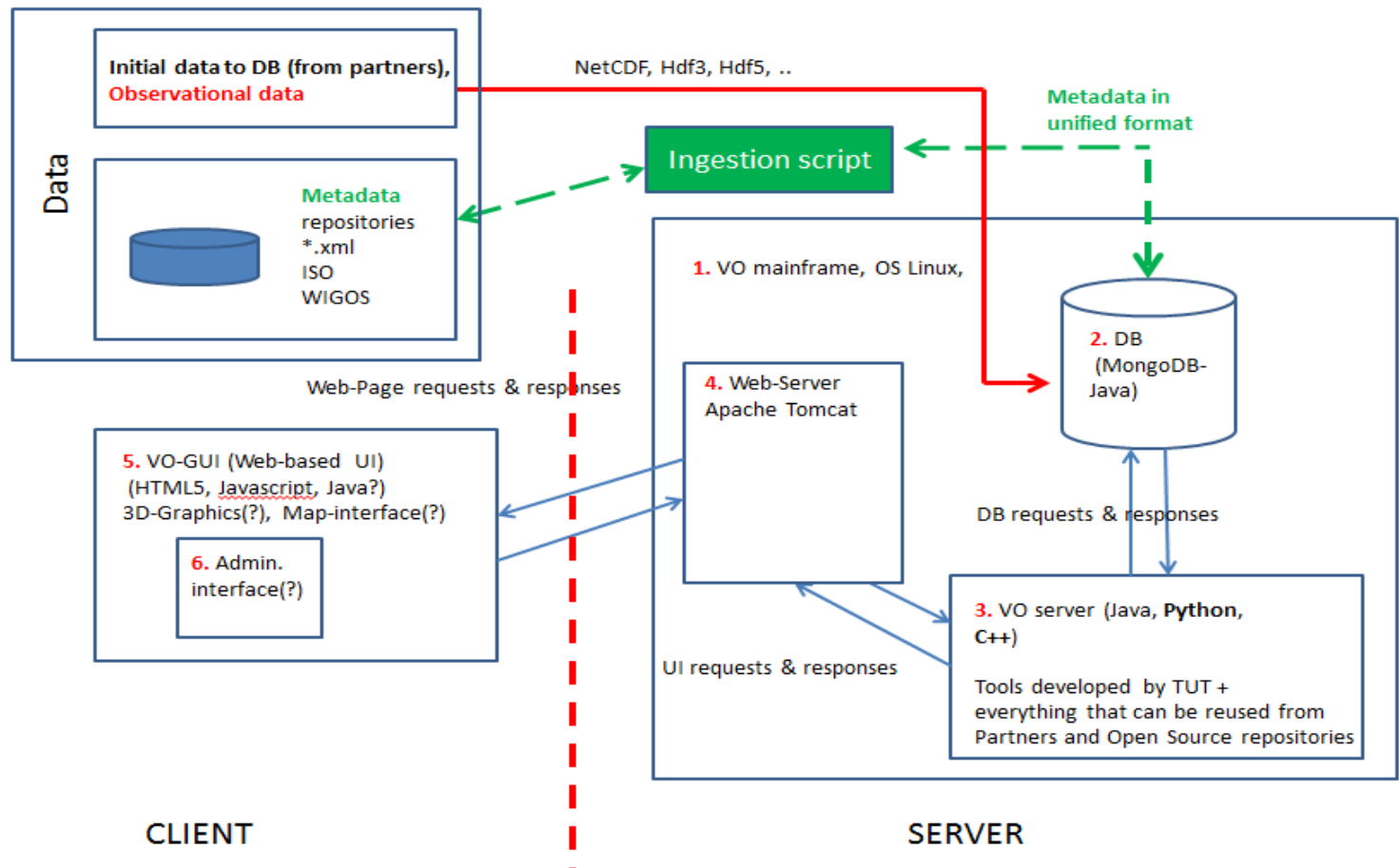
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GAIA-CLIM Reference Observation Readiness Table

	measurement technique	ECV	Readiness of uncertainty chain	Smoothing & Mismatch errors
Task 2.1.1	LIDAR	aerosol	ready	OSSSMOSE: target is mid 2017 Empirical methods: tbd
	LIDAR	H2O profiles	ready within GAIA-CLIM (mid-2017)	OSSSMOSE: late 2017 Empirical methods: tbd, but possibly earlier with STAT4COLL
	LIDAR	O3 profiles	ready	Target: ready by end of 2016 (OSSSMOSE)
	LIDAR	temp profiles	partially ready, remaining part ready within GAIA-CLIM (mid 2017)	Early 2017
Task 2.1.2	MWR	water vapour profiles	not ready within GAIA-CLIM	Late 2017
	MWR	temperature profiles	not ready within GAIA-CLIM	Early 2017
	MWR	total water vapour content	not ready within GAIA-CLIM	Early 2017
	MWR	total liquid water content	not ready within GAIA-CLIM	tbd
Task 2.1.3	FTIR (NDACC)	CH4	ready	Possible by end of 2016
	FTIR (NDACC)	O3	ready	Target: ready by end of 2016

	FTIR (NDACC)	MUSICA H2O	ready	OSSSMOSE: not ready within GAIA-CLIM Errors to be derived from NWP (WP4) and STAT4COLL results - 2017
	FTIR (NDACC)	MUSICA H2O isotopologues	ready	not ready within GAIA-CLIM
	FTIR (TCCON)	CH4	ready	Possible by end of 2016
	FTIR (TCCON)	CO2	ready	tbd
Task 2.1.4	UV-vis/ DOAS Dobson/ Brewer EUBREWNET	O3	ready within GAIA-CLIM (mid-2017) selected stations earlier	Smoothing: Ready Co-location mismatch: ready for comp. with GOME-2A/B
Task 2.1.5	MAX-DOAS/Pandora	Trop. O3	not ready within GAIA-CLIM	Possible early 2017
Task 2.1.6	GNSS	total column water vapour	to be determined	Unlikely within GAIA-CLIM
---	NDACC ozonesonde	O3 profiles	early 2017	Target: ready by end of 2016 (OSSSMOSE)
---	GRUAN radiosonde	Humidity & Temp profiles (Level 2)	ready	OSSSMOSE: not ready within GAIA-CLIM Errors to be derived from NWP (WP4) and STAT4COLL results - 2017

Architecture of the VO



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Satellite sensors targeted

Measurand	Satellite instrument
Level 1 Satellite Data Comparison	
Brightness Temperature (from GRUAN sondes)	Infrared Sounding: IASI, HIRS (FIDUCEO) Infrared Imaging: MVIRI, SEVIRI, (A)ATSR Microwave Sounding: MHS, AMSU-B, SSMIS, SAPHIRE Microwave Imaging: GCOM-W AMSR-2, FY-3C, GPM-GMI / MTVZA
Level 2 Retrieval Comparison	
Water vapour total column	CM-SAF products (SSM/I, ATOVS) Products available from GEWEX Water Vapour Assessment
H2O profiles	EUMETSAT and NOAA Metop IASI L2
upper troposphere humidity	CM SAF MVIRI, MSG/SEVIRI, (CM SAF AMSU-B, MHS)
Aerosol	(A)ATSR (ESA CCI), Parosol, MODIS (AQUA+TERRA), CALIPSO, ALAMO, EUM PMAP (GOME-2, IASI, AVHRR, SENTINEL3, SLSTR, OLCI)
Ozone and other trace gases	EUM L2 products GOME-2, IASI, O3M SAF , OMI, (TROPOMI)



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Status of the VO

- The common data base for metadata and observational data (MongoDB) has been established
- Harmonization of different metadata formats and data-sets (developed “unified metadata format for VO” supporting the ISO, WIGOS, CCI-CF standards). Our thanks to WP1 for providing most of this.
- The Ingestion of discovery metadata is complete.
- Back-end utilities are in place to support http-requests to the DB.
- Realised the root principle of data handling in the VO – reaching observational data over its metadata
- Basic functionality for selecting and visualizing metadata has been established
- Export of search results (.json)



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GUI of the VO: Reference Site Info

Home Overview Networks Methods Documentation Help

Networks

Earlinet

Data type

Metadata

Geometry

Polygon

Polygon coordinates, type: long, lat, long, lat..

16.008,69.278,-
7.912,38.568,33.04,34.67,27.54
3,62.738,16.008,69.278

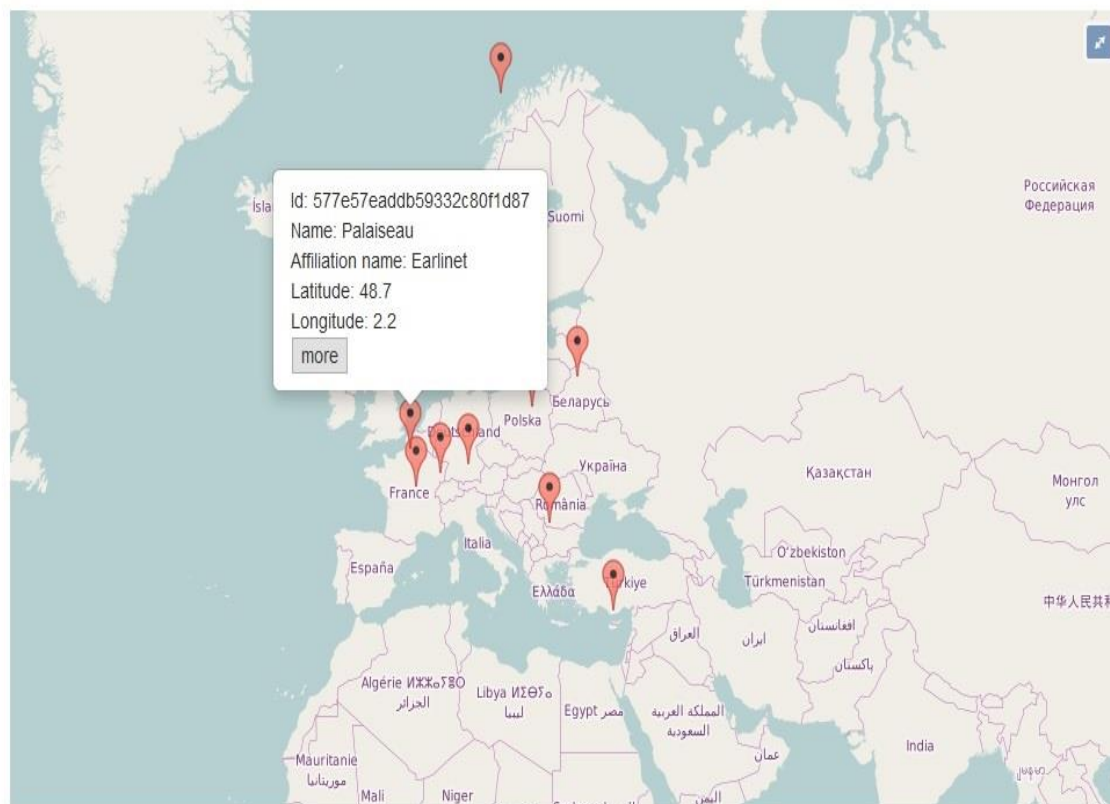
Measurand

Aerosol

☐ Layering by Network

☐ Layering by ECV

Show



Save as Image

Save as CSV



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GUI of the VO: Maturity Matrix

Home Overview 1 Overview Networks » Methods Documentation Help

Compile data

Server URL

TUT

Data type

metadata

Search by Name

GRUAN

Search geometry

rectangle

circle: [lon,lat]

[lonMin,latMin]

-130.0,10.0,3

Measurand [ECV]

temperature

Measurand [min, max]

Layering by Network

Some GIF to here..

Metadata	Documentation	Uncertainty characterization	Public access, feedback and update	Usage	Sustainability	Software (optional)
Standards	Formal Description of Measurement Methodology	Traceability	Access	Research	Strong environment	Coding standards
Collection level	Formal Validation Report	Comparability	User feedback mechanism	Public and commercial exploitation	Scientific and expert support	Software documentation
File level	Formal Measurement Data User Guidelines	Uncertainty Quantification	Updates to record		Programmatic support	Portability and numerical reproducibility
		Routine Quality Management	Version control			Security
			Long term data preservation			

Legend

1 2 3 4 5 6 Not applicable

5000 km

Layering: Network



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Status of the VO (continued)

- The GRUAN processor (RTTOV radiative transfer model) from WP4 has been installed on the VO Linux workstation and it has recently been upgraded to version 4.3 (RTTOV 11.3)
- >4000 GRUAN radiosonde sounding data and corresponding RTTOV derived brightness temperature profiles as well as matching NWP simulations from the UK MetOffice Model have been ingested into the VO database.
- GUI: The menu structure has been largely decided and implementation is ongoing.
- Observational data can be selected by Measurand, Reference Network/Instrument, Monitored Satellite Instrument (in progress) and/or NWP as well as by time interval and or site(s)
- User selected co-location criteria have not been implemented just yet
- Basic 2d plotting of e.g. radiosonde profiles is working
- Any parameter in the data file can be plotted against altitude or pressure
- Implementation of plotting of time series or statistical analysis of data is still in progress

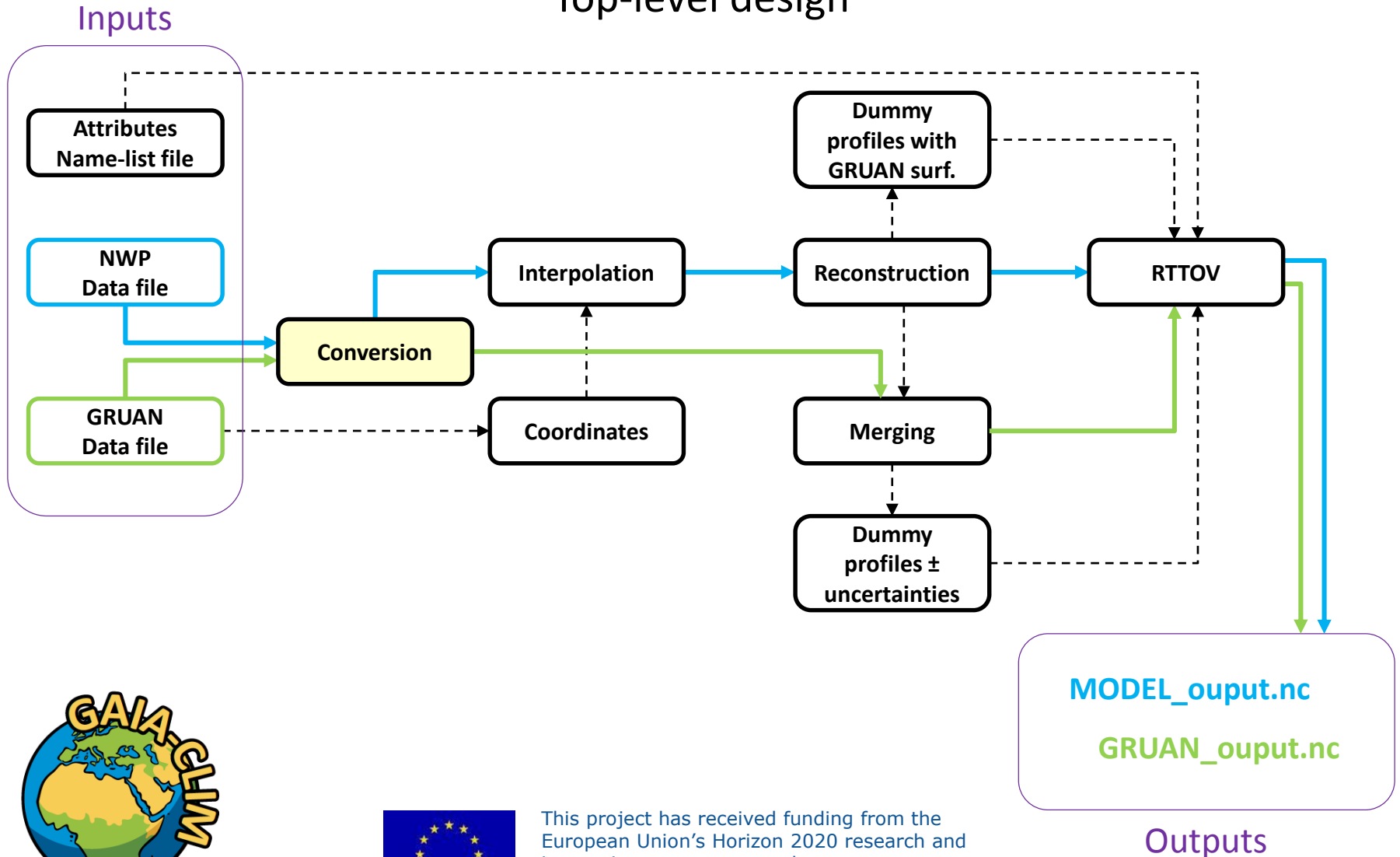


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The GRUAN Processor

Top-level design



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Status of the VO (continued)

- Reference data for ozone:
- NDACC UV-VIS DOAS, sample data from Harestua & Jungfraujoch from 2015/2016; data description at <http://avdc.gsfc.nasa.gov/index.php?site=1876901039> and http://avdc.gsfc.nasa.gov/index.php?site=1876901039#current_template
- NDACC FTIR, sample data from MUSICA sites Kiruna, Izana and Reunion from 2015; data description at <http://avdc.gsfc.nasa.gov/PDF/GEOMS/geoms-1.0.pdf>
- Dobson Brewer, sample data from Eubrewnet network from 2015/16; <http://rbcce.aemet.es/eubrewnet>, awaiting description of samples from wp2
- ECC ozone sonde sample data from Sodankyla from August 2015: <ftp://ftp.cpc.ncep.noaa.gov/ndacc/station/sodanky/ames/o3sonde/so150820.b11>, Izana <ftp://ftp.cpc.ncep.noaa.gov/ndacc/station/izana/ames/o3sonde/iz140917.b11>, Hohenpeissenberg <ftp://ftp.cpc.ncep.noaa.gov/ndacc/station/hohenpei/ames/o3sonde/ho160817.b05>



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T5.2 Graphical User Interface

- ..will be presented in detail in the presentation by Kalev



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OSSSMOSE: Calculation of smoothing error

- WP3 is providing Look-up tables (LUTs) based on OSSSMOSE simulations for the total ozone columns smoothing and co-location uncertainties. These are provided as files in hdf5 format.
- Calculations have been completed for Dobson/Brewer (direct sun) and uv-vis DOAS (aka SAOZ, ZSL-DOAS) type instruments. Similar calculations for FTIR and ozone sonde reference observations are expected to be completed soon.
- Direct sun instruments, like Dobson, Brewer and FTIR spectrometers depend on the solar zenith angle (SZA); hence LUTs are prepared for a series of different SZAs. DOAS instruments (scattering light) require only one LUT each for sunset and sunrise.
- **Smoothing** errors can be calculated within the VO with the help of the LUTs at the time of data ingestion. They are specific for that type of reference observation (e.g. Brewer or DOAS) and given observation geometry.



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OSSSMOSE: Continued

- The Look-up tables allow to calculate the smoothing errors readily within the VO as needed
- The errors introduced by using LUTs adds very little to the overall error budget

Co-location uncertainties can only be calculated once the matching satellite observation is available and paired up with the reference observation. Calculation of these uncertainties are using the second set of LUTs once the user has chosen his/her co-location criteria – or at least once the matching co-located observation from space is known for a specific reference observation.

A LUT for the co-location uncertainty has the following 5 dimensions:

- time of year (weekly or monthly resolution)
- lat (resolution tbd)
- lon (resolution tbd)
- spatial co-location criterion (e.g. 10 - 1000km in 5 steps or so)
- temporal co-location criterion (0 - 12h in hourly steps or so)

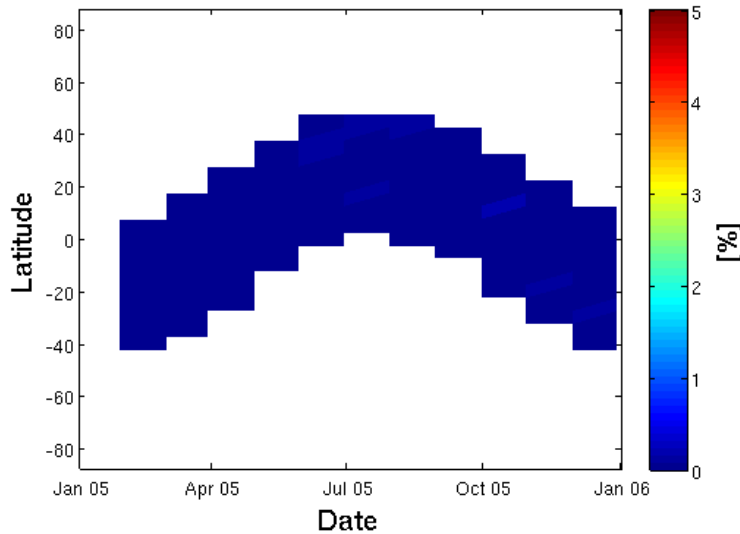


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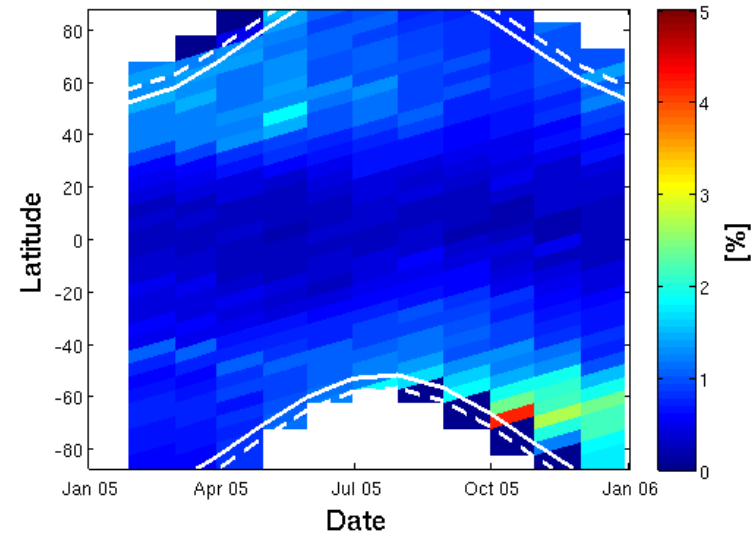
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Smoothing uncertainties: LUT examples

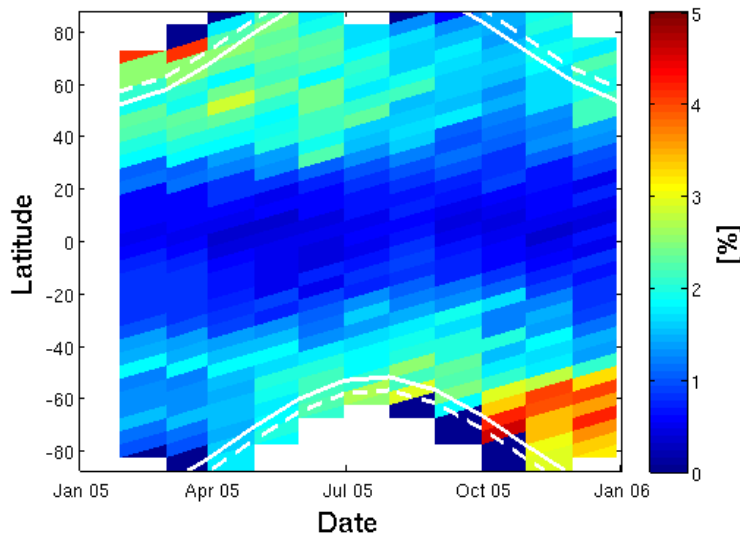
Spread on smoothing errors for
Brewers and Dobsons at $0\text{deg} < \text{SZA} < 20\text{deg}$



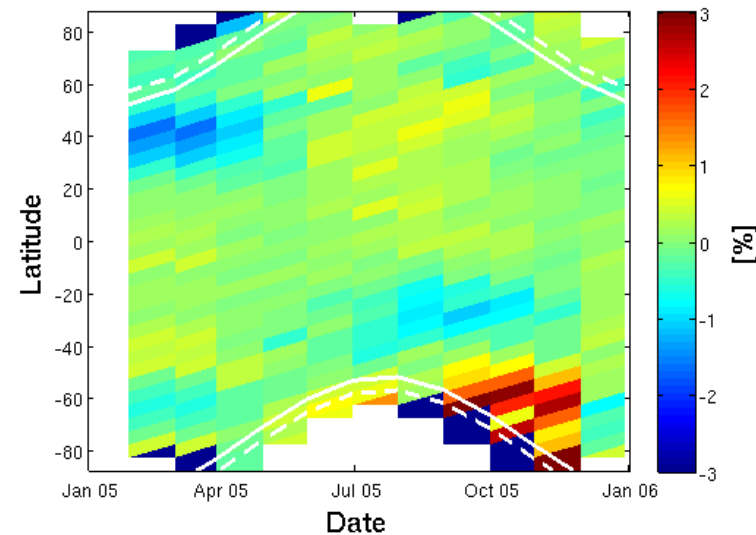
Spread on smoothing errors for
Brewers and Dobsons at $70\text{deg} < \text{SZA} < 80\text{deg}$



Spread on smoothing errors for
Brewers and Dobsons at $80\text{deg} < \text{SZA} < 85\text{deg}$

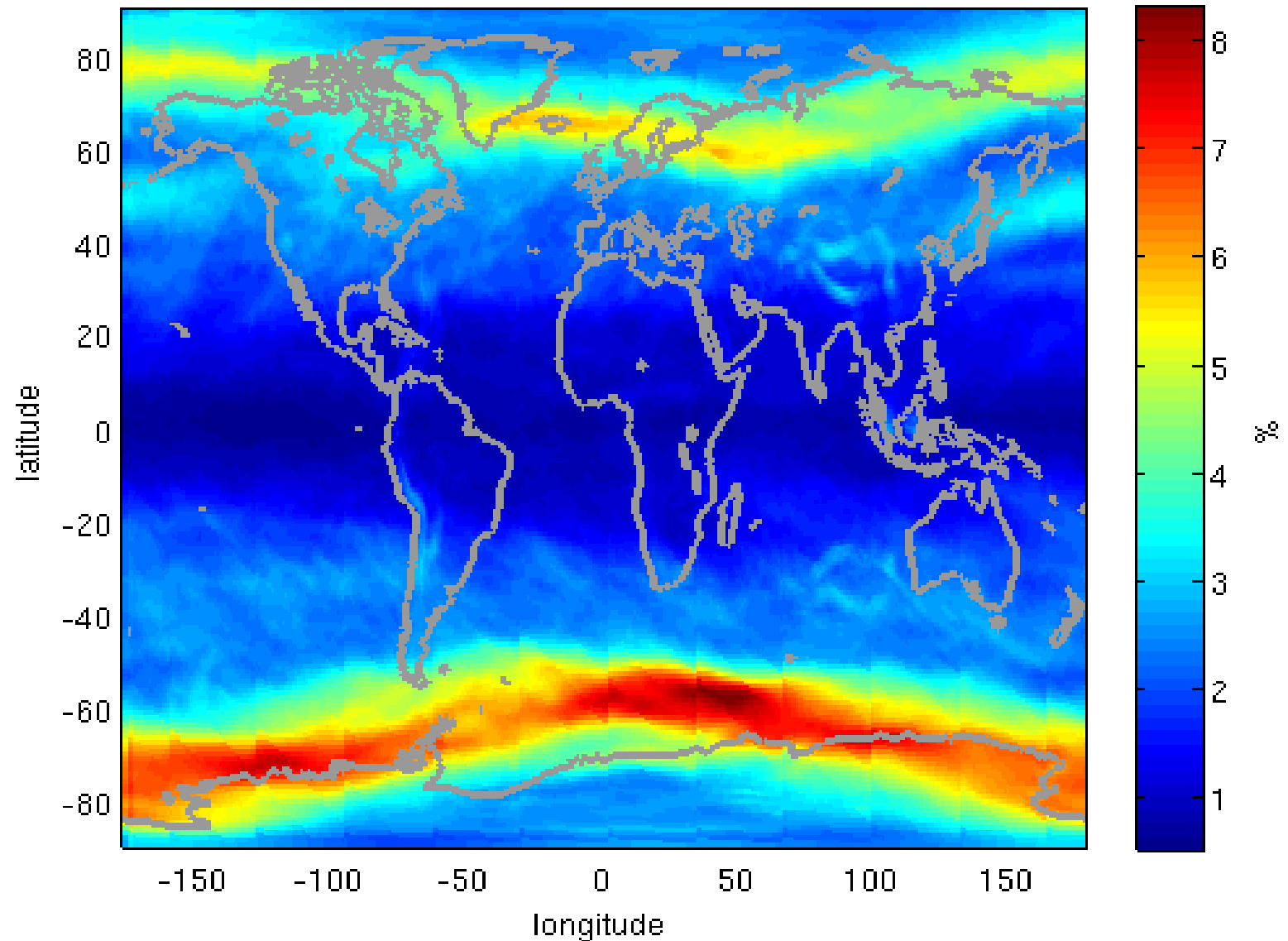


Mean smoothing error for
Brewers and Dobsons at $80\text{deg} < \text{SZA} < 85\text{deg}$



O3 Collocation uncertainties (3°, 3hrs): LUT examples

Co-location uncertainty at (3deg,3hour) max separation, October



Feed-back from user workshop

- The feed-back from the user workshop in November has been collated and converted into an [action item list](#) with currently 47 entries and assigned priorities and workloads.

VO action items - details

Last modified:

4.27E+04

keys: A) priority 1=high, 2=normal, 3=low B) People AM=Arndt, HK=Hannes, IS=Inna, AG=Artur, NN=to be decided later, tut=TUT to decide on a TUT staff including the new staff planned

item	priority	Task	difficulty	people	when ready
1	1	Collocation algorithm working for ingestion	a little more work	AM	22
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
5	1	The second selector should be the "Reference Network/Observational Platform" where we have GRUAN radiosondes, Processed GRUAN radiosondes (BT), EARLINET Aerosol LIDAR, NDACC FTIR, NDACC ECC ozone sondes, NDACC uvvis/DOAS, EUBREWNWT Brewer, NDACC Dobson/Brewer for a start.	normal		22
6	1	3rd selection area "Include/show model data" tickboxes for "UK MetOffice NWP", "ECMWF NWP" (others may follow later)	normal	??	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		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
10	3	we will possibly dream up more like "pool latitude bands"	normal	??	26



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Live Demo

- A live demo will be presented after Kalev and Hannes' presentation
- During breaks you can try out the VO (early alpha stage)



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Issues and Outlook

- Readers for all NDACC and GRUAN observations exist on the VO
- Currently finalising the collocation software
- Integration of partners' software (CESIUM) can be started
- Decision to be taken on plotting engine (home-made, CISUM or VISAN)
- GUI needs to be tidied up and must become easier to use
- The feed-back from the user workshop in November has been collated and converted into an [action item list](#) with assigned priorities and workloads.
- Missing functionality needs to be added (Will show some of the functionality developed, but that is not integrated into the website yet)
- Plotting of co-location data needs to be implemented to show differences in meaningful ways and their respective errors
- Statistical analysis tools need to be implemented
- Educational aspects of the VO have not been considered up to now but resources are very limited.
- Plans for TUT, CNR and EUMETSAT key staff to have a common coding session



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Spare slides for questions



Testing of initial prototype of the VO

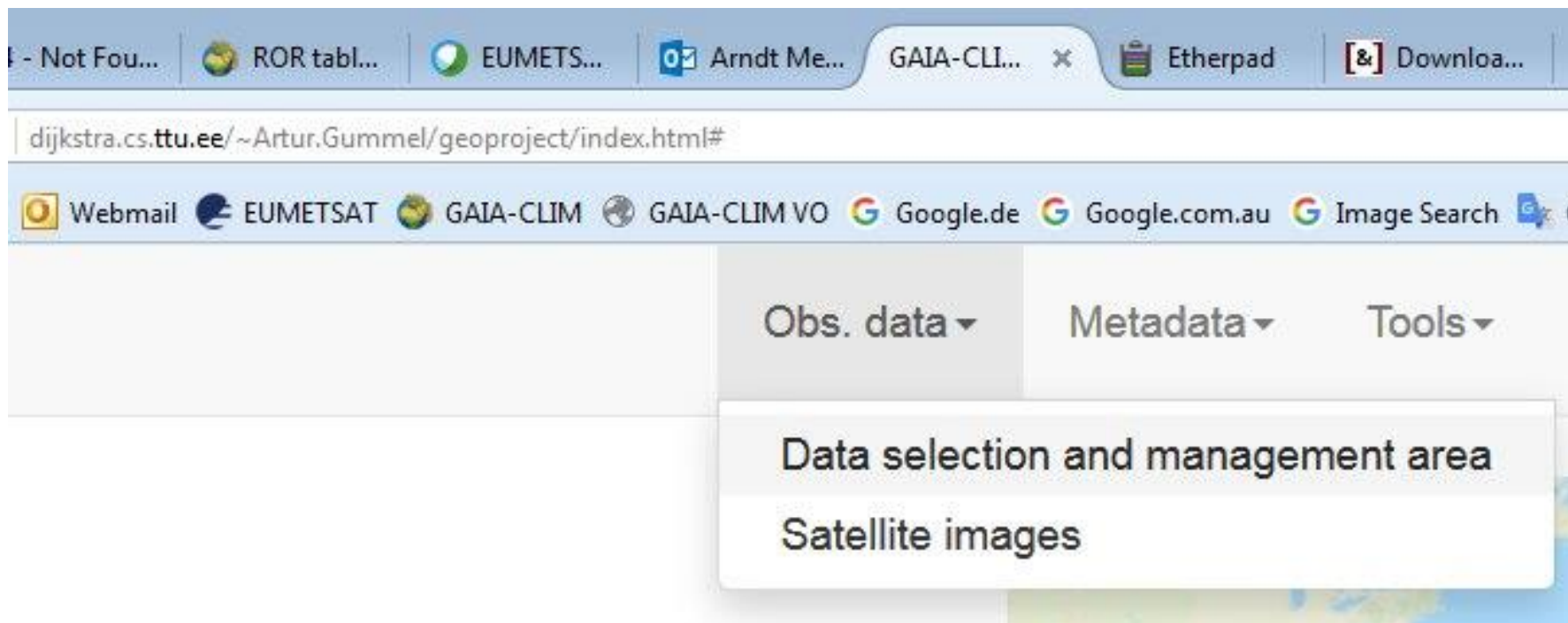
- On the next few slides we are illustrating the menu structure for the Virtual Observatory as a web-based service.



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Plotting observational data - 01



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Plotting observational data - 02

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dijkstra.cs.ttu.ee/~Artur.Gummel/geoproject/index.html# Search

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Data Selection and management area

Reference Network of Reference Instrument

GRUAN radiosonde

Measurand

Additional quality control information

From Date (YYYY-MM-DD)

To Date (YYYY-MM-DD)

From Time (HH:MM:SS)


To Time (HH:MM:SS)

Metadata standard (data format)

Metadata CCI CF

Geometry

All



Plotting observational data – 03

Data Selection and management area

Reference Network of Reference Instrument

GRUAN radiosonde

GRUAN radiosonde

GRUAN processor

WOUDC ozonesonde

UK MetOffice NWP model

EARLINET aerosol lidar



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Data Selection and management area

Reference Network of Reference Instrument

GRUAN radiosonde

Measurand

Additional quality control information

Additional quality control information

Altitude

Ascent/descent speed

Brightness temperature

Correction of air temperature

Correction of relative humidity

Correlated uncertainty of relative humidity

Correlated uncertainty of temperature

Frostpoint

Geopotential altitude

Land-sea mask

Latitude

Level code

Longitude

Meridional wind

Meridional wind at 10m

Ozone concentration

Pressure

Quality control flag

Relative humidity

Plotting observational data – 04

Data Selection and management area

Reference Network of Reference Instrument

GRUAN radiosonde

Measurand

Relative humidity

From Date (YYYY-MM-DD)

2013-08-01|

August 2013						
Su	Mo	Tu	We	Th	Fr	Sa
28	29	30	31	1	2	3
4	5	6	7	8	9	10
11	12	13	14	15	16	17
18	19	20	21	22	23	24
25	26	27	28	29	30	31



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Plotting observational data – 05

dijkstra.cs.ttu.ee/~Artur.Gummel/geoproject/index.html#

Home Webmail EUMETSAT GAIA-CLIM GAIA-CLIM VO Google.de Google.com.au Image Search Google Translate

Data Selection and management area

Reference Network of Reference Instrument

GRUAN radiosonde

Measurand

Relative humidity

From Date (YYYY-MM-DD)

2013-08-01

To Date (YYYY-MM-DD)

2013-08-03

From Time (HH:MM:SS)

00:00:00

To Time (HH:MM:SS)

23:59:59


Metadata standard (data format)

Metadata CCI CF

Geometry

All

Send data request



Data Selection and management area**Reference Network of Reference Instrument**

GRUAN radiosonde

Measurand

Relative humidity

From Date (YYYY-MM-DD)

2013-08-01

To Date (YYYY-MM-DD)

2013-08-03

From Time (HH:MM:SS)

00:00:00

To Time (HH:MM:SS)

23:59:59

Metadata standard (data format)

Metadata CCI CF

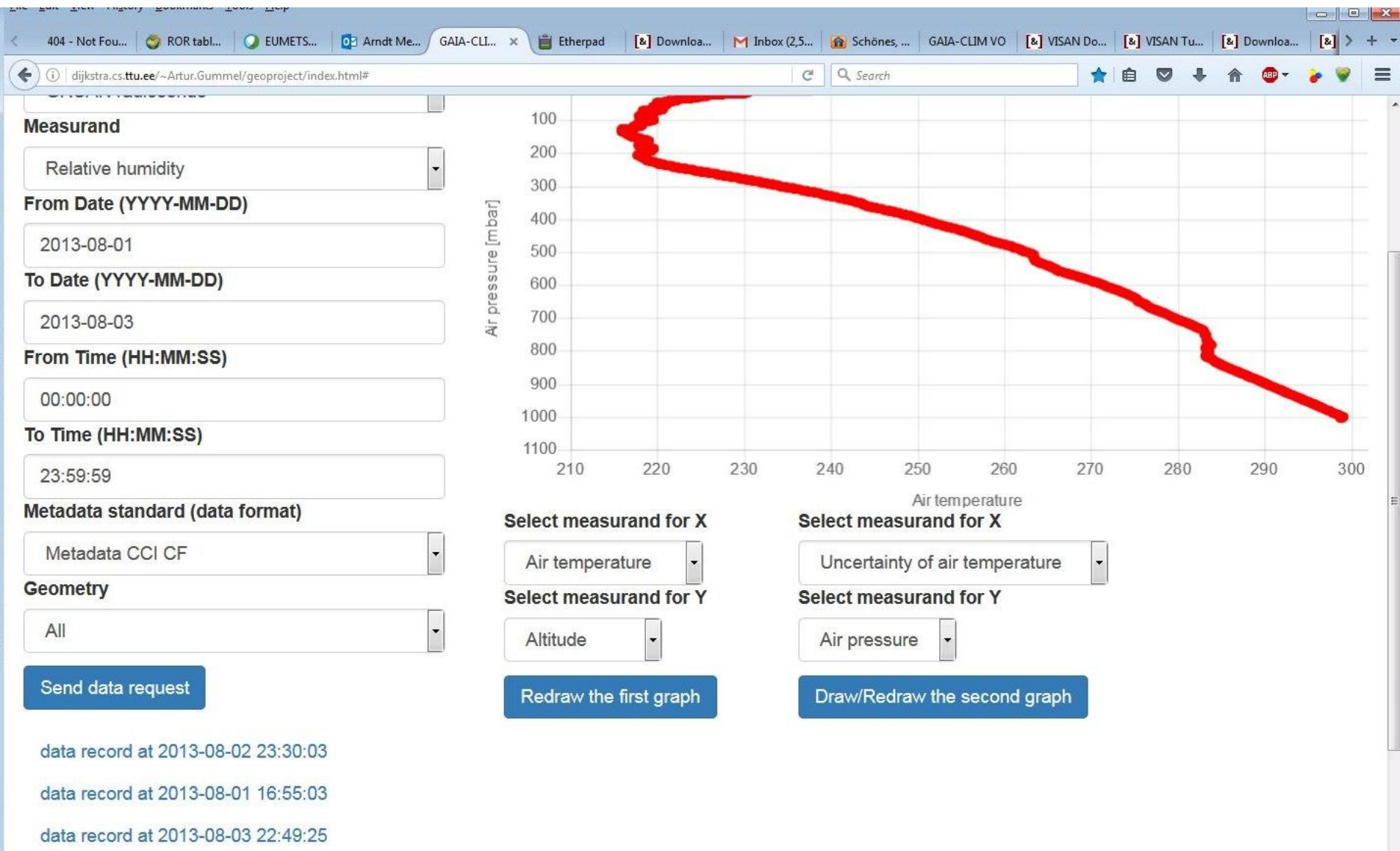
Geometry

All

Send data request

data record at 2013-08-02 23:30:03

Plotting observational data – 07

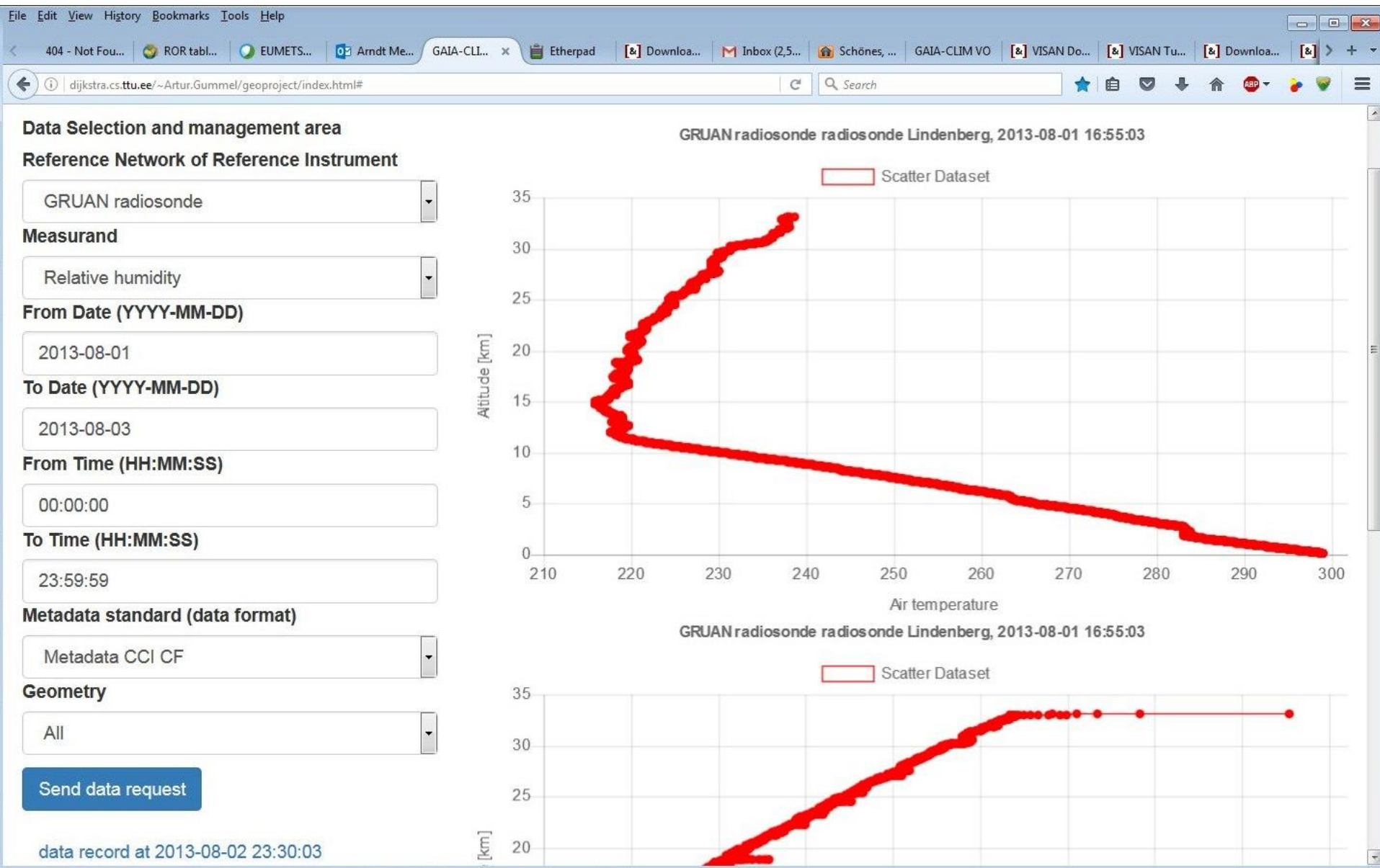


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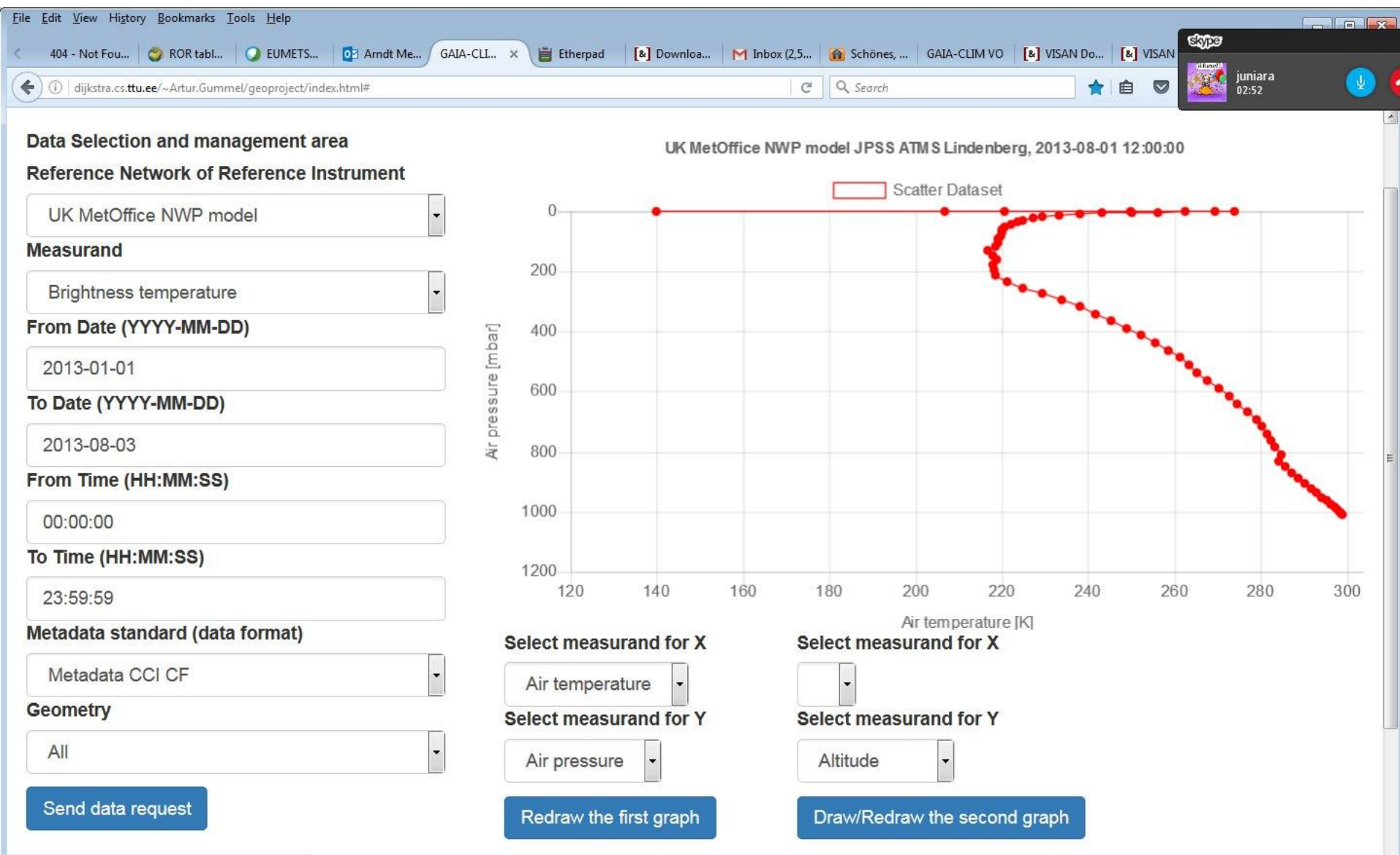
Plotting observational data – 08



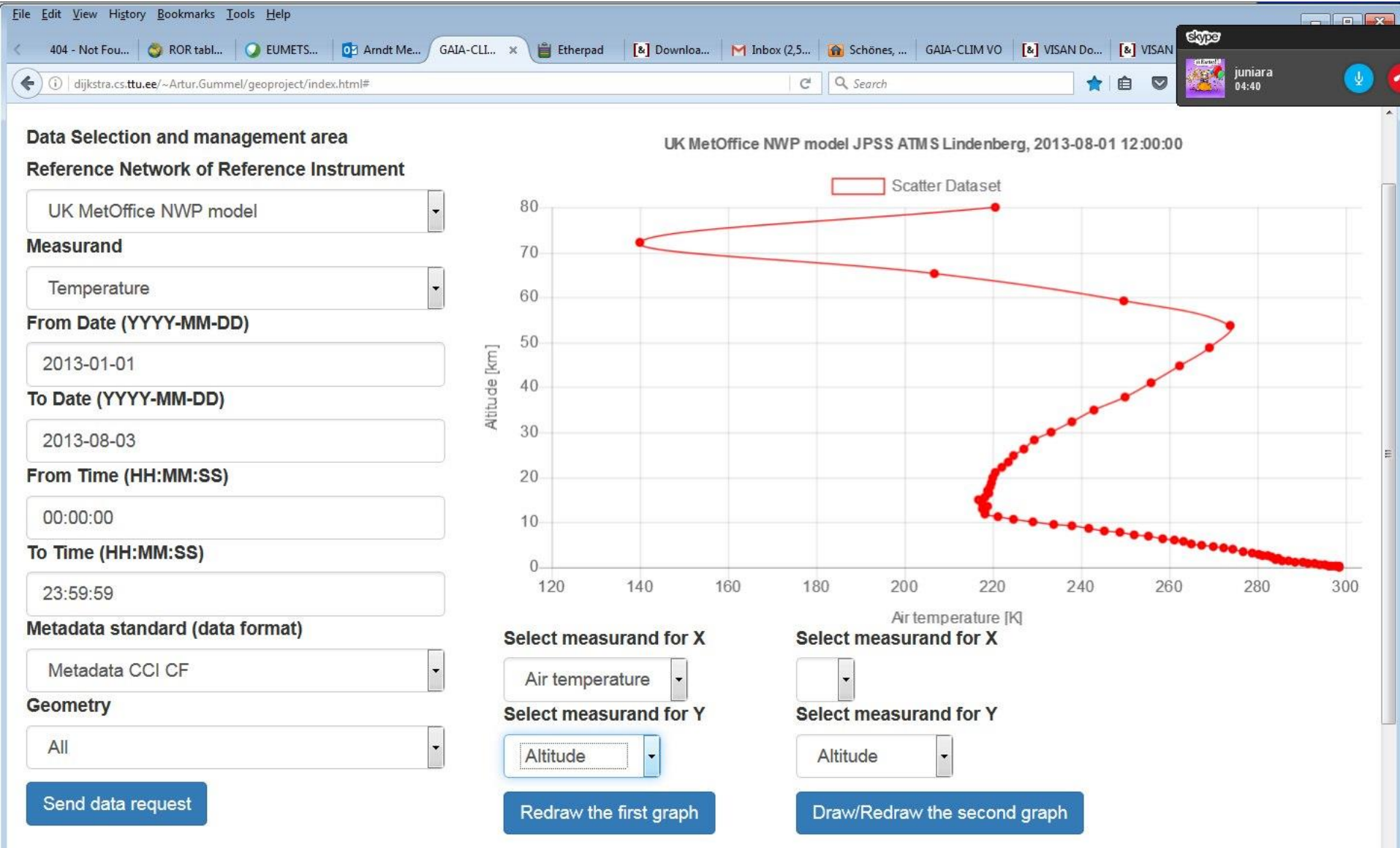
Plotting observational data – 09



Plotting observational data – 10



Plotting observational data – 11



innovation programme under grant agreement
No 640276.