Deliverable Report
D2.1

Project acronym	**IGAS**
Project full title	**IAGOS for the GMES Atmospheric Service**
Grant agreement no.	**312311**
Funding scheme	**Collaborative Project**
Deliverable title	**Specifications of the requirements for interoperable IAGOS data services**
Project start date:	**01.01.2013**
Project duration:	**3 years**
Call topic:	**SPA.2012.1.3-01**
Project web-site:	**Igas-project.org**

Document	
Deliverable number:	2.1
Deliverable title:	Specifications of the requirements for interoperable IAGOS data services
Due date of deliverable:	month 10 (Oct 31st, 2013)
Actual submission date:	November 27, 2013
Editors:	M.G. Schultz
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Reviewers:	P. van Velthoven, C. Gerbig, A. Petzold
Participating beneficiaries:	JÜLICH, UPS, MPG, DLR
Work Package participants:	2
Estimated person-months for deliverable:	12
Dissemination level:	P
Nature:	report
Version:	1.0
Draft/Final:	Final
No of pages (including cover):	14

Specifications of the requirements for interoperable IAGOS data services

This report summarizes the information gathering that has taken place in preparation for the construction of a network of interoperable databases for IAGOS aircraft data. The network shall include the central IAGOS database in Toulouse which will host IAGOS-core and IAGOS-CARIBIC data, the flight campaign archive at DLR, and the MACC data archive in Jülich from which all data shall be accessible via the Jülich OGC Web Services Interface (JOIN).

Interoperability is a broad term which encompasses various ways for discovering and accessing data over the internet. Several standards have been developed for describing geospatial data sets (a necessary requirement for discovery), and other standards exist for formatting and transporting data among services or to the end user. Unfortunately, these standards are not always fully developed (and introducing changes can be a slow and painful process), they are sometimes ambiguous or even contradict each other, and they are often not cleanly implemented. Therefore, the team working on WP2.1 in the IGAS project decided to take a practical approach which will firstly aim to satisfy the user needs. Several interfaces to access IAGOS data will be developed which will follow existing standards where possible, but also contribute to the further development of such standards by providing reference implementations for functional interoperable data services.

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1. The IGAS data network architecture

The primary data centre for IAGOS data will be the central IAGOS database in Toulouse, which already hosts the database for MOZAIC and IAGOS-core data. IAGOS-CARIBIC data will be added to the Toulouse database so that there will be one central access point for all IAGOS data. In addition, the aircraft campaign database in Oberpfaffenhofen and the MACC database in Jülich will be linked to the central IAGOS database so that a one-stop access using the same data protocols, formats, and metadata standards will be achieved for these three sites (in the following referred to as the "IGAS data network"). Furthermore, by exposing IAGOS metadata to large international geospatial catalogues (e.g. EuroGEOSS-Broker), the data from these three data centres shall be easily discovered and accessed from outside the IGAS data network as well. Figure 1 presents an overview of the data and service architecture that shall be built during the IGAS project. The remainder of this report discusses various elements which need to be defined and implemented in order to create a data network which provides the best possible services to the users under the constraints of available hard- and software, cost efficiency, legal issues and data protocols, etc.

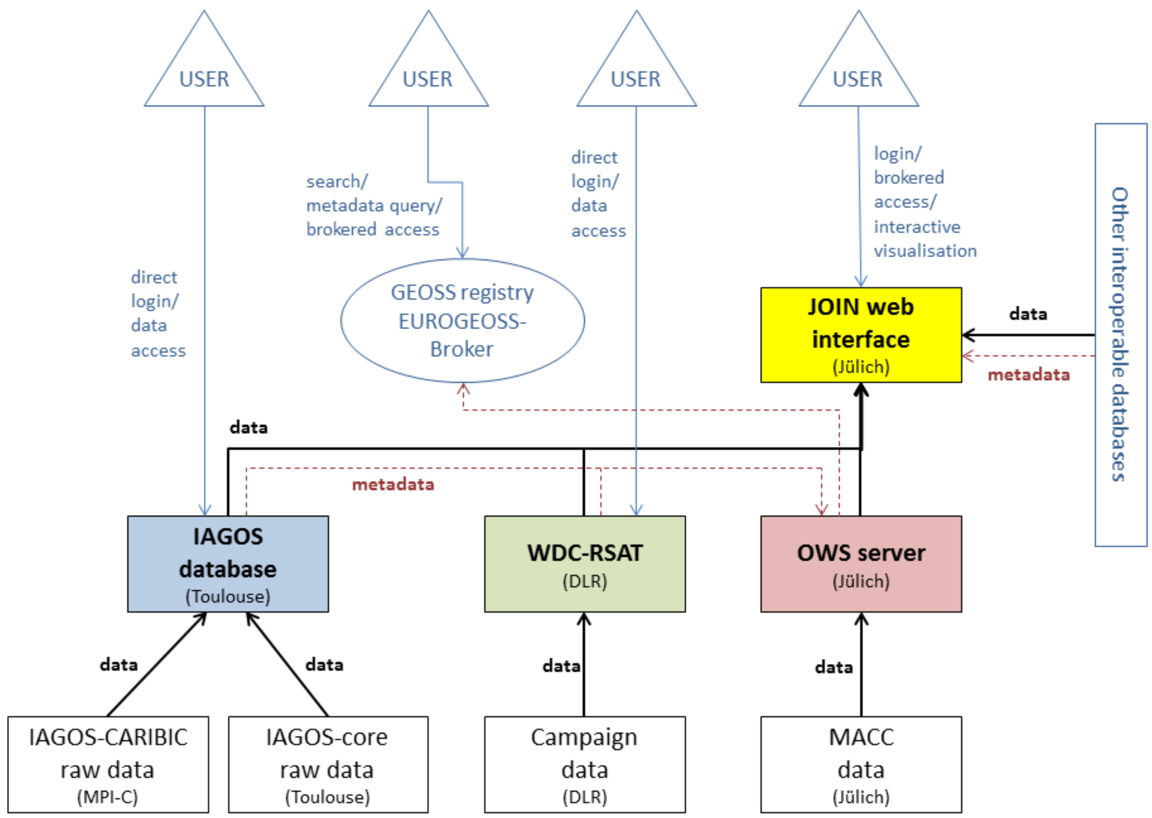

Figure 1: Architecture of the IGAS data network

2. Functionality of the interoperable IAGOS data services

In order to define the requirements for the IGAS data network and to explore possible software solutions, the WP2.1 team established three scenarios describing typical use cases of IAGOS data. These are not meant to be complete, but mainly serve to define the necessary requirements, data formats and processing steps that need to be implemented at the nodes of the IGAS data network. Additional scenarios can be developed once the network is in place and when it has demonstrated its usability.

Case 1: access to high-resolution data for specific episode analysis
Requirements:
- need data quality information stored in the metadata record (instead of having to ask the PI by email)
- precise definition of terms like "missing value" and "limit of detection" and the implications of these
- traceability of instrument (serial number) and calibration
- precise geolocation (and time) information; information about the time zone used (UTC)
- available instruments, etc.; allow queries such as "have there been flights near the Bahamas on April 20th, 2013 (+/- 2 days) which carried a (working) aerosol probe?"

Case 2: Copernicus atmospheric service model evaluation
Requirements:
- NRT access and established update mechanism for validated data
- highly standardized format and data transmission protocol

Notes:
- The MACC project currently uses averaged profiles with a standardized altitude grid; it might be helpful to continue this service even if in the future raw vertical profiles will be delivered
- potentially useful to have averaged data (e.g. 5 minutes) along cruise altitude portion of the flight
- there may be other users interested in NRT data in the future

Case 3: statistical model evaluation, e.g. of chemistry climate models
Requirements:
- need for a stable reference dataset with little detail (e.g. climatological monthly mean profiles); possible variants: relative to tropopause height or interpolated onto PV levels (these could be IGAS products, see OBS4MIP: http://obs4mips.llnl.gov:8080/)
- general information about data quality and representativeness

While case 2 requires special handling because of the near-real-time nature of the data and the format and processing demands of the Copernicus Atmosphere Service, the other two cases shall be handled through user-friendly web interfaces. It is foreseen that a user can log onto one single web interface to find, access, visualize and download IAGOS data, DLR aircraft campaign data, and MACC model data. Other data use scenarios, such as batch processing of large amounts of data, are outside the scope of interoperable services (at least during this stage) and will have to be dealt with individually. However, the standardisation of data access and data formats which will be achieved within IGAS will also help to facilitate such requests.

3. The IGAS data centres and their connections

This section describes how the three IGAS data centres manage their data internally and how they envision sharing data among themselves.

The central IAGOS database in Toulouse

The central IAGOS database is the main access point for atmospheric observations made on a fleet of currently seven airliners. The database contains almost 40000 flights since 1994. During each flight measurements are taken every four seconds from take-off to landing by automated instruments onboard the aircraft. IAGOS-core data are automatically transmitted via GSM network to a reception server immediately after the aircraft lands. The database also includes data from the former MOZAIC project that were transmitted to the reception server and integrated into the database in the same way as IAGOS-core data.

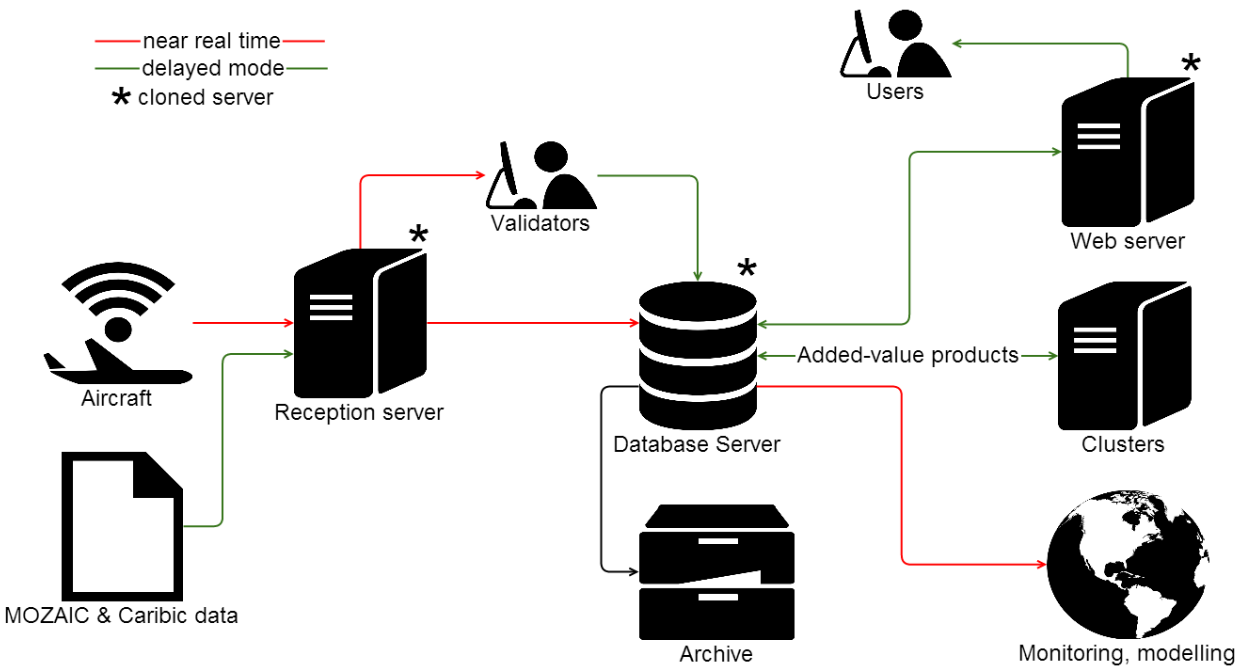

Figure 2: Data flow and architecture of the central IAGOS database. Note that IAGOS data are also used for modelling in delayed mode; however, in this case the users access data via the web server and not directly from the database server

Unprocessed IAGOS-core data first undergo automated validation procedures before being inserted into the database. They are available in near real time within 12 hours of landing for operational users such as climate monitoring services (GMES/Copernicus). Yet data need to be further validated by the relevant PI to improve automatic validation and after the calibration of instruments. These delayed-mode data or final data will be available within a maximum of twelve months for end-users. Added-value products are created on clusters using analyses from ECMWF (European Centre for Medium-Range Weather Forecasts) and emission inventories.

The central IAGOS database also contains metadata, measurements and instrument parameters. Data access is handled by an unrestrictive access policy after a registration procedure. The exact terms of the new IAGOS data policy are currently being discussed within the IGAS project.

The central IAGOS database relies on a user-friendly web interface providing scientific users and policy makers with:

- in-situ observations of atmospheric chemical composition (greenhouse gases, aerosols, cloud particles...) and meteorological parameters (pressure, wind speed, …)
- added-value products: back-trajectories allowing for determination of the geographical origin of air, averaged profiles, climatology, etc.
- quick visualizations: vertical profiles over visited cities, flight time series, maps, etc.

Users can execute the following actions, depending on their user status:

- retrieve data within a location bound box, a time period, selection parameters, etc.
- retrieve data related to an airport location, a time period, selection parameters, etc.
- choose the format of output files
- display flight tracks on a map
- quick visualization of flight observations
- manage metadata (for administrator)
- validate data (for validators)
- manage instruments (for validators)

The central IAGOS database is accessbile to the users via a web interface at : http://www.iagos.fr/extract. The interface has been developped using Java language and J2EE frameworks (JSF2, hibernate, spring). Major update are expected in 2014 to improve the database model and the functionnalities of the web interface.

Web links:
IAGOS central database: http://www.iagos.fr

The DLR aircraft flight campaign archive in Oberpfaffenhofen

The DLR database is the central access point for atmospheric observations made during scientific campaigns with the DLR research aircraft HALO and Falcon. The key tasks of this database are:

- to serve the communities of the single campaigns as an exchange platform of the scientific data during the first years after the campaign
- to give easy access to metadata and to primary data via an online front-end
- to provide extended search functions to explore the entire database
- to disseminate the data to the public after the initial period (usually two years)
- to serve as a long-time archive for scientific data

Short technical description:
The scientific data are parsed during upload by the system software. The system checks if a valid data-format is used and subsequently extracts extensive metadata, see Figure 3. It adds additional information such as arrival airport and departure airport and tries to connect the uploaded data to a specific flight. These metadata are stored in an object relational database with geospatial extension (PostgreSQL/PostGIS) which allows one to perform a geospatial search on the metadata. The primary data are stored in a mass storage with a carefully designed backup strategy and additional information including a checksum to ensure the integrity of the data.
For the user to access the database a dynamic web front-end had been developed. This website (https://halo-db.pa.op.dlr.de) is realized with the Perl catalyst framework. It gives the user an intuitive access to the object relational database in the back.

Interoperability:
Currently, the database is only accessible to the public and the partner databases via the website. That means that a query on the database has to be encoded into a URL and the feedback will be given in plain html. To enable true interoperability, the metadata has to be made available via OGC (Open Geospatial Consortium) services. The DLR database will be connected in the next months with the infrastructure of the World Data Center for Remote Sensing of the Atmosphere (WDC-RSAT) at DLR. After this connection is established, the metadata and also the primary data will be accessible via OGC-services provided by the WDC-RSAT.

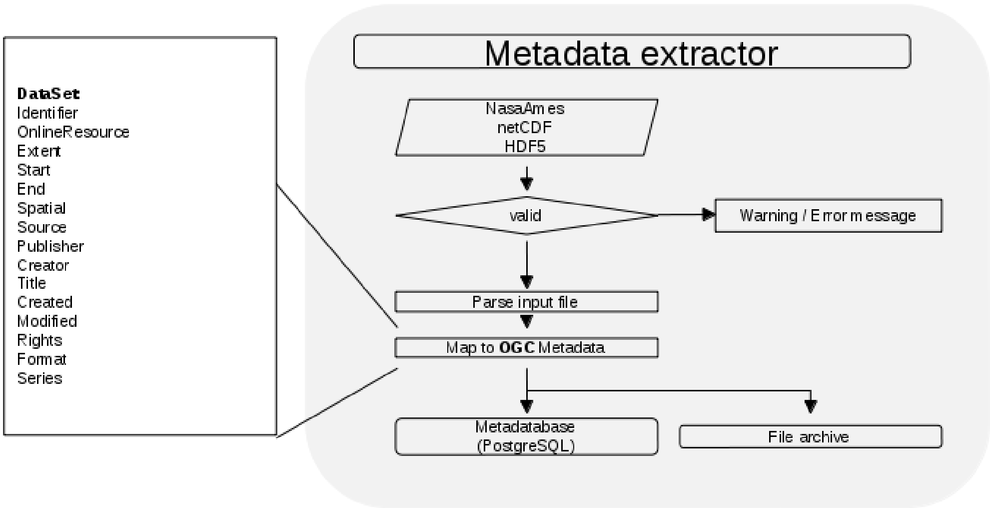

Figure 3: Workflow of metadata extraction that is active during the upload of scientific data into the DLR-database.

The DLR database is accessible to the public via a web front end at https://halo-db.pa.op.dlr.de . At this site the user can explore the content and the relations between the datasets in an interactive and intuitive manner. Most recently the database system has been extended to include sophisticated geospatial searches. The interaction is intended to be that of a human using a standard web browser. No dedicated machine-to-machine interface is currently available.

The MACC database in Jülich

Jülich hosts current atmospheric composition forecasts and reanalysis data from the MACC project, i.e. the precursor service of the Copernicus Atmosphere Service. These data are automatically transferred from ECMWF once per day and reprocessed to form daily forecast files, annual time series, and monthly mean datasets in netcdf 4 format with attributes compliant with CF-1.5 (Climate and Forecast convention, version 1.5. These data files are then accessible via an open-source WCS (Web Coverage Service) server developed jointly between Washington State University, St. Louis and JÜLICH, and also through WebDAV (web distributed authoring and versioning). WCS access is facilitated by the Jülich OWS (OGC web services) interface (JOIN) which allows users to graphically select regions, variables, time ranges, etc. and either visualize data online or download the selected portions of the netcdf files. In addition, JÜLICH stores some observational data from surface monitoring sites in a POSTgres (an open source object-relational database management system) database. These data can be visualized, but not downloaded because of legal restrictions. Finally, JÜLICH also hosts data from the 2006 TFHTAP (Task Force on Hemispheric Transport of Air Pollution) multi-model intercomparison experiment, and allows access to ECCAD (Emissions of atmospheric Compounds and Compilation of Ancillary Data) emissions data and a few other external datasets through JOIN.

JÜLICH is currently investigating the installation of a Unidata THREDDS (**Fehler! Hyperlink-Referenz ungültig.**) server for the MACC data files. This would allow for a more flexible storage structure and also for inter-conversion among various data formats.
The JOIN web interface encapsulates all necessary exchange of metadata and search queries and provides the user with easy access to a variety of datasets hosted in Jülich and elsewhere as long as these data are accessible via the OGC WCS protocol. JOIN was developed during the TFHTAP multi-model intercomparison activity and forms an essential element for data provision in the MACC project. The web interface is currently undergoing a major overhaul whereby its underlying web framework is being changed from web.py (http://webpy.org/) to DJANGO (https://www.djangoproject.com/). The new version of JOIN will feature user login and user sessions, it will allow for a better integration of different datasets, and data visualization should become faster because more of the plotting will be performed on the client side.

Web links:
Jülich WCS server (current forecasts): http://ows-server.iek.fz-juelich.de/MACC_fnyp_fc-3hourly_ModelLevel?service=WCS&acceptversions=1.1.2&Request=GetCapabilities&sections=Contents
Jülich WebDAV service (MACC data): http://macc.iek.fz-juelich.de/data/
JOIN: http://join.iek.fz-juelich.de/macc/
THREDDS: http://www.unidata.ucar.edu/software/thredds/current/tds/
Open-source WCS server package: http://redmine.iek.fz-juelich.de/projects/geo_aq_cop_community_web_server

Integration of IAGOS-CARIBIC data into the Toulouse database

After the common definition of IAGOS-core and IAGOS-CARIBIC parameters, the integration of the CARIBIC data into the central IAGOS database in Toulouse will be done in 2014. The relevant subset of the CARIBIC data will be transmitted from MPI-C in Mainz as NASA AMES text or as netCDF files by FTP to the IAGOS reception server in Toulouse and processed in the same way as MOZAIC data.

For the greenhouse gases CO_2, CH_4, N_2O and SF_6, the data are provided for each discrete sample collected along the CARIBIC flight tracks. For the CARIBIC in situ instruments, the data are provided as a continuous data stream along the flight path. Most in situ data are available with a time resolution of around 1 s. It is yet to be determined which time resolution, i.e. 1 s, 4 s or 10 s, is suitable for integration into the central IAGOS database to be compatible with the IAGOS-core and MOZAIC data streams.

During the coming months, procedures for updating and versioning IAGOS-CARIBIC data need to be developed. Initial discussions about this topic took place during the WP2.1 meeting in Jülich (19-20 June 2013).

Data connections between Toulouse, Oberpfaffenhofen and Jülich

There are two different types of connections which must be ensured in order to achieve full interoperability among different databases. The first aspect involves the transfer and interpretation of metadata, which is essential to query the database and to obtain additional information about a specific dataset. Secondly, the data centres must agree on formats and protocols to transfer the actual data among themselves. Note that the standardisation that is involved here can be different from the way that data and metadata are delivered to the end user or to other data centres outside the project. For the "internal" connections the efficiency of accessing and transporting data is the most relevant criterion, whereas communication with the outside world requires adherence to more widely accepted metadata standards and data formats and a broader variety of choices. Nevertheless, adherence to standards even for internal communications will facilitate the brokering of data services and potential modifications of data streams and shall therefore be applied to the extent possible.
In order to enable a smooth interoperable data exploration by the end user, the primary requirements for data transfer among the three IGAS databases are low latency and high transfer rates. When querying the existence of a specific dataset or subset, the database centres exchange metadata information comprising of a defined set of parameters. A single query will be tiny in size and can generally be coded for example into a URL. On the other hand, depending on the activity on the sites of the data centres, there can be a huge number of such queries. The response to such a query varies according to the protocol employed and may consist of either an ephemeral web link or a more or less extensive XML document which could even contain the requested data in ASCII encoding (e.g. in the OGC SOS protocol).
A severe shortcoming of current OGC protocols is the lack of metadata information on the expected size of a requested data transfer. Geophysical datasets as they are produced and

distributed in IAGOS and MACC can be as large as several gigabytes, which can easily cause timeouts or memory exceedances of interactive services, or at least disrupt the interactive experience of a user who tries to analyze or visualize data over the internet. The data centre connections within the IGAS network will have to take this into account and define a mechanism through which it becomes possible to estimate the approximate data volume that is associated with a user request so that appropriate action can be taken *before* the actual data transfer (e.g. display a warning, cancel the request, offer an archived file (zip or tar.gz) instead, etc.).
Most of the standard protocols which would be suitable to openly exchange aircraft (and model) data come with substantial overhead (parsing of large XML files) and use ASCII encoding for data values, which increases the volume and requires a translation process. It will therefore be necessary to define a data transfer protocol among the IGAS partner institutions which is more efficient and transfers data in binary form. A final decision on this has not yet been made. The following options are being considered, and a number of test cases will be set up in order to establish the optimum solution:

1. Direct database access: in this model, the web interface in Jülich would be registered as a (read-only) user to directly access the databases in Toulouse and Oberpfaffenhofen and retrieve data from there via SQL requests. This requires detailed knowledge of the database structures. Since the Jülich interface would act "on behalf" of a registered user, it must be ensured that this user is actually allowed to retrieve data from either database. We will explore a solution to this which resembles the technology used in web certificates.
2. THREDDS access: The Unidata THREDDS data server enables direct access to (netcdf) data files via OpenDAP, WMS, and WCS. This technology is used at several sites in the US to host and serve vast collections of data, often with near-real-time access. Jülich will explore the installation and use of a THREDDS server and the team will discuss if this could be a way to implement fast data transfer among the IGAS data centres.
3. For the 'query mode' communication the query parameters can be encoded into the URL of an HTTP-request (for example, a URL similar to http://igas-datacentre.eu/search?xml&count&BoundingBox=354.7,44.5,15.2,64.2& TimeSequence=2012-10-01T00:00/2012-10-31T23:59&species=ozone,carbondioxide could be used to inquire about the number of available observations of ozone and carbon dioxide in a bounding box over Central Europe in October 2012 and the response format shall be an xml file). The exact syntax of such requests depends on the adopted standard, its version, and the software that is used to implement the web services. For IGAS it is important to define which requests can be made to which data centre and how each of these requests shall be answered.
   The responses could be encoded into different formats such as xml, plain html, json, depending on the requirements of the querying system.
4. Sensor Observation Service (SOS): This is a web service to query real-time sensor data and sensor data time series. The offered sensor data comprises descriptions of sensors themselves, which are encoded in the Sensor Model Language (SensorML), and the measured values in the Observations and Measurements (O & M) encoding format. The web service as well as both file formats are open standards and specifications of the same name defined by the Open Geospatial Consortium (OGC). Partner UPS is exploring the possibility of using this service to exchange aircraft data.

Authentication methods and restrictions on the access of the primary data that exist in each data centre shall not be bypassed by the interoperable network. Several ways of satisfying this requirement are available but no final decision has been made so far. Applying an Open Data policy by setting the content of the databases under a public license would make this process much easier but due to the nature of the scientific data (preliminary and final state, "first publication" rights) this cannot be achieved. However, following on a request from WP2.1, the IAGOS PIs have agreed to make aircraft position and time information freely available without access restrictions. This is essential in order to enable metadata queries such as those given in Case 1 or the example in point 3 above.

Concerning the exchange format for data transfer between the IGAS data centres, netCDF appears to be a reasonable option, unless we decide for direct SQL access (option 1 above). Smaller amounts of data might be transferred efficiently enough in ASCII formats, but for larger datasets a binary format is mandatory. In order to avoid having to support multiple formats it will probably be easiest to encode all transfers in netCDF.

4. Data delivery to users

Direct access to either the IAGOS or DLR databases will remain possible. Users need to be registered for access and follow the instructions provided at these sites. At DLR the primary data are in general available to the public two years after the observation. This period is needed by the scientists to prepare the data into its final state (calibration, quality control, etc.) and to publish their work connected to this data. After that time the Open Data policy is applied to the data. However, the metadata are available to the public as soon as the data enter the database.

Similarly, IAGOS data on the Toulouse server are accessible to registered users after screening and quality control of the data. In the past there has not been extensive support for the provision of metadata information for database queries and interoperable applications. This shall be implemented within the IGAS project.

In addition, through the IGAS project, users will get interoperable access to aircraft data via the Jülich web interface JOIN or through web services that will be implemented at all three sites. At DLR, the campaign database will be linked to the World Data Center for Remote Sensing of the Atmosphere (WDC-RSAT). As a result the full content of the DLR database will be made available through OGC-services operated by the WDC-RSAT. Toulouse and Jülich will provide these web services either through the open source WCS server or through THREDDS. JOIN will provide a one-stop access point to all data, which will also allow users to reformat data, package data into netcdf groups, and ultimately to process data (e.g. averaging, calculation of combined variables, etc.).

The current JOIN interface (http://join.iek.fz-juelich.de/macc/) has been written in Python and Javascript and allows for access to gridded data that have been entered into a catalogue (see Data services – Data access), and comparison of model data to selected station measurements from the German environmental monitoring network (Data services – Data comparison). The user can select the geographical domain and time extent of the data and choose the variables for download or display. The gridded data (generally model data) are transferred to a workspace from which they can be either downloaded or visualized. Current visualisation options comprise time series (for the station comparison), maps, and vertical cross sections. Several fields can be overlaid and individually controlled with respect to color schemes, ranges, transparency, etc. The current version of JOIN has limitations in terms of the data model and ease of use. It does not allow for user login and cannot save sessions. Therefore, JÜLICH has started to re-program JOIN, including a complete re-design of the underlying data model and web module. The new JOIN will be based on the DJANGO framework which includes modules for user management, session management and interface administration.

5. Data discovery

The discovery of IAGOS data is foreseen to proceed along different lines. Some users who may have worked with MOZAIC or IAGOS data in the past may know what they are looking for and request, for example, all data for a specific flight in the original time resolution. For these users, the new capabilities of interoperable access may improve the information content that is delivered with the dataset, and the brokered approach may allow them to obtain the data directly in, for example, the NASA AMES format or as a fully CF compliant netCDF file without having to first download and then convert the files.

With the help of the PIs, we are currently compiling the list of the parameters of IAGOS-core, IAGOS-CARIBIC, and MOZAIC datasets (actual parameters and from future packages 2). For each parameter we are defining three names:

- the standard name which refers to the CF convention and will be only used in the NetCDF files (e.g. mole_fraction_of_ozone_in_air)
- the short name (e.g. O3_P1)
- the long name which will be used for display in plots or web pages (e.g. ozone mole fraction measured by IAGOS package 1)

An open issue at this point is the level of detail to be included in the description of the instrument which performed the measurement.

A more generic approach to IAGOS data discovery involves searching one of the larger international web catalogues, such as the GEOSS registry or the EuroGEOSS Broker, NASA's Global Change Master Directory, etc. These catalogues provide web interfaces allowing the user to restrict their query by specifying a geographic domain, time interval, variables, keywords, or free text search. The response to such a query will generally consist of XML files which are then displayed as icons, web links, or informative text. The XML files generally follow the ISO 19115 standard and/or the INSPIRE directive. Through collaboration with MACC and other initiatives, the IGAS WP2.1 team members hope to establish a community metadata profile for atmospheric composition data which will clarify some of the ambiguities that are inherent in the ISO and INSPIRE standard documents.

The metadata for IAGOS data shall be made available to catalogue services like EuroGEOSS Broker. Initially we will use the Jülich WebDAV server for this purpose, from where

EuroGEOSS broker can harvest the information at regular intervals. Later, the difficulty of implementing an actual web catalogue service shall be explored.

Another aspect that shall be worked on in IGAS is the definition of metadata discovery facets, i.e. groups and terms of controlled vocabulary that could be used in dataset queries. Here it is essential to establish realistic user scenarios, i.e. ask users what information they might like to use for identifying specific datasets. In addition to the standards position, time and variable, this could be items like aircraft number, departure and arrival airport, etc.

As documented for the DLR database above, scripts will be developed to automatically generate metadata for custom-tailored datasets that are generated based on specific user requests.

6. Data analysis

In order to allow users a meaningful analysis of aircraft data, the actual datasets must be accompanied by a comprehensive set of “descriptive metadata”. These metadata include more information than the “discovery metadata” mentioned above, such as calibration records, information about the specific instrument that performed the measurements, dataset versions, etc. Initially such metadata will be purely informational. In the distant future (i.e. beyond IGAS) it may then become possible to link such information, for example in order to retrieve and display all calibration records of one particular instrument or apply different corrections for individual instruments “on the fly”.

7. Data access restrictions

The central IAGOS database requires registration of users before they can access data. This user registration shall be facilitated such that a user can register at any of the three sites (or at least at Toulouse and JÜLICH) and the registration information will be shared among the data centres.

The IAGOS-CARIBIC PIs are still discussing which parts of the CARIBIC data set beyond the metadata may be made freely available to the general public (Open Data). However, all CARIBIC data are and will remain available for scientists upon request to the CARIBIC PIs. The CARIBIC user registration shall be harmonized with the IAGOS-core registration so that the same procedure, web form and mechanism for exchanging license information can be used.

The campaign data at the DLR follows a separate data policy (see section 4 above).

A new data policy for IAGOS and MOZAIC data is currently under discussion in the IGAS project.