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Deliverable 6.2.1 – Specifications of the data storage

Work Package	**WP 6 : Ocean use case**
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Dissemination Level

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Versioning and contribution history

Version	Date	Author	Notes
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1.5	11.03.2020	Corrections after review Joel Sudre (CNRS)	Deliverable version (with revision marks)
1.6	11.03.2020	Gilbert Maudire (Ifremer)	Final version (taking in account the review and remarks on deliverable D6.1.1)

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TERMINOLOGY

Terminology/Acronym	Description
CSW	Catalogue Service for the Web (ISO/OGC Protocol)
DIAS	Data Information and Access Service
DIVA	Data Interpolating Variational Analysis
DIVAnd	DIVA in n dimensions (new version of DIVA)
EMODnet	European Marine Observation and Data Network
EOSC	European Open Science Cloud
EUDAT	Collaborative Data Infrastructure in Europe
HPC	High Performance Computing
HPDA	High Performance Data Analytics
OGC	Open Geospatial Consortium
OPeNDAP or OpenDAP	Open-source Project for a Network Data Access Protocol
SeaDataNet	European Research Infrastructure for Marine Data Management
WCS	Web Coverage Service (OGC Protocol)
CSV	Coma Separated Values, Flat Text File Format
CF-convention	Climate and Forecast convention
NetCDF	Network Common Data Form
BGC	Bio-Geo-Chemical variables
DOI	Data Object Identifiers
IFCB	Imaging FlowCytoBot
API	Application Programming Interface
ORCID	Open Researcher and Contributor Identifier
iRODS	Open Source Data Management Software (irods.org)

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Executive Summary

This document provides the specifications of the Data Storage of the "Ocean use case" defined and developed in WP6 of the PHIDIAS project. This version has been reviewed by Joël Sudre (CNRS). It is the first deliverable version.

It presents the use case context before detailing the technical requirements in order to present the main components to readers.

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1 Objectives of the WP6 – Ocean use cases

The general objective of the WP6 - Ocean use case is to improve the use of cloud services for marine data management, data service to users in a FAIR perspective, data processing on demand, taking into account the European Open Science Cloud (EOSC) challenge and the Copernicus Data and Information Access Services (DIAS).

Since the marine environment is evolving continuously, and because marine observation is still expensive, observation data are unique and must be well preserved and easy to be retrieved.

In practice, several functions (cf. Fig. 1) have been implemented either in France, by the Ocean – Odatis cluster of the French Earth Observation Research Infrastructure DataTerra and, in Europe, by the SeaDataNet Research Infrastructure, the European Marine Observation and Data Network for in-situ data and the Copernicus Marine Environment Monitoring Service for Operational Oceanography and Satellite Data:

- Distributed Data and Services Centres manage data that are acquired in routine modes**.** Those data centres have established a direct interface with observation systems: satellite missions, in-situ observatories, research fleets in relationship with National Oceanographic Data Centres.

- Data that are acquired more occasionally ("long tail data") or data that require manual work at laboratories to be elaborated are often not directly interfaced with data centres. In order to facilitate the ingestion of these data in the marine data management infrastructure, **publication/archiving services** have been provided to scientific teams.

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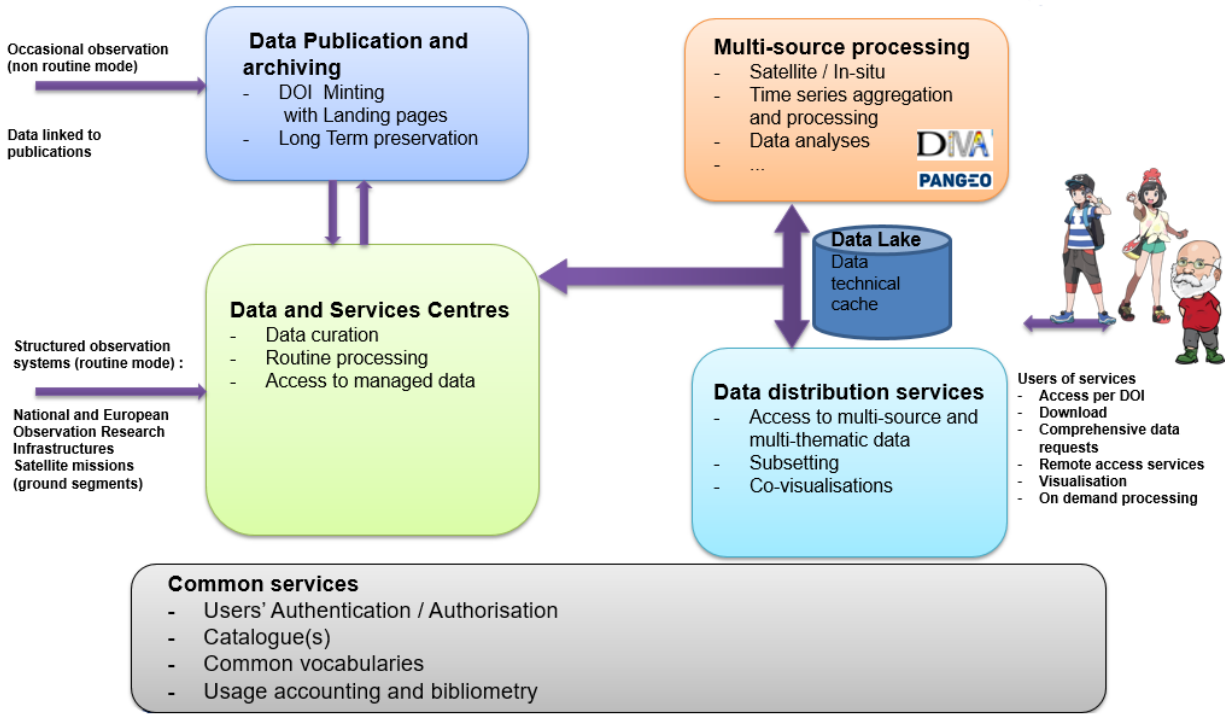

Figure 1: General architecture of services provided by French and European Marine Data Infrastructures

Most of these services are already implemented by the French Ocean Data Management Cluster (Odatis) and by European Infrastructures such as SeaDataNet and EMODnet. However, upgrades are necessary to facilitate and to speed-up response time of data access and data browsing, to enlarge data management capacities, and to improve the long-term stewardship of marine data, especially for the long tail in-situ observations.

In this context, the technical objectives (cf. Fig. 2) of the WP6 - Ocean Use Case are, by making an adapted use of HPC (high-performance computing) and HPDA (high-performance data analytics) capacities:

1. **Task 6.1: Improvement of long-term stewardship of marine in-situ data**
2. **Task 6.2: Improvement of data storage for services to users**
   - For two contexts :
     - 1- Fast and interoperable access for visualization and subsetting purposes (web portal)
     - 2- Parallel processing within dedicated high-performance computing
3. **Task 6.3: Marine data processing workflows for on-demand processing**

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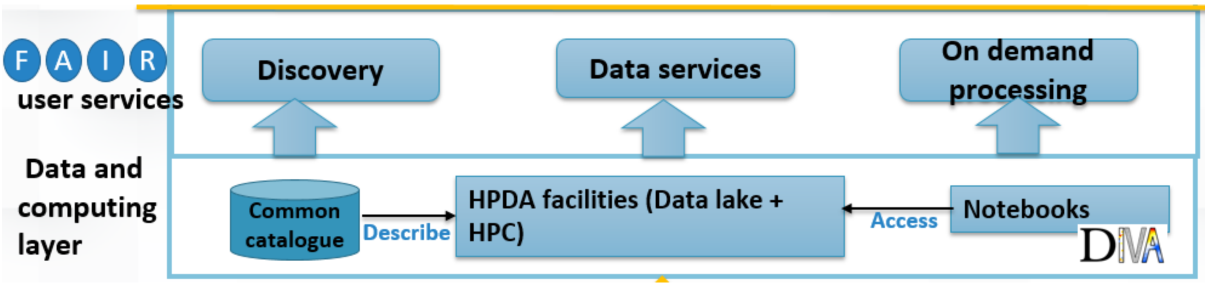

Figure 2: General sketch of the WP6 - Ocean use-case

In respect of those objectives, two main requirements have been identified about data storage:

1. Reinforce the long-term preservation capacities of observational data;
2. Manage a work copy of data with adapted structure in order to speed up and facilitate data retrieval and data processing. This working copy can be considered as a "**technical cache**" (called "**Data Lake**" in this document) that accelerates and harmonizes data requests and data processing, and may be consider as the **work copy of data**.

The need 1 – "Long-term preservation capacities" will be described by the deliverable 6.1.1 - Specifications for long-term data archiving procedures in respects of RDA recommendations, since this deliverable will focus on the "Data Lake", which is the work copy of data.

The specifications of the need 2 (Data Lake) will be considered in this document.

Because, the marine data, especially in-situ observations, are managed in very distributed systems, it is difficult to provided services to users that require data from different data sources such as in-situ and satellite data or to assemble multidisciplinary datasets on a specific data areas. In this context, one of the ambitions of the present use-case is to facilitate the discovery and the assembling of data from distributed data management systems, in two cases:

- On line data distribution services such as:
  - Discovery, selection, assembling and subsetting of multi-sources data;
  - Visualization of data from different sources to allow visual comparisons.
- On-demand data processing:
  - Using Notebooks;
  - With Diva interpolation software;
  - With Pangeo Python components library for specific data browsing and analysis.

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2 Managed data

Marine observations are made up of several data types, with different characteristics:

- Satellite data (large datasets, covering only the sea surface);
- In-situ observations (many small datasets, often with measurements below the sea surface).

And from distributed data repositories, such as:

- Operational oceanography observations that are, for example, stored in the DIAS Wekeo;
- Scientific observations that are, for example, stored using EUDAT services (SeaDataNet European infrastructure) or by the Data Centre themselves;
- Long tail data sources that are partly managed by online publication/archiving services.

Access conditions may differ from one data source to another one, for instance for some repositories, access is only granted to registered users (MarineID for SeaDataNet, Mercator Ocean International for Copernicus …).

Most of those data are recorded using one of these formats: NetCDF (following the CF-Conventions), Ocean Data View spreadsheet (CSV compatible + semantic header). Other formats must also be considered such as Geographical Shape Files (SHP) and imagery formats (TIFF, Geo-TIFF, JPEG and MPEG for the animations).

This use case will target only two specific areas: the North Atlantic (North-East for the Chlorophyll-a) and the Baltic Sea. These 2 regions represent 10 millions of observations in the North Atlantic and the Baltic Sea, accounting for a total of approx. 250 GBytes. However, the progresses achieved during the Phidias project will be extended to other data sources and data types as far as possible.

The following data sets will be considered at a first stage by the use case:

2.1 In-situ Data

- SeaDataNet and EMODnet-Chemistry marine in-situ data collections, managed at EUDAT partner CSC (Finland), especially:
    - Temperature & Salinity
    - Chlorophyll-a concentration
    - Access conditions at https://www.seadatanet.org/Data-Access
- Copernicus in-situ data collections, managed by DIAS-WEKEO, Ifremer and FMI, especially:
    - Temperature & Salinity
    - Chlorophyll (BGC Argo & FerryBox)
    - Access conditions at http://www.marineinsitu.eu/access-data/

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- Euro-Argo data managed by Ifremer, especially:
  - Temperature & Salinity
  - Chlorophyll (BGC Argo)
  - Access services:
    - ftp servers
      ftp://ftp.ifremer.fr/ifremer/argo
    - DOI (Data Object Identifiers)
      http://www.argodatamgt.org/Access-to-data/Argo-DOI-Digital-Object-Identifier
    - synchronization service (rsync)
      http://www.argodatamgt.org/Access-to-data/Argo-GDAC-synchronization-service
  - Thredds server API
    http://tds0.ifremer.fr/thredds/catalog/CORIOLIS-ARGO-GDAC-OBS/catalog.html
- Imaging FlowCytobot (IFCB): in-situ automated submersible imaging flow cytometer at Utö field station
- Long-tail observations managed by EMODnet Ingestion and SeaNoe online publication/archiving service

2.2 Remote Sensing Data

- SMOS Sea Surface Salinity products, managed at Ifremer
  - De-biased 10-day average & monthly salinity field products from SMOS satellite (mixed orbits)
  - Access services :
    - ftp server: ftp://ext-catds-cpdc:catds2010@ftp.ifremer.fr/
    - DOI: 10.12770/0f02fc28-cb86-4c44-89f3-ee7df6177e7b
  - 20 MBytes per day
- Sentinel-3 imagery, managed at ESA-DIAS (variables to be defined)
  - Sentinel 3 (OLCI) service
  - Two datasets: 1) Full resolution with 300 m spatial resolution and 2) Reduced Resolution is approximately 1.2 km on ground. Resolution 20m
  - access conditions at https://sentinel.esa.int/web/sentinel/user-guides/sentinel-3-olci

2.3 Output Data

Products will be 4-D gridded fields (latitude, longitude, depth, time) or 3-D (fixed depth of fixed time) recording using netCDF according to the CF conventions (Climate Forecast, http://cfconventions.org/).

Examples may be found at: https://www.seadatanet.org/Products#/search?from=1&to=30.

See also figure 3 and 4 below.

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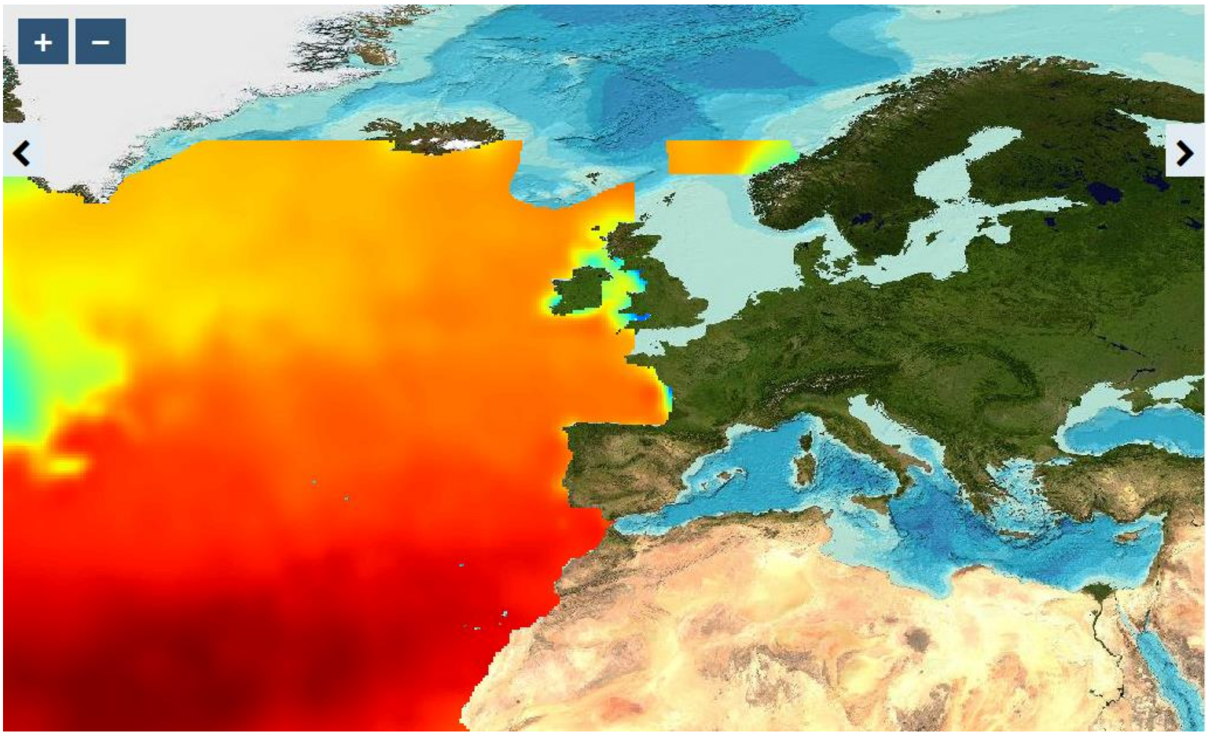

Figure 3: North-East Atlantic Mean Salinity at surface in January (Ocean Browser – ULiege)

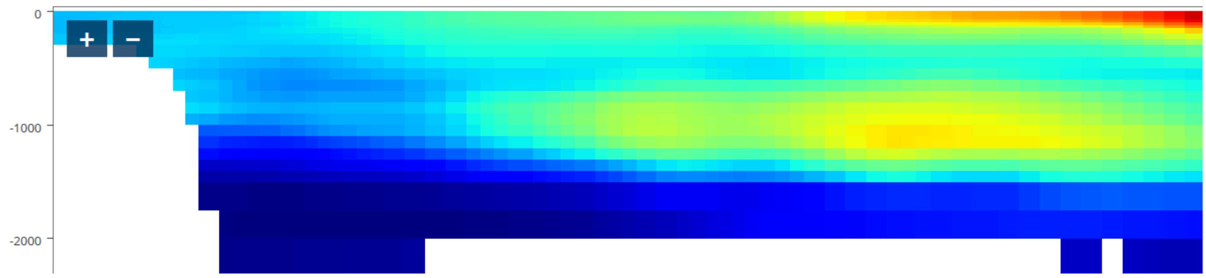

Figure 4: Vertical section of North-East Atlantic Mean Salinity at longitude 20°W, with Mediterranean water bodies (Ocean Browser – ULiege)

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3 Specifications of the data storage ("Data Lake")

The "Data Lake" will assemble data from several in-situ and satellite data sources, which may face different issues:

- In-situ datasets are not extremely large. However, managed data types are heterogenous : vertical profiles, times series, underway data... In addition, due to this heterogeneity, data are often managed in separate files or relationnal databases, that leads to very large amount of files (> hundreds of millions of individual observations). Browsing such a large number of observation is really ineficient.
- Satellite datasets may be very large (> several tens of petabytes at total), that leads to difficulties to transfer them over networks.

The "Data Lake" will be periodically synchronized (e.g. daily) with the Data Centres. Since it is impossible to transfer all data at each synchronization period, the Data Lake has to be persistent.

Important notice: The management of the original copy of the datasets assembled in the Data Lake will remain under the responsibility of the Data Centres. The Data Lake is considered as a work copy of the data.

3.1 Data structures within the Data Lake

Data structures within the data lake will have to be adapted to the targeted uses. Two main uses are targetted:

- Online selection and vizualization of data using a two-step discovery service via a common catalogue : 1) Selection of "Data collections" / Datasets , and then 2) selection of the subset of data of interest. This common catalogue will have to be stored. Access to data will have to be optimized to select and retreive a small amount of data amoung a large number of data, using different selection criterions : geographical, temporal... This case will be mainly oriented towards in-situ datasets.
- On demand data processing of large data subsets using DIVA or Pangeo,

Providing storage infrastructures for these two requirements will probably necessitate two different data structures :

- One data structure adapted for selecting a few amount of data within a large number of data (e.g. NoSQL databases), especially for in-situ data;
- One data structure adapted for processing large subsets of data, in parallel mode if necessary (e.g. "Data Cubes" such as Xarray, Parquet...).

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3.2 Storage of the common catalogue

- **Input** : Existing data indexes from SeaDataNet & EMODNET (CDI-Common Data Index, https://www.seadatanet.org/Metadata/CDI-Common-Data-Index, including planned development of an API in the framework of ENVRI-FAIR) and CMEMS in-situ data index (e.g. API https://fleetmonitoring.euro-argo.eu/swagger-ui.html)

- **Objective** : Interoperability of metadata between SeaDataNet (Common Data Index) and Copernicus Marine Services including fast detection of co-localized data, and improvement of long term preservation especially for "Long Tail" data using publication services (such as SeaNoe which is used by SeaDataNet / EMODNET).

- **Output**: 2-Step Discovery service for in-situ marine observations via a common catalogue : 1) Selection of "Data collections" / Datasets , and then 2) selection of the subset of data of interest. Storage of the common catalogue required (already partially managed with the help of EUDAT).

- **Prototyping** : Set up of the common catalogue and of a prototype user interface for selecting observations.

- **Storage** : The common catalogue will be stored as an **Elastic Search** NoSQL database, in order to allow facetting of the web selection portal, with optimized response time.

3.3 Data Lake for selection and visualization

- **Input** : Existing in-situ data sources from SeaDataNet, EMODNET, CMEMS, EuroARGO and the French Odatis Ocean data cluster. Satellite data are less used that way.

- **Objective** : Create and populate and adapted data structure within the "**Data Lake**" that facilitates and improves access to data (especially for in-situ data) for fast and interoperable access for visualization and subsetting purposes (web portal) : **"access few data among many data".**

- **Output** : "Small" extracted data subsets and web-based maps and diagrams (representation of time-series and of vertical profiles).

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- **Prototyping** : set up of the Data Lake by implementing *NoSQL* Data base (e.g. Cassandra). This includes the synchronization procedures from distributed data sources to the adopted data structure within the Data Lake.

- **Storage** : The adopted data structure will be, in this case, a **Cassandra** NoSQL database, which is able to retreive data using different selection criterions. Using the same data structure than the structure adopted for on demand-processing will be also considered and tested in order to discard the need of data duplication in several structures.

3.4 Data Lake for on-demand processing

- **Input** : Existing data sources from SeaDataNet, EMODNET, CMEMS, EuroARGO and the French Odatis Ocean data cluster, including both in-situ data and . Satellite data are less used that way.

- **Objective** : Create and populate and adapted data structure within the "**Data Lake**" that facilitates and improves browsing and processing of large amount of data (e.g. salinity and chlorophyll), preferably in parrallel: **"access many data among many data".**

- **Output** : Gridded fields of Salinity and Chlorophyll.

- **Prototyping** : Data processing will be conducted using both DIVAnd software and Pangeo software component suite. These software tools will be used within notebooks for providing direct user interaction. The users will launch the processing on demand. DIVAnd will be adapted to be interfaced with the provided data structures in the Data Lakes. Tests will be conducted for exploiting HPC facilities (parallel processing using a compiled version of DIVAnd).

- **Storage** : The adopted data structure will be, in this case, a **"Data Cubes"** which are used to access data using Pangeo software components suite : e.g. zarr format, Xarray, Parquet, Arrow. In order to facilitate identification of avalaible data sets from a Python Script, an Intake interface will be set up on top of the (https://github.com/intake/intake). Intake is a lightweight package for finding, investigating, loading and disseminating data.

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4 Synchronisation mechanisms

Routine software will be developped and set up to synchronize source datasets with the "Data Lake". This sofware will have to manage:

- Identification of the new data or the data that have been modified or deleted from the last synchronisation, using the common catalogue;
- Data transfert from data source to the Data Lake over the network;
- Reformatting of the datasets according to the data structure(s) adopted for the Data Lake.

Use of iRODS dataflows seems to be well adapted to synchronise source datasets and the Data Lake.

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