New Developments in ACTRIS Surface In-Situ Data Flow and Handling

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Norwegian Institute for Air Research

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Proposed ACTRIS VOC Data Flow in a Nutshell

1. Data is quality assured at the station, including tools provided by ACTRIS
2. Data are submitted to ACTRIS DC / EBAS via submission portal (ensures homogeneous format low in errors), associated with project "ACTRIS_preliminary".
3. Data are moved to a read-only FTP site at ACTRIS DC for download by the ACTRIS VOC QA group.
4. ACTRIS VOC QA group checks data, and either:
    1. logs issues found in issue tracker, and associates issue with responsible PI / submitter. Data are corrected by submitter, change documented in issue tracker. Back to 2.
    2. Finds the data to pass all QA tests, i.e. closes all issues on dataset (or creates a closed issue if pass at first submission). Go to 5.
5. Data are taken from FTP site, and imported into EBAS with project association "ACTRIS".

Note: for NOx, the whole QA procedure will be handled by NOx QA centre. Will NOx QA centre give feedback via issue tracker?

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Requirements for Organising Data QA and Feedback

2 related requirements when organising data QA and data feedback:

1. **VOC**:
   Issues found with submission of a station by QA group need to be recorded, station PI notified, correction followed up, DC notidied when issues are solved.
2. **Aerosol**
   Issues are found when data are screened for larger studies (e.g. trend analysis, model inter-comparison). Issue needs to be documented, assigned to responsible PI, correction followed up, and corrected in archive.

→ Issue tracker at http://ebas-feedback.nilu.no. To be used for project / framework QA, but also general feedback on EBAS / ACTRIS system.

EBAS Feedback: Organising Quality Assurance and Feedback on Data

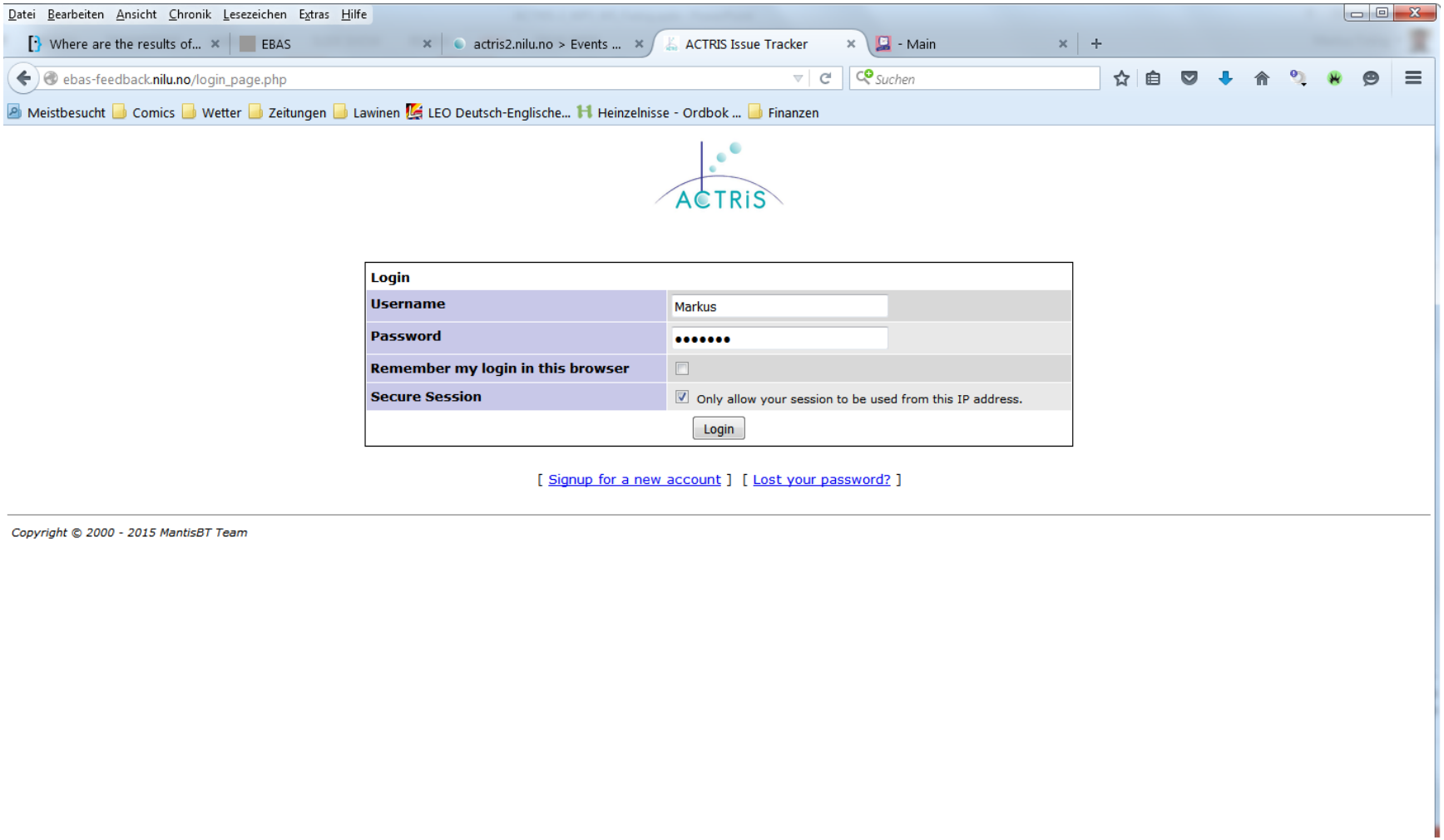
What is an issue tracker?

- Web portal for organising and keeping track of issues and tasks in a project.
- Issues are described in text, attachments allowed for illustration & documentation.
- Issues can have 4 statuses reflecting work flow: open, assigned, resolved, closed.
- All users need to have an account!
- Each user has a “role” (set of rights): anybody can report issues or set issue to “resolved”
- Only “managers” (members of QA group) can assign or close an issue.

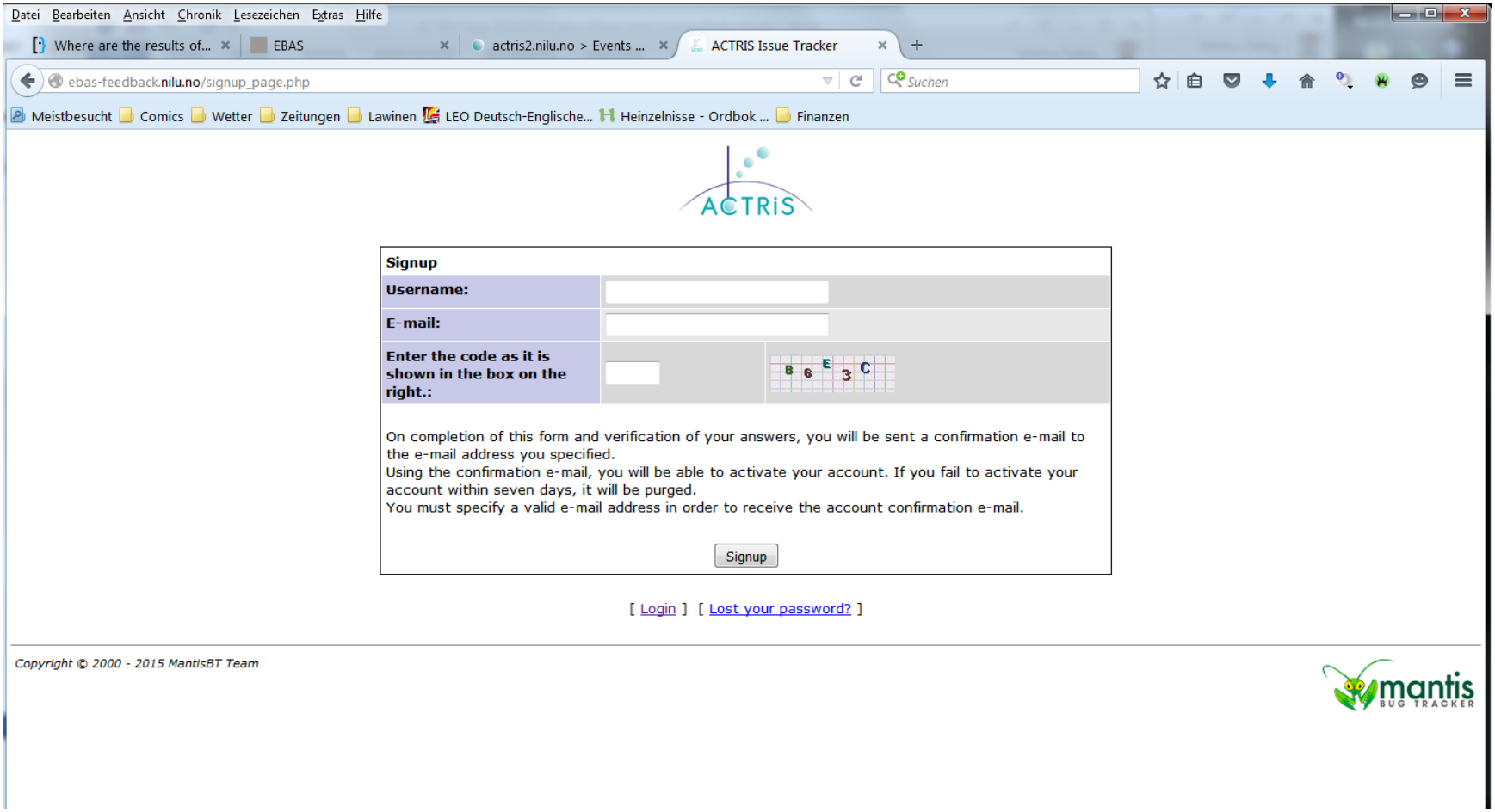
HOMEWORK:

- Every station / data PI & submitter to create account at ebas-feedback.nilu.no
- Use syntax for login name: <First Name>_<Last Name>

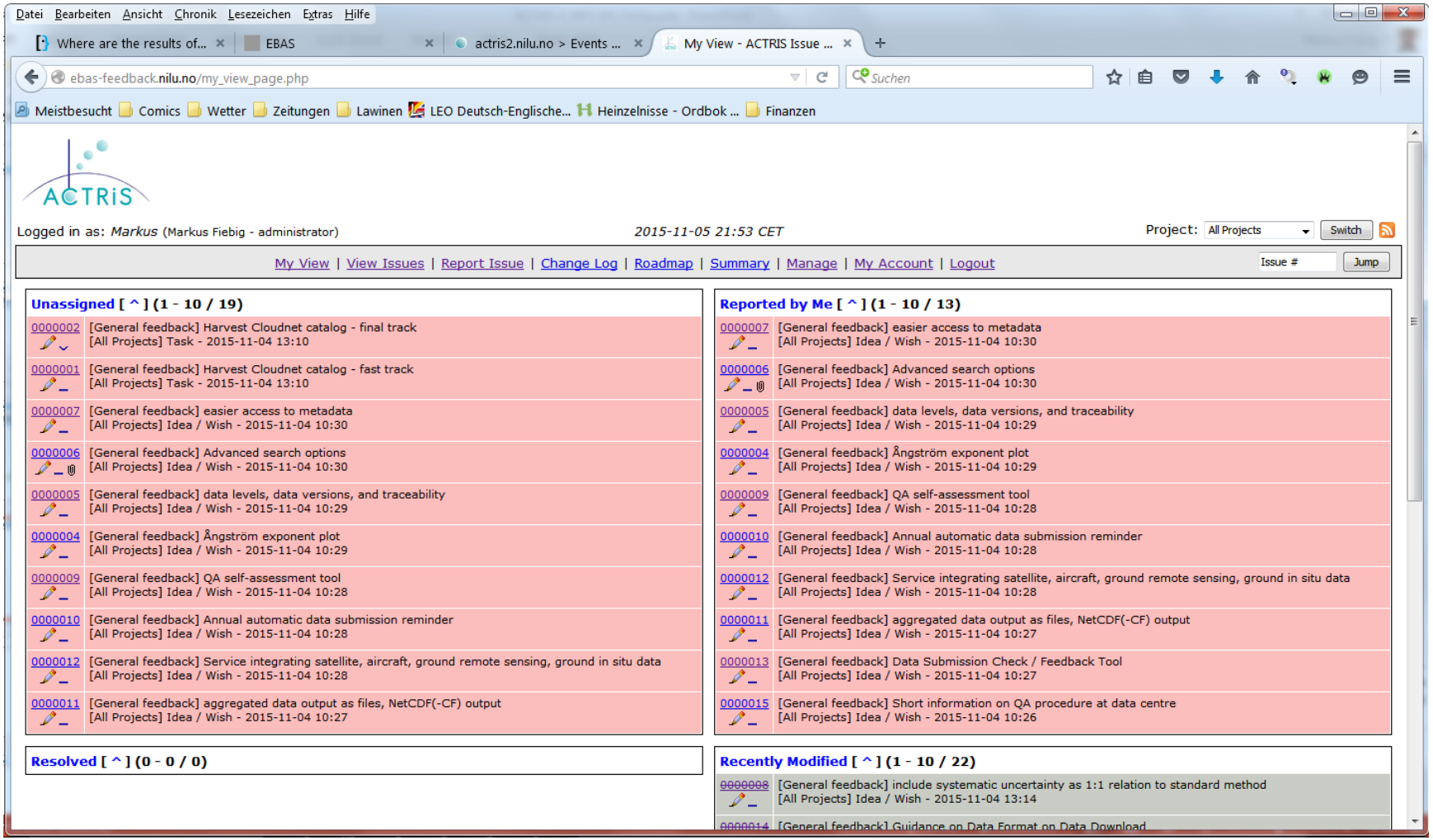
EBAS Feedback: Organising Quality Assurance and Feedback on Data



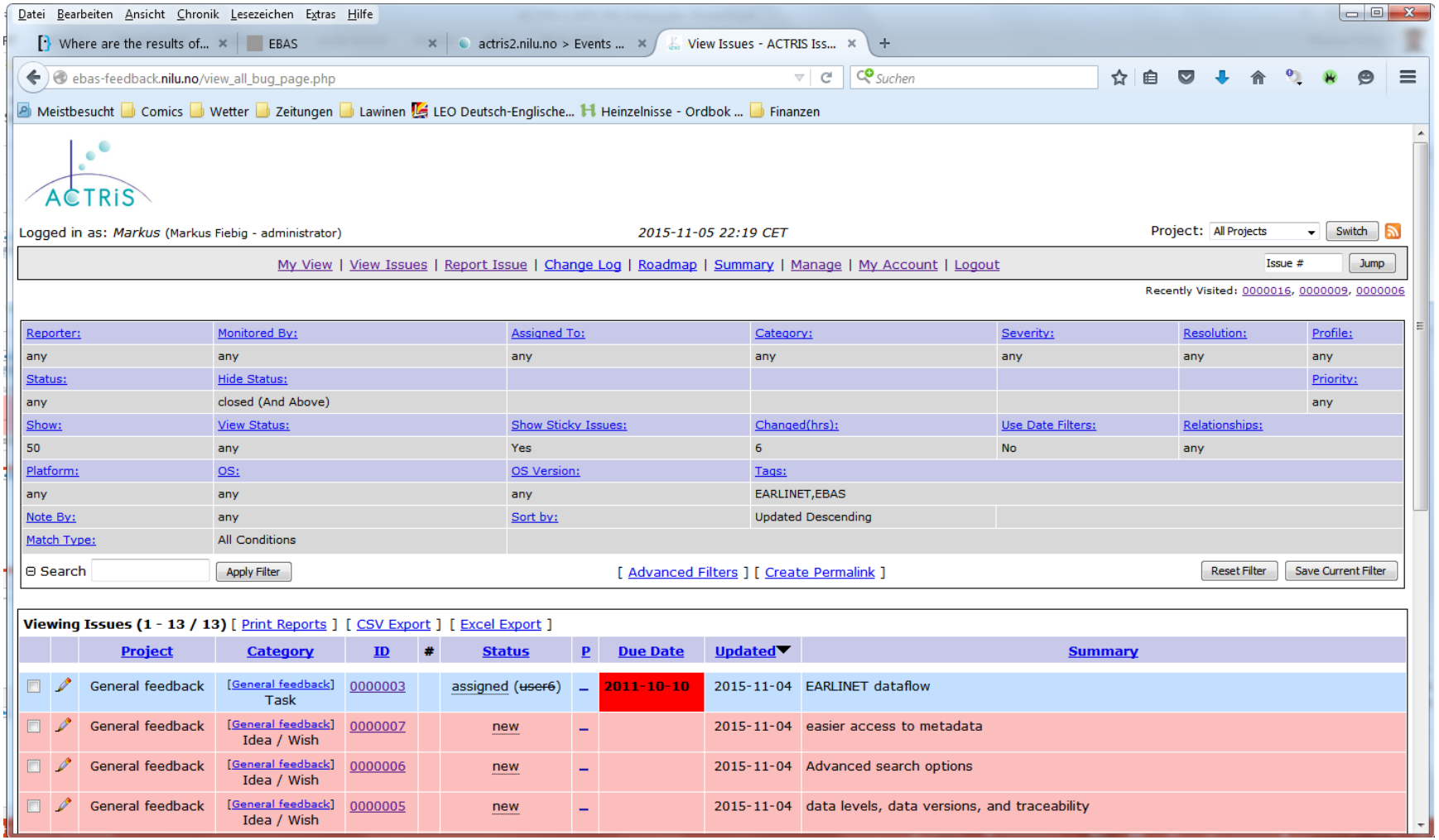
EBAS Feedback: Organising Quality Assurance and Feedback on Data



EBAS Feedback: Organising Quality Assurance and Feedback on Data



EBAS Feedback: Organising Quality Assurance and Feedback on Data



Datei Bearbeiten Ansicht Chronik Lesezeichen Extras Hilfe

Where are the results of... | EBAS | actris2.nilu.no > Events ... | View Issues - ACTRIS Iss...

ebas-feedback.nilu.no/view_all_bug_page.php

Meistbesucht Comics Wetter Zeitungen Lawinen LEO Deutsch-Englische... Heinzelnisse - Ordbok ... Finanzen

ACTRiS

Logged in as: *Markus* (Markus Fiebig - administrator) *2015-11-05 22:19 CET* Project: All Projects Switch

My View | View Issues | Report Issue | Change Log | Roadmap | Summary | Manage | My Account | Logout Issue # Jump

Recently Visited: 0000016, 0000009, 0000006

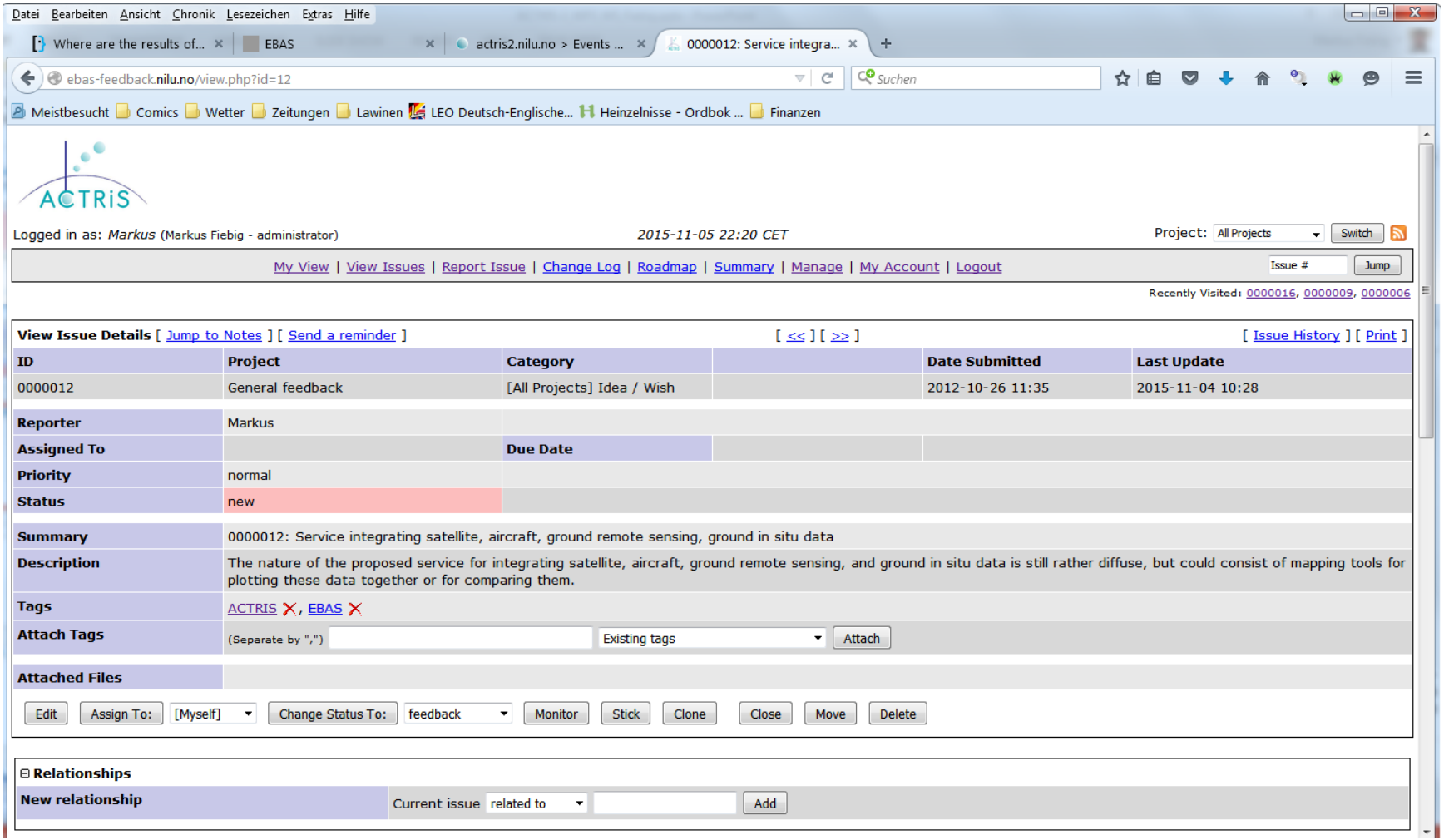
Reporter:	Monitored By:	Assigned To:	Category:	Severity:	Resolution:	Profile:
any	any	any	any	any	any	any
Status:	Hide Status:					Priority:
any	closed (And Above)					any
Show:	View Status:	Show Sticky Issues:	Changed(hrs):	Use Date Filters:	Relationships:	
50	any	Yes	6	No	any	
Platform:	OS:	OS Version:	Tags:			
any	any	any	EARLINET,EBAS			
Note By:	any	Sort by:	Updated Descending			
Match Type:	All Conditions					

⊟ Search Apply Filter [Advanced Filters] [Create Permalink] Reset Filter Save Current Filter

Viewing Issues (1 - 13 / 13) [Print Reports] [CSV Export] [Excel Export]

Project	Category	ID	#	Status	P	Due Date	Updated	Summary
General feedback	[General feedback] Task	0000003		assigned (~~user6~~)	_	2011-10-10	2015-11-04	EARLINET dataflow
General feedback	[General feedback] Idea / Wish	0000007		new	_		2015-11-04	easier access to metadata
General feedback	[General feedback] Idea / Wish	0000006		new	_		2015-11-04	Advanced search options
General feedback	[General feedback] Idea / Wish	0000005		new	_		2015-11-04	data levels, data versions, and traceability

EBAS Feedback: Organising Quality Assurance and Feedback on Data



Datei Bearbeiten Ansicht Chronik Lesezeichen Extras Hilfe

Where are the results of... | EBAS | actris2.nilu.no > Events ... | 0000012: Service integra...

ebas-feedback.nilu.no/view.php?id=12

Meistbesucht Comics Wetter Zeitungen Lawinen LEO Deutsch-Englische... Heinzelnisse - Ordbok ... Finanzen

ACTRiS

Logged in as: *Markus* (Markus Fiebig - administrator) *2015-11-05 22:20 CET* Project: All Projects Switch

My View | View Issues | Report Issue | Change Log | Roadmap | Summary | Manage | My Account | Logout Issue # Jump

Recently Visited: 0000016, 0000009, 0000006

View Issue Details [Jump to Notes] [Send a reminder] [<<] [>>] [Issue History] [Print]

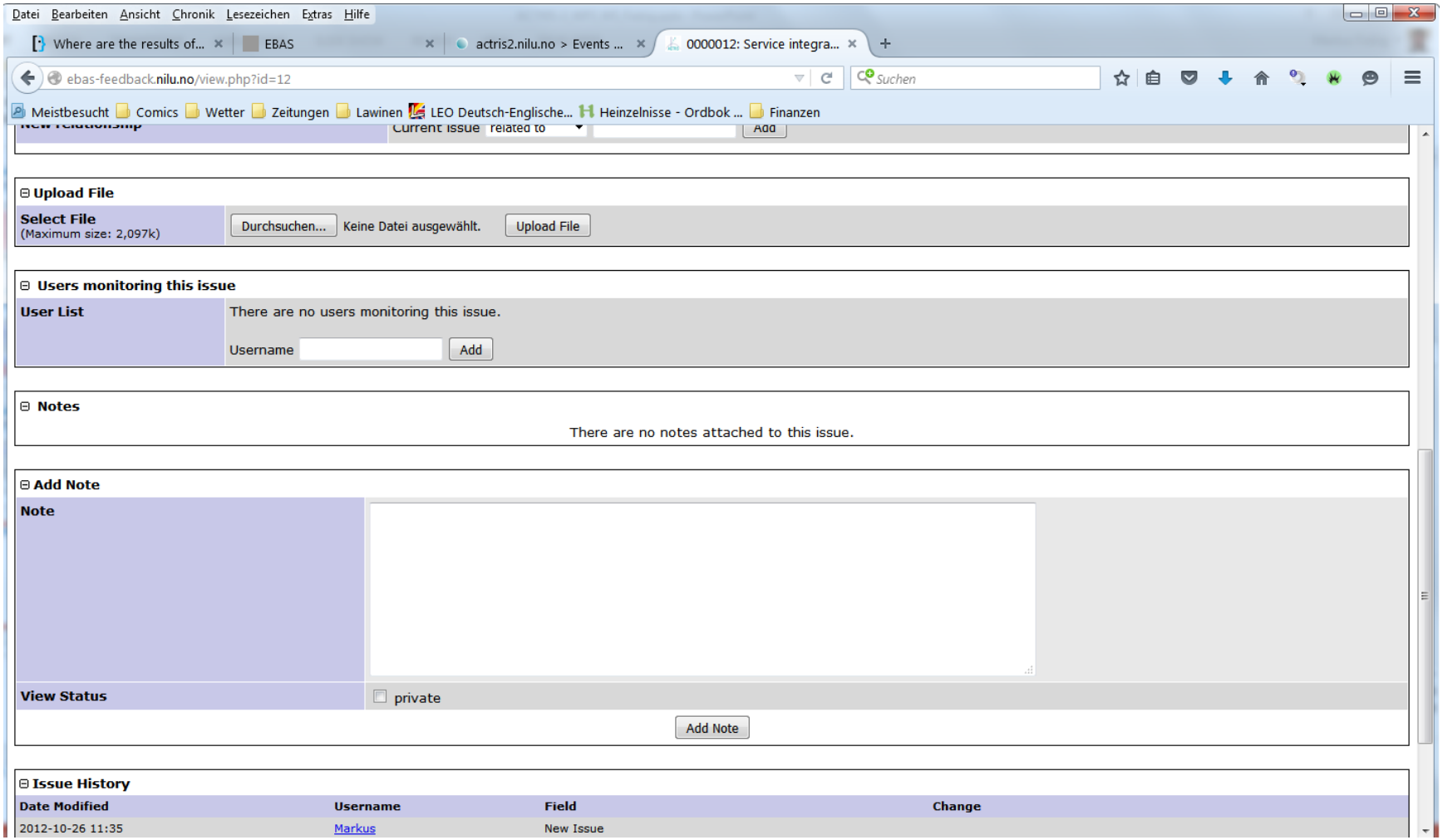
ID	Project	Category		Date Submitted	Last Update
0000012	General feedback	[All Projects] Idea / Wish		2012-10-26 11:35	2015-11-04 10:28
Reporter	Markus				
Assigned To		**Due Date**			
Priority	normal				
Status	new				
Summary	0000012: Service integrating satellite, aircraft, ground remote sensing, ground in situ data				
Description	The nature of the proposed service for integrating satellite, aircraft, ground remote sensing, and ground in situ data is still rather diffuse, but could consist of mapping tools for plotting these data together or for comparing them.				
Tags	ACTRIS, EBAS				
Attach Tags	(Separate by ",") Existing tags Attach				
Attached Files					

Edit | Assign To: [Myself] | Change Status To: feedback | Monitor | Stick | Clone | Close | Move | Delete

Relationships

New relationship Current issue related to Add

EBAS Feedback: Organising Quality Assurance and Feedback on Data



Quality Assurance Metadata: Why Do We Need That?

- So far, quality metadata has focused on uncertainty of individual data points.
- A huge fraction of ACTRIS' work is around QA measures:
  - inter-comparison workshops
  - round-robin experiments
  - on-site inter-comparison
  - on-site audit
- ACTRIS markets itself as RI for high-quality data – we need to "show-off" and document that.
- Motivation for stations to participate in QA measures.

Metadata Documenting Quality Assurance

- Measure master data:
  - Unique ID of QA measure (issued by EBAS)
  - Type of QA measure (on site intercomparison, off-site intercomparison, round-robin, on site audit)
  - Entity issuing QA measure (name, address, URL)
  - Date of QA measure
  - Reference to test procedure used (title, URL).
- Requested from data provider:
  - Unique ID of QA measure (issued by EBAS)
  - Date of QA measure
  - Outcome:
    - pass / no pass,
    - uncertainty found (number, unit)
  - reference document (title, date, URL)
  - Will depend on component, at least for gases
- Consistent with ISO19115 DQ metadata items.

To Do: Defined Interface between QA Centre and Data Centre:

- Public documentation of QA measures and results at QA centre website.
- Documentation in machine-readable format

Data Levels Defined in ACTRIS: Use for VOC & NOx?

Data Level	Description		Used for
0	• Annotated raw data • format instrument specific • all data / information for processing to final value.	• contains all parameters provided by instrument as provided • ”native” time resolution	NRT
1	• processed to final parameter • invalid data removed	• ”native” time resolution • format property specific	intercom-parisons
1.5	• aggregated to hourly averages • variability quantified • format property specific • STP correction if necessary	auto-processed	NRT
2		manual QA	regular collection

- SOP describes steps from one to the next level.
- All levels use EBAS NASA-Ames format.

Why Do We Have Data Levels?

- **Traceability**: Whole chain of data acquisition / processing / QA can be traced back to the time of measurement.
- Allows to reprocess the data.
- Separates DAQ / processing / QA chain into well defined steps, great tool for finding the cause of failing intercomparison.
- Data is documented also for a user in 15 years from now.
- Higher level frameworks are moving to requiring this feature.

How to Make Use of Data Levels for NOx & VOCs

NOx:

- Similar to online aerosol observations: make use of all levels?
- Draft templates exist, expert / stake holder overhaul needed.

VOCs:

- Offline measurement, levels normally not used.
- Calibration & target gas measurements should be documented, but may confuse end-user
- Use level 0 & 2, almost identical templates, except:

  Level 0: contains all calibration / zero / target gas measurements, respective data points use respective flags.

  Level 2: same data, but excluding calibration / zero / target gas measurements
- Level 0 archived offline, level 2 accessible in EBAS-web
- Expert / stake holder input needed.

Use of Flags in Data Submission: The General Philosophy

So far, data archives are often single purpose – ACTRIS is multi-purpose:

- Data are flagged invalid only with non-quantifiable instrument malfunction or severe local contamination (paint job on station, smoking under inlet) – non-representative even for close surroundings, can't be corrected.
- Other conditions of local influence are to be flagged with respective flag, but data are reported as valid, e.g.:
  - Farming activity
  - Dust storm
  - Biomass burning episode
  - Volcanic eruption

Comparison of Data Flags, 1/2

Flag	V/I/M	Description	VOC use	NOx use	Aerosol use
000	V	Valid measurement	no obvious local influence or technical/instrumental problems		
110	V	Episode data checked and accepted by data originator.	-----	-----	Used to validate outlier
147	V	Below theoretical detection limit or formal Q/A limit, but a value has been measured and reported and is considered valid			-----
185	V	Possible local contamination indicated by wind direction or velocity	-----	-----	
186	V	Possible local contamination indicated by single scattering albedo	-----	-----	
187	V	Possible local contamination indicated by occurence of new particles.	-----	-----	Used in a setting where new particle formation indicates contamination)
188	V	Possible local contamination indicated by low wind speed.	-----	-----	Used in case of auto-contamination by station
189	V	Possible local contamination indicated by wind from contaminated sector.	-----	-----	Used if flag 185 is too unspecific.
390	V	Data completeness less than 50%	Needed for averaged values, SOP uses 66%		
392	V	Data completeness less than 75%			
394	V	Data completeness less than 90%			
410	V	Saharan dust event	-----	-----	
459	I	Extreme value, unspecified error	-----	-----	Unexplained extreme values, technical problem suspected.

Comparison of Data Flags, 2/2

Flag	V/I/M	Description	VOC use	NOx use	Aerosol use
499	V	Inconsistent with another unspecified measurement.	-----	-----	Inconsistent e.g scattering coefficient calculated from particle size distribution.
559	V	Unspecified contamination or local influence, but considered valid	unexpected values, no instrumental or technical failure.		
599	I	Unspecified contamination or local influence	-----	-----	
640	V	Instrument internal relative humidity above 40%.	-----	-----	Used to signal possible hygroscopic growth of aerosol particles (neph, MPSS)
652	V	Construction / activity nearby.	-----	-----	Includes disturbance by other lab activity.
662	V	Too high sampling flow, data considered valid.	-----	-----	E.g. aerosol flow rate out of range but considered valid.
676	V	station inside cloud (visibility < 1000 m).	-----	-----	
677	I	Icing or hoar frost in the intake.	-----	-----	
699	I	Mechanical problem, unspecified reason.	-----	-----	E.g. problems with flow, leaks.
797	V	Data element taken from co-located instrument			-----
980	M	Missing due to calibration or zero/span check	-----	-----	e.g. neph zero checks
999	M	Missing measurement, unspecified reason	missing measurements, outliers, technical problems, non-ambient contamination, definetly unusable for known reason (smoking, …)		
???	I	Missing due to zero/span check	Zero/span gas applied		-----
???	I	Missing due to target gas check	Target gas applied		-----
???	I	Missing due to calibration	Calibration gas applied		-----

2 Routes For Data Submission

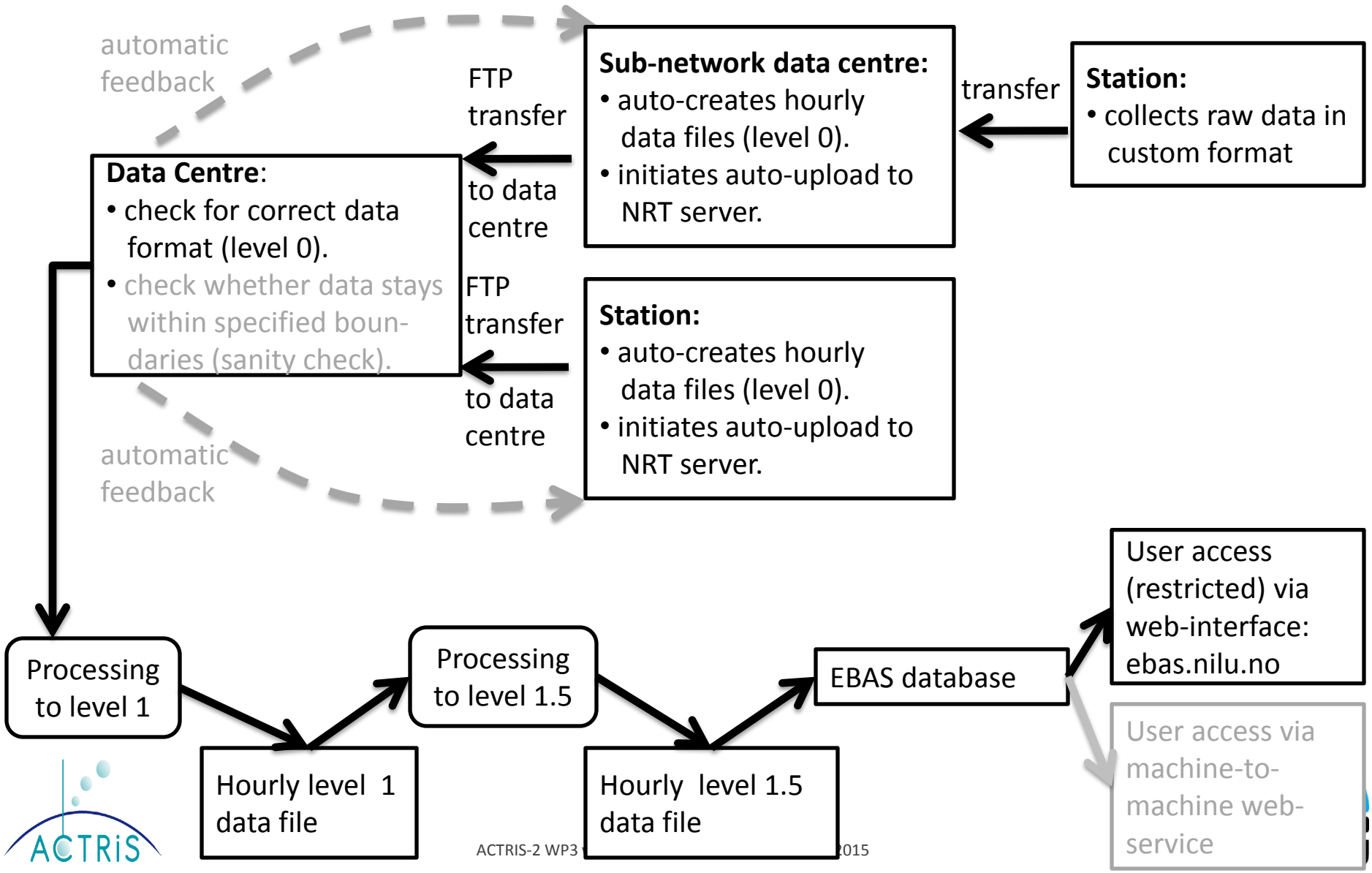
Regular, annual submission:

- Submission of annual dataset by **30 June** the following year.
- Data shall have highest level of QA possible.
- Dataset assembled by data originator, because detail knowledge resides here.

Near-Real-Time Data Submission:

- Submission shall be collected and disseminated within max. 3 hours of measurement.
- Compromise on data quality due to auto-processing accepted.
- Alert service for provider if instrument “misbehaves”.
- Central data processing to ensure uniform dataset and implement alert service.

NRT data collection flow chart



Near-Real-Time Reporting for Reactive Gases!?

NOx:

- Technically, NOx data can be phased into the ACTRIS NRT infrastructure.
- Previous efforts (MACC) need to be considered.
- Who will be doing the processing, or specify the SOP for NRT processing?

VOCs:

- "NRT" VOC submission would in fact be rapid delivery, suitable for validation, but not operational services.
- NRT data submissions don't receive feedback – import only when 100% correct.
- VOC rapid delivery would need dedicated tool for stations to submit 100% correctly formatted files.

Online Checks For Incoming (NRT) Data: Current Status

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Online Outlier Check for Incoming Data

- Original plan: online check of VOC concentration ratios – proves difficult to specify.
- Plan B: implement outlier check for data submitted via submission portal
- Check will be based on comparison with running percentiles.
- Outliers found will need to be flagged valid (flag 110 - Episode data checked and accepted by data originator) or removed as invalid for file to be accepted.
- Fine-tuning threshold for outliers will be based on feedback from submitters.

BUT:

- How do we proceed with online check of VOC ratios?

Closure studies for particle light scattering coefficient

- Slowly degrading instrument performance often difficult to diagnose.
- Closure of scattering coefficient between nephelometer measurement and calculation from size distribution can help to diagnose instrument performance.
- Focus on NRT submissions, option for use on regular (annual) data submissions.
- Additional incentive to participate in NRT programme

Elaborate implementation options:

- Conditions at stations (observed size ranges, occurrence of coarse-mode particles) too heterogeneous to set strict thresholds for alerts.
- Instead, users receive weekly scatter plot of scattering coefficient measured over calculated from MPSS.

Why Is Increasing the Number of Near-Real-Time Stations All Important for ACTRIS?

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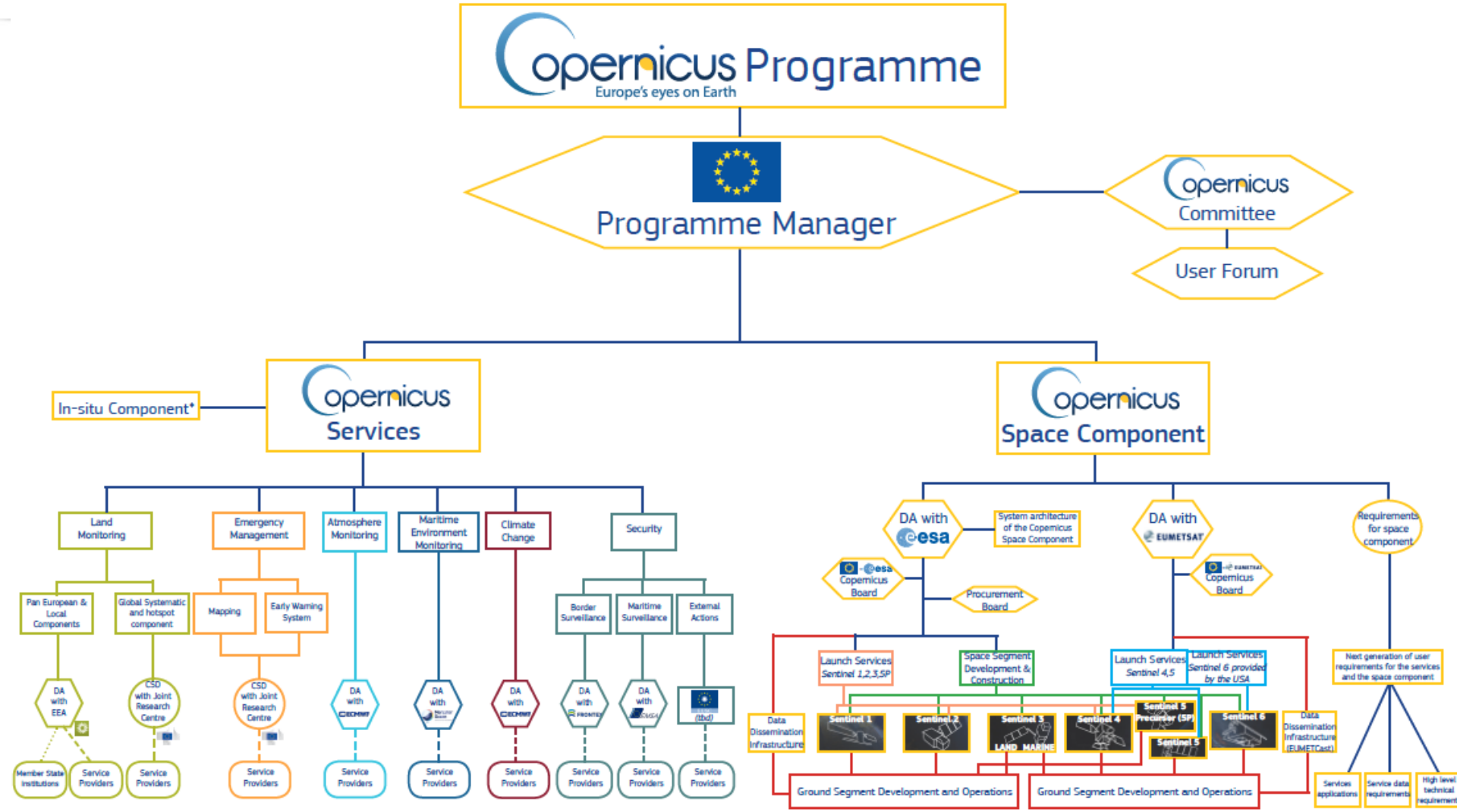
The Big Picture: The EC Digital Agenda

"Quite simply, knowledge is the engine of our economy. And data is its fuel."

(Neelie Kroes, former European Commission Vice President in charge of the Digital Agenda)

EU Commission's Digital Agenda:

- Digital technologies are to be used for generating economic growth (next Facebook, Google, Air BnB, …)
- Data has to flow as freely as possible to be available for new products and services.
- A whole General Directorate is working on this!
- Every project funded has to demonstrate how it fits into digital agenda (section on socio-economic impact).



Source: Copernicus.eu

Which will be the future users of Copernicus?

- EO Professionals
- Other Private Services (e.g Transport, Tourism, …)
- Public Authorities
- Policy and Decision Makers
- Research
- Education (including schools)
- …
- Public (all citizens) ??

Open to new market opportunities – from few to many users

BUT

Each different category could have different requirements for data management

Source: Alessandro Annoni, JRC

GMES

gmes SERVICES

GMES
Global Monitoring for Environment and Security

kopernikus
Observing our planet for a safer world

opernicus
The European Earth Observation Programme

Gmes
Observing our planet for a safer world

~2004

Present

PROMOTE

SEVENTH FRAMEWORK PROGRAMME

SEVENTH FRAMEWORK PROGRAMME

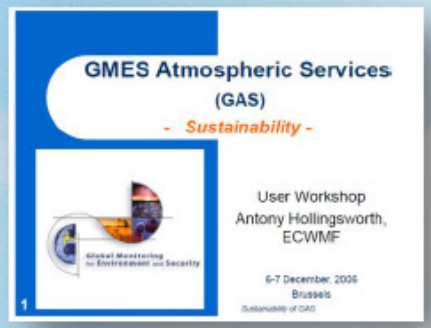
GEMS

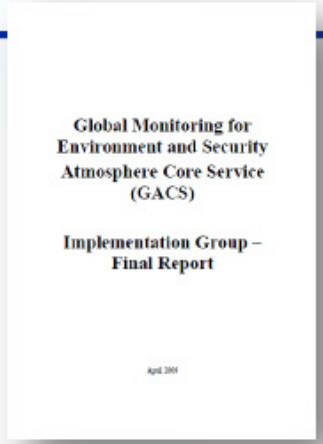
macc
Monitoring atmospheric composition & climate

macc
Monitoring atmospheric composition & climate – II

~2006

Present

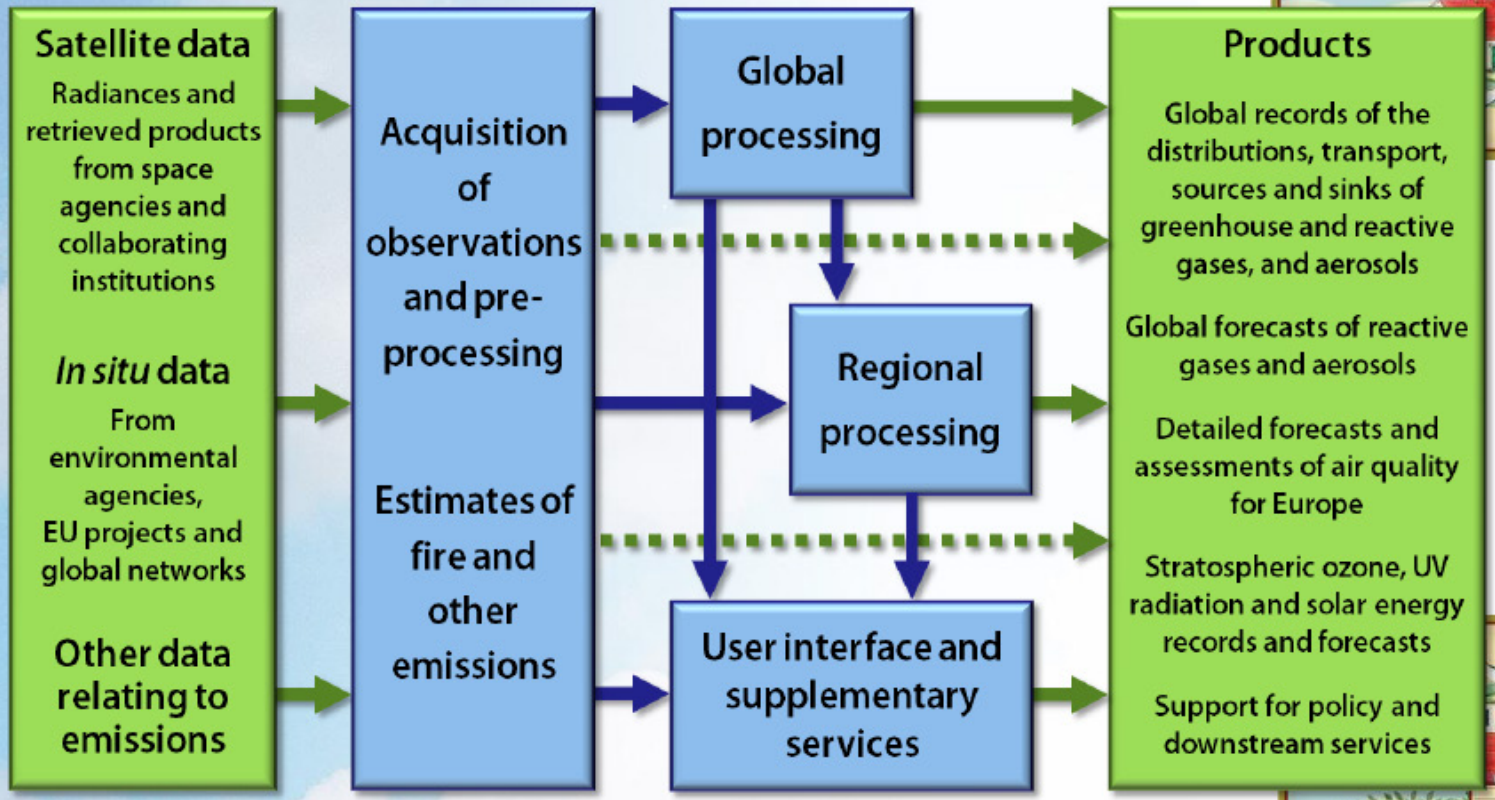


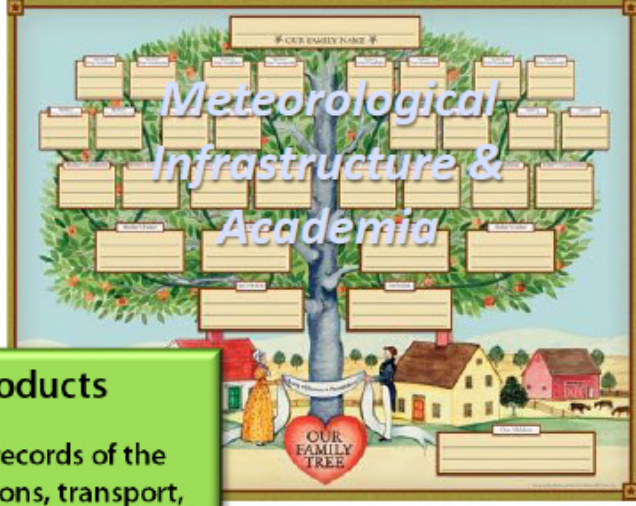

Global Monitoring for Environment and Security
Atmosphere Core Service
(GACS)

Implementation Group – Final Report

Source: Vincent-Henri Peuch, ECMWF

Transforming observations into information





Source: Vincent-Henri Peuch, ECMWF

The global observing system for atmospheric composition

Balloons

Airplanes

Satellites

Trains

Ground-based stations

Ships

...

GEO

GLOBAL ATMOSPHERE WATCH

ICOS integrated carbon observation system

IAGOS

ACTRiS

EEA

AERONET Aerosol Robotic Network

Source: Vincent-Henri Peuch, ECMWF

Key elements of the data and information policy

- *Free, full and open access*
  - **No restriction on use nor on users**

    Reproduction, redistribution with or without adaptation

    Commercial and non-commercial purposes
  - **A free of charge version of any dataset is always available** (under pre-defined format on Copernicus dissemination platform)
  - **Worldwide without limitation in time**

Source: Astrid-Christina Koch, Copernicus

This policy applies to

A. Data (and information) generated inside Copernicus

Sentinel mission data

Service information

Does not apply to

B. Data (and information) generated outside Copernicus

Contributing Mission data

In situ and reference data and information

Copernicus sets the rule for A and follows (or negotiates) the rules for B set by the data providers

Source: Astrid-Christina Koch, Copernicus

Operational Services: What's In It For The Station?

Success for ACTRIS-ESFRI:

- ACTRIS-ESFRI will establish ACTRIS (stations & facilities) as permanent infrastructure.
- Will be successful only if relevant (for digital agenda / Copernicus)

Funding & Visibility at national level:

- Your national funding agency can demonstrate they are contributing to Copernicus (with your station)
- Increased chances of getting national funding on ACTRIS ticket.

Visibility:

- Work towards visibility of network and station in final product.

Increasing the number of NRT stations and instruments

- Follow-up on stations that have NRT upload procedures ready.
- Take one instrument type at a time, focus first on nephelometers, then absorption photometers, then MPSS.

Within ACTRIS WP3, we should provide & share DAQ software that:

- collects data from instrument
- displays incoming data graphically,
- writes data to hard drive in level 0 format
- uploads hourly level 0 files to NRT account at NILU.
- auto-start of the software, e.g. after a power failure.

Need volunteers to write, provide, and maintain such software!!!

Increasing the number of NRT stations and instruments

Volunteers:

Instrument	Responsible
TSI 3563 nephelometer	NILU (ready!)
ECOTECH nephelometer	U. Crete
MAAP	JRC?
Magee AE31	NILU
Magee AE33	NILU
Radiance Res. PSAP	NILU
TROPOS SMPS	TROPOS
Custom DMPS / SMPS	Stations themselves

AeroCom INSITU PNSD: Comparing Climate Model Particle Size Distributions with Surface InSitu Observations

M. Fiebig & S.M. Platt

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Previous Work: