Blue-Cloud

Piloting innovative services for Marine Research & the Blue Economy

D2.7 Blue Cloud Architecture (Release 2)

Work Package	WP2, developing the Blue Cloud discovery and access service and overall Blue Cloud architecture
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0.1	27.07.2020	MARIS	First version
0.2	29.05.2021	CNR-ISTI	Adding new VRE aspects
0.3	31.05.2021	MARIS	Review and adding new Data Discovery and Access service aspect
1.0	31.05.2021	TRUST-IT	Deliverable submission
2.0	30.09.2021	MARIS, CNR-ISTI, TRUST-IT	Revised Deliverable submission

Contents

Executive summary

This deliverable D2.7 describes the Blue Cloud architecture as it is known at Month 20. It is the second release of the architecture and an update of the earlier 1st release of the Blue-Cloud architecture document D2.6. It is expected that there will be further developments and refinements to the Blue Cloud system. For that purpose, one more release of the architecture document is planned, namely report D2.8 in Month 27.

In order to make it easier for readers and reviewers, a table is included as part of Chapter 1, which indicates the elements and sections of this Deliverable 2.7, which have been updated or added in comparison with the earlier Deliverable 2.6.

The technical framework of the pilot Blue-Cloud features:

1) **the Blue Cloud Data Discovery and Access service** component to serve federated discovery and access to blue data infrastructures
2) **the Blue Cloud Virtual Research Environment (VRE)** component to provide a Blue Cloud VRE as a federation of computing platforms and analytical services.

In this report, the current architecture and functionalities of each of these components are described in detail as well as the roles of partners that are developing and hosting modules.

The Blue Cloud Data Discovery and Access service architecture is based upon a combination of the DAB metadata broker service of CNR-IIA, and the SeaDataNet CDI service modules as developed by MARIS, IFREMER, and EUDAT in the framework of the EU SeaDataCloud project. For the Blue-Cloud Data Discovery and Access service and its modules, additional developments were needed such as adapting and upgrading of existing services, adding new services, testing modules, integrating modules, and testing the integrated service, in order to achieve the planned functionality.

The Blue Cloud VRE is largely based upon the existing **D4Science e-infrastructure** as developed and managed by CNR-ISTI. This e-infrastructure from the start hosted already multiple Virtual Labs and offered a variety of services. These services have been adopted and adapted for the Blue Cloud and new services have been added, while also new Virtual Labs have been constructed and deployed as part of the Blue-Cloud Demonstrators. The D4Science e-infrastructure also already had proven solutions for connecting to external computing platforms and means for orchestrating distributed services, which are instrumental for smart connections to the other e-infrastructures in the Blue-Cloud system.

The Blue Cloud demonstrators are developed as Virtual Labs embedded in the D4Science VRE e-infrastructure and supported by data input from the Blue Cloud Data Discovery and Access service and other data resources, and additional computing services. The demonstrators are worked out in a cooperation between WP3 and WP4, analysing their scientific workflows and technical set-up, and considering the D4Science VRE infrastructure and services that provide the basis platform. As part of their development, the demonstrators have required upgrading of existing functionality and development of additional services. This is described, where relevant, in this document.

In addition, consideration is given to integration aspects, such as two-way linking between the 2 Blue Cloud components, and expanding the VRE with additional platforms for computing and algorithms, and where needed for specific demonstrators, direct access to data infrastructures. Moreover, aspects of authentication and monitoring are considered on full Blue Cloud scale.

The Blue Cloud architecture as described in this report, is designed to be scalable and sustainable for near-future expansions, such as connecting additional blue data infrastructures, implementing more and advanced blue analytical services, configuring more dedicated Virtual Labs, and targeting more (groups of) users.

1 Introduction

The technical framework of the pilot Blue-Cloud features:

1) **the Blue Cloud Data Discovery and Access service** component to serve federated discovery and access to blue data infrastructures
2) **the Blue Cloud Virtual Research Environment (VRE)** component to provide a Blue Cloud VRE as a federation of computing platforms and analytical services.

A major challenge in the Blue-Cloud project is to establish federations at the levels of data resources, computing resources and analytical service resources. The federation of data resources by means of the Blue Cloud Data Discovery and Access service should facilitate sharing of multi-disciplinary datasets from existing blue data infrastructures with external users as well as providing these as a major resource of data input for the Blue Cloud VRE. In addition, VRE users should be able to ingest data sets from other external sources, including their own data sources, using internal VRE functionality for data ingestion and for setting up and running direct access to selected remote blue data infrastructures. Overall, data input could be in-situ data, earth observation data, and model outputs. The federation by means of the Blue Cloud Virtual Research Environment (VRE), should facilitate that computing and analytical services can be shared and combined for specific applications. Analytical services can be various algorithms and generic services, for instance for sub setting, pre-processing, publishing, and viewing data and data products.

In the project, the Blue Cloud Data Discovery and Access service will be configured and deployed for a selected number of blue data infrastructures, represented in the Blue Cloud consortium. And the Blue Cloud VRE will be dimensioned to drive five high-level demonstrators whereby for each demonstrator a so-called Virtual Lab will be configured as a combination of analytical and generic services, selected from the overall service portfolio. As there was already a large portfolio of existing services managed by the Blue Cloud founders, these are used for developing and configuring the VRE and the Virtual Labs. Thereby, upgrading of selected existing services and developing additional services takes place for providing the planned Demonstrators their full requested functionality.

An important prerequisite for the Blue Cloud architecture has been that it should be designed to be scalable and sustainable for near-future expansions, such as connecting additional blue data infrastructures, implementing more and advanced blue analytical services, configuring more dedicated Virtual Labs, and targeting more (groups of) users.

A start with detailing the Blue Cloud architecture was made at the 1st Blue Cloud TCOM meeting in Amsterdam – The Netherlands, 22 – 23 January 2020, where the overall concept of the Blue Cloud system with its two main components, the development of five demonstrators as Virtual Labs, the use of a brokerage service, and the EUDAT and D4Science e-infrastructures were presented and discussed. Following the TCOM, the concept of the Discovery and Access service was further elaborated and documented in D2.1 - Blue Data Infrastructures – Services Description Report. This was followed by detailed analyses and trying out of web services and APIs as provided by blue data infrastructures. This was reported in D2.2 - Blue Data Infrastructures – Services Analysis Report, which was released in M14.

The development of the β-version of the Blue-Cloud Data Discovery and Access service has nearly been completed and its launch is planned in the course of June 2021. Its development has recently been documented in D2.4 - Blue Cloud Data Discovery and Access Service -, which was released in M20.

Also, recently, the analysis was concluded on how the Blue-Cloud Data Discovery and Access service will be connected to the European Open Science Cloud (EOSC) by means of exchanging Blue-Cloud metadata with the EOSC B2FIND data catalogue service. This is documented in D2.5 - Interfacing Blue Cloud Data Discovery and Access with EOSC -, which was released in M20.

More input for the design of the Blue Cloud system architecture was gathered from the Blue Cloud demonstrator teams, asking for their perspective concerning the input, output, and workflow processes that they envisioned for demonstrator Virtual Labs. These requirements were documented in D3.1 - Demonstrator general technical requirements, which was released in M5.

The Blue Cloud VRE was planned to be primarily based upon the existing D4Science e-infrastructure, which already hosted multiple Virtual Labs and offered a variety of services, which could be adopted for the Blue Cloud, while new services could be specified and developed for full support of the Blue Cloud demonstrators. Further insights into the D4Science e-infrastructure, in particular from the perspective of how to configure Virtual Labs for deployment of the Blue Cloud demonstrators, were given as part of D3.2 – Demonstrator Implementation Guidelines, which was released in M5.

Following the actual development of the five Blue-Cloud Demonstrators and associated Virtual Labs, another deliverable has been prepared, D3.3 - Blue Cloud Demonstrator Users Handbook V1 -, which was released in M15. It is the first version of the handbook and guidelines on how to use the five Virtual Labs. For each Blue-Cloud Demonstrator, it describes the objective, the targeted users, a summary of their provided services, and the guidelines of how to use the respective Virtual Lab. The handbook describes the β-version of the Virtual Labs, which were not fully complete and finalised yet at the time of writing of the Deliverable.

The development of the Blue-Cloud Virtual Research Environment (VRE) takes place in WP4 and in M13 a report was released, D4.2 - Blue Cloud VRE Common Facilities (Release 1) -. It presents the Blue-Cloud Virtual Research Environment constituents by focusing on both new services and revised existing services that have been developed in the meantime since Blue-Cloud project start to serve the needs of the Blue Cloud community. In M17 a further report, D4.1 - Blue Cloud VRE Operation Report (Release 1) -, was released, complementing what was already described in D4.1. In particular, this deliverable focuses on how the components have been exploited and operated to support the development of the Blue Cloud gateway https://blue-cloud.d4science.org, its underlying infrastructure, and the VLabs.

At the same time in M17, a report, D4.3 - Interfacing EOSC Report (Release 1) –, was released. The Blue-Cloud platform will feature a variety of services that can be used for undertaking world-class science via the Blue-Cloud VRE, but also via the European Open Science Cloud (EOSC) framework. The D4.3 deliverable describes how a Blue-Cloud service catalogue will be build and how it will be integrated in the EOSC Portal.

Based upon all these deliverables and discussions at several additional TCOM meetings and WP meetings since the 1st TCOM, and following the actual developments of the Blue-Cloud components, steadily the insight and common understanding about the Blue Cloud architecture have increased. A first description of the architecture was described in D2.6 – Blue Cloud architecture (1st release) - in M9. The current report, D2.7, is an update of D2.6 and describes the Blue-Cloud architecture as it is known at Month 20.

As it is expected that there will be further developments and refinements to the Blue-Cloud system, one more release of the architecture document is planned, namely report D2.8 in Month 27.

Table of changes between first release of architecture Deliverable D2.6 and current second release D2.7

In order to make it easier for readers and reviewers to follow updates and new developments in the architecture description in this Deliverable D2.7 in comparison with the description in the earlier release Deliverable D2.6, the following table gives an overview of major changes.

Subject	Type of Change	Chapter
Blue-Cloud Data Discovery & Access service (DD&AS)	D2.6 describes the initially planned concept and its early developments for establishing the DD&AS, while D2.7 describes and gives much more details on the actual developments and deployments that have taken place in the meantime between M10 and M20, and which have resulted in a near operational β-version of the DD&AS at M20. The analysis of existing web services from each of the Blue Data Infrastructures (BDIs) has been finalised and documented in D2.2. Those results have been used to set-up level 2 query interactions with most of the BDIs, while also the set-up of the Data Brokerage service in combination with the shopping mechanism and delivery service have progressed considerably. This major progress in development of	2.1 and 2.2

Subject	Type of Change	Chapter
	the DD&AS has been documented in more detail in Deliverable D2.4 (M20).	
Blue-Cloud Data Discovery & Access service (DD&AS)	More information is given of each of the DD&AS architecture components, which are detailed in D2.7. The common level 1 metadata model is described which is applied by the DAB metadata brokerage on the metadata output from each of the BDIs. The protocols as used by the Level 2 Databrokerage service are detailed per BDI. The draft GUI for the DD&AS is explained and illustrated with screendesigns.	2.3
Blue-Cloud Data Discovery & Access service (DD&AS)	A new element is how the DD&AS will connect with EOSC. This will be done by DD&AS API which will facilitate the EUDAT B2FIND service to harvest Blue-Cloud Level 1 metadata records for inclusion in the EOSC metadata catalogue service. Each metadata record will include a path to the DD&AS for drilling down to Level 2 and the actual data retrieval. This is detailed in D2.5 (M20).	2.4
Blue-Cloud Virtual Research Environment (VRE)	The description of the gCube frameworks and the image with high-level architecture of the D4Science infrastructure, enabled by gCube, which provides the basis for the Blue-Cloud VRE, has been updated with some extra components which will be highlighted below.	3.1
Blue-Cloud Virtual Research Environment (VRE)	The image with Enabling Framework Architecture has been updated with some extra components which will be highlighted below.	3.3.1
Blue-Cloud Virtual Research Environment (VRE)	Compared to the situation as described in D2.6, the VRE now has fully adopted state of the art industry standards for authentication and authorization. In particular, it fully adopts OIDC (OpenID Connect) for authentication and UMA (User Managed Authorization) for authorization flows. Both protocols	3.3.3.4

Subject	Type of Change	Chapter
	are specializations of the generic OAuth 2.0 specification. A new IAM (Identity and Authorization Manager) has been adopted to enhance the initial gCube architecture. These upgrades are described in detail.	
Blue-Cloud Virtual Research Environment (VRE)	The storage layer of the Auditing framework was enhanced to use TimeScaleDB, i.e. a relational database for time-series data that relies on the rock-solid reliability of PostgreSQL. It fully replaced the previous implementation based on CouchBase.	3.3.3.5
Blue-Cloud Virtual Research Environment (VRE)	The continuous growth of the gCube platform in terms of complexity and size has highlighted the necessity to better govern complex service interactions. In order to untangle user administration workflows and make them more future proof, a new micro service orchestrator has been introduced which is described in detail.	3.3.3.6
Blue-Cloud Virtual Research Environment (VRE)	The Shared Workspace System provides a remote (Cloud) folder-based file system, supporting sharing of folders and different item types. Compared to the situation in D2.6, the Shared Workspace System was heavily redesigned with the aim of increasing its scalability and overall performance. This is described in detail.	3.6.3.2
Blue-Cloud Virtual Research Environment (VRE)	The publishing framework, making it possible for providers to document (by rich metadata) any research outcome and publish it following FAIR principles, has been upgraded. A new Catalogue System is described, provides its users with facilities for documenting and publishing items as well as searching and browsing across the published items to access them.	3.7
Blue-Cloud Virtual Research Environment (VRE)	The range of Third-Party Frameworks, supported by the VRE, is expanded with JupyterHub, a web-based interactive	3.8

Subject	Type of Change	Chapter
	development environment for Jupyter notebooks, code, and data. It allows users to configure and arrange the user interface to support a wide range of workflows in data science, scientific computing, and machine learning.	

Table 1.1: Major changes in architecture as described in D2.7 versus earlier D2.6

2 Architecture of Blue Cloud Discovery and Access service

2.1 Overall concept

The **Blue-Cloud Data Discovery and Access service** is one of the two main components of the Blue-Cloud technical framework, next to the **Blue Cloud Virtual Research Environment (VRE)**. The Blue Cloud service will facilitate discovery and retrieval of data sets and data products for external users in stand-alone mode, and for users of the VRE through connectivity. These data sets are managed in blue data infrastructures that will be connected to the Blue Cloud service to serve federated discovery and access. The development of the Blue Cloud Data Discovery and Access service is undertaken as part of WP2.

The pilot Blue-Cloud Data Discovery and Access service project aims at federating initially in total 10 blue data infrastructures. Each of these existing infrastructures have been described in deliverable D2.1 - Blue Data Infrastructures – Services Description Report, in particular with a focus on their current content and data discovery and access mechanisms. While deliverable D2.2 - Blue Data Infrastructures – Services Analyses Report – describes the web services and APIs that each of the blue data infrastructures is providing and maintaining.

The overall concept is that the Blue-Cloud Data Discovery and Access service will make use of web services and APIs, following protocols such as CSW, OAI-PMH, ERDDAP, or otherwise, as provided and maintained by the blue data infrastructures. These will be used to deploy machine-to-machine interactions for harvesting metadata, submitting queries, and retrieving resulting metadata, data sets and data products.

The Blue Cloud Data Discovery and Access service should then provide a common interface for discovery and retrieval of data sets and data products from each of the federated blue data infrastructures. The GUI should also include facilities for mapping and viewing the locations of data sets, as this will be part of the query dialogue.

Moreover, conceptually it has been decided to set up the query mechanism as a two-step approach:

- The first step has a focus on identifying interesting data at an aggregated collection level, with free search, geographic and temporal criteria as main query operators;
- The second step has a focus on drilling down within identified collections to get more specific data at granule level, using again free search, geographic and temporal criteria, but this time at granule level, and including additional search criteria which are specific per blue data infrastructure
- Finally, users should be able to download and store the retrieved data collections on their own machines or in a data pool as part of the Blue Cloud VRE.

The two-step approach for data discovery and access is effective to go from coarse to fine and to determine in an early stage which of the blue data infrastructures might have interesting data sets. It is also effective to keep the number of entries relatively limited in the exploratory first step of discovery. The granule level as a second level is applicable to several of the blue data infrastructures, in particular in cases with observation (raw) data which often can be very large collections with numerous data sets. For instance, the SeaDataNet CDI service currently gives discovery and access to more than 2.5 million individual observation data sets for physics, chemistry, geology, biology, geotechnics, and bathymetry. At first level, there are circa 800 CDI aggregated records at collection level, which then give access to the more than 2.5 million granule records, which in the end can be downloaded.

There are also cases, when one step can be sufficient, such as in case of specific data products, that a user wants to download as a complete file. The second level then gives ways for some additional criteria to distinct better between data products and to allow the actual downloading.

In both cases, the overall principle is that queries at level 1 will be applied to search on level 1 over all connected blue data infrastructures and on a common metadata profile, while queries at level 2 will be applied with specific search profiles for each individual blue data infrastructure. For each blue data infrastructure selected records can be included in a shopping basket that then can contain a mix of requested data sets from multiple blue data infrastructures. The shopping basket, once submitted, will deliver the requested data files in a data package, directly linked to the shopping order.

In the Blue Cloud project for the first level use is made of the DAB metadata brokerage service software kit as developed and managed by CNR-IIA. The mappings are made against the common DAB metadata model, and the DAB service has been set up by CNR-IIA to generate, maintain, and provide a common Blue-Cloud level 1 catalogue as an internal service in a dynamical way with the latest entries as derived from the blue data infrastructures.

For the data access part of the Blue-Cloud data discovery and access service, a data brokerage service has been developed, integrating the internal Blue Cloud level 1 metadata catalogue (see above), a series of machine-to-machine interfaces to the blue data infrastructures for level 2 queries, and a shopping mechanism to support the actual discovery and retrieval functions. This part makes use of the experience and software services that MARIS, IFREMER, and EUDAT have developed and are managing for the SeaDataNet CDI service. For the Blue Cloud selected services will be adopted and/or adapted.

Implementing this approach largely depends on the interfaces of blue data infrastructures, that should be supportive. As part of D2.2 the existing web services and APIs of each blue data infrastructure were analysed, tested and documented. In the follow-up further testing and analysis was applied, inter alia for finding the best ways for the deployment of level 2 queries and how to construct the download URLs.

The developments for the Blue-Cloud Data Discovery and Access service have made great progress and launching of the β-version is planned in the course of June 2021. Its development has recently been documented in D2.4 - Blue Cloud Data Discovery and Access Service -, which was released in M20.

Once fully complete, the resulting Blue Cloud Data Discovery and Access service will facilitate users:

- to search and discover interesting data sets
- to complete and submit a shopping basket with interesting data sets
- to stay informed about the progress of the shopping requests
- to download the data sets once ready for downloading
- to ingest data sets into the VRE data pool for use in VRE applications.

It will facilitate managers of blue data infrastructures:

- to stay informed about the shopping requests and associated users for their repository
- to prepare periodic management reports

This way, the Blue Cloud Data Discovery and Access service will provide a delayed mode service to oversee and to select interesting data sets from the connected blue data infrastructures, followed by downloading and using of the selected data sets by external and VRE users. Next to the offer provided by the blue data infrastructures, the Blue Cloud Data Discovery and Access service will also index and make available selected data products, resulting from the Blue Cloud demonstrator Virtual Labs, to support a wider distribution and publishing. This will be implemented in a later stage, once the VRE Products Catalogue has been populated with a critical mass of contents.

2.2 Involved blue data infrastructures

The following blue data infrastructures are pillars under the initial Blue-Cloud developments and services:

- SeaDataNet (physics, bathymetry, chemistry, geology, geophysics, and biology)
- EMODnet Bathymetry (bathymetry)
- EMODnet Chemistry (chemistry)
- EurOBIS – EMODnet Biology (marine biodiversity)
- Euro-Argo and Argo GDAC (ocean physics and marine biogeochemistry)
- ELIXIR-ENA (biogenomics)
- EuroBioImaging (microscopy)
- EcoTaxa (bio images)
- WekEO (CMEMS ocean analysis and forecasting and C3S climate analysis and forecasting)
- ICOS-Marine (carbon)

These blue data infrastructures are mostly complementary to each other, dealing with other data originators and/or different stages in the processing chains from data acquisition to data products to knowledge. Each of them has been described in deliverable D2.1 - Blue Data Infrastructures – Services Description Report.

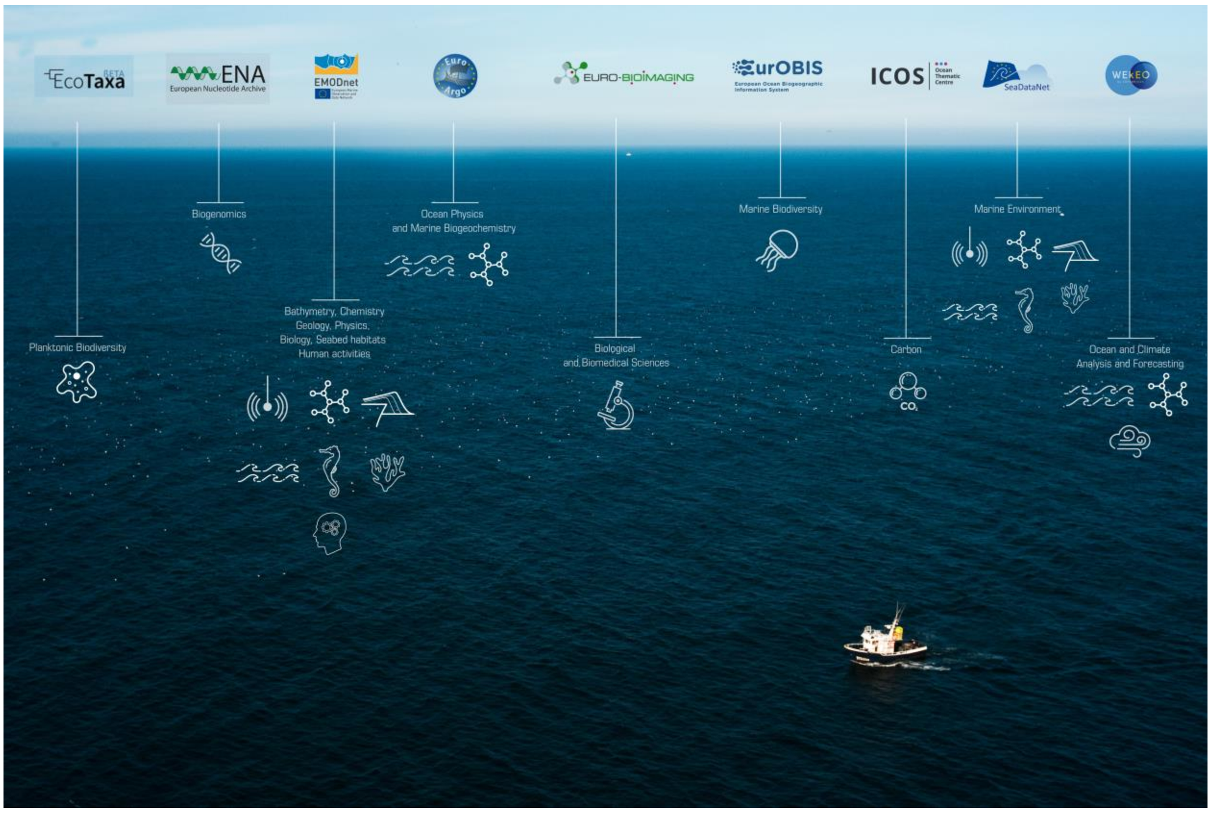

EcoTaxa
ENA European Nucleotide Archive
EMODnet
Euro Argo
EURO-BIOIMAGING
EurOBIS
ICOS
SeaDataNet
WEkEO
Planktonic Biodiversity
Biogenomics
Bathymetry, Chemistry Geology, Physics, Biology, Seabed habitats Human activities
Ocean Physics and Marine Biogeochemistry
Biological and Biomedical Sciences
Marine Biodiversity
Carbon
Marine Environment
Ocean and Climate Analysis and Forecasting

Figure 2.1: Blue data infrastructures as included in initial Blue Cloud discovery and access service

The Blue-Cloud project initially aimed at federating these 10 blue data infrastructures (BDIs). To get a better understanding, each of these existing BDIs infrastructures have been described extensively in deliverable **D2.1 - Blue Data Infrastructures – Services Description Report** - which was released in February 2020. In the report there is a particular focus on their current data discovery and access mechanisms, how these work, types and volumes of data, used formats, which are relevant information as each of the BDIs has to provide endpoints for the federated Blue-Cloud service. From this initial analysis it appeared that the list of BDIs needed to be refined to the following infrastructures: SeaDataNet CDI data service, SeaDataNet Data Products service, EMODnet Chemistry Products service, EurOBIS – EMODnet Biology data collections service, Euro-Argo - Argo GDAC data services, ELIXIR-ENA data service, EuroBioImaging data service, EcoTaxa data service, WekEO (CMEMS) data products service, ICOS-Marine data service and ICOS-SOCAT data service.

As part of the activities for Deliverable D2.2 - Blue Data Infrastructures – Services Analysis Report, further analyses and tests were undertaken for each of the BDIs, focusing on their existing data delivery mechanisms and their fitness-for-purpose. During the developing and deploying of the data brokerage component, a further analysis activities were undertaken, in particular by MARIS and CNR-IIA, in dialogue with the operators of each of the BDIs. The analysis focused on gathering more technical information concerning the existence and functioning of web services and APIs for detailed queries with additional criteria and at granule level, where relevant, and for actual access to associated data sets. During these analyses also several of the web services and APIs were tried out, testing if and how these services could be used for supporting the machine-to-machine interactivity as required. Some BDIs provide multiple web services, sometimes with different results. In those cases, preferred services were selected in communication with their operators. Some use authentication for use of web services and APIs and this could be overcome by registering the Blue-Cloud service as a user, while agreeing to build KPI records of usage as part of the Blue-Cloud shopping component.

From these deeper analyses it appeared that a few of the BDIs cannot be taken onboard of the Blue-Cloud Data Discovery & Access service. This applies for the **EuroBioImaging** service which is being upgraded by EBI and which currently cannot provide the required web services. Hopefully, this BDI can be added later in the remainder of the Blue-Cloud project. It also applies for **WEkEO** which has a well-developed API (so-called HAD). However, WEkEO hosts and gives access to large data products which are resulting from satellite observations, numerical forecast models, and large in-situ collections. These products itself are too big (GBs to TBs) to download as units and are increasing in volume in time. For that reason, the WEkEO API is set-up as a subsetting service, which allows users to compose and run dedicated queries for extracting slices of data from the large products, which then can be downloaded. Emulating this API in the Blue-Cloud discovery service is highly impractical. However as alternative, the WEkEO API is very fit for configuring specific data extraction tasks, for instance in a Jupyter notebook, and this way being included in some of the Blue-Cloud Virtual Labs that require regular input from WEkEO. Therefore, together with MOI, operator of WEkEO, and CNR-ISTI, developer of the Blue-Cloud VRE, it was decided to make a direct coupling of the WEkEO service with the Blue-Cloud VRE using their API embedded in an i-notebook. This is being worked out and tested by CNR-ISTI as part of WP4 developments. Finally, from the analyses it also appeared that ICOS provides two interesting services, namely the ICOS Marine data service and the SOCAT (Surface Ocean CO_2 Atlas) service. It was decided to include both in the Blue-Cloud Data Discovery and Access service.

Following these analyses and observations, the list of BDIs to be incorporated in the first release of the Blue-Cloud Data Discovery & Access service has been confined to:

- SeaDataNet CDI data service (including also CDI entries for EMODnet Chemistry, Bathymetry, and Physics)
- SeaDataNet Data Products service
- EMODnet Chemistry Products service
- EurOBIS – EMODnet Biology data collections service
- Euro-Argo - Argo GDAC data services
- ELIXIR-ENA data service
- EcoTaxa data service
- ICOS-Marine data service
- ICOS-SOCAT data service

So, a total of 9 BDIs for the first release.

2.3 Architecture and modules

The following image gives the architecture of the Blue-Cloud Data Discovery & Access service. The developments are led by MARIS, with contributions of CNR-IIA and EUDAT partners (DKRZ, CINECA, and CSC). MARIS is responsible for the overall system and its integration, while CNR-IIA and EUDAT each deliver components and contributed to the conceptual design, also involving IFREMER and CNR-ISTI. MARIS for a major part makes use of earlier developments and experiences gained during the upgrading of the SeaDataNet CDI service as part of the H2020 SeaDataCloud project. EUDAT develops the Blue-Cloud data delivery component, also using the earlier achievements and experience built up during the SeaDataCloud project.

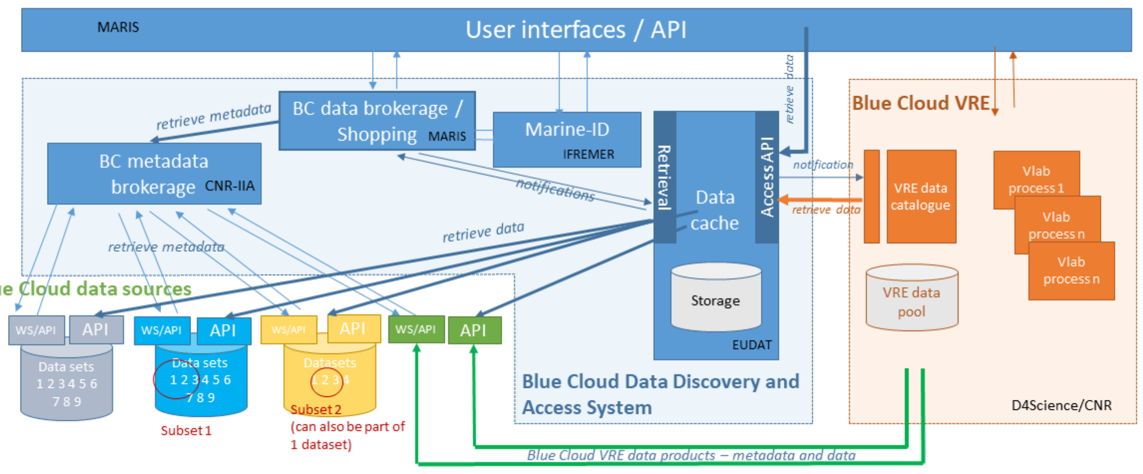


Figure 2.2: Architecture of the Blue Cloud discovery and access service

The Blue Cloud Data Discovery and Access service will consist of a number of modules (services) as indicated in the figure above:

- **Blue Cloud metadata brokerage**, operated by CNR-IIA, dynamically interacting with each of the blue data infrastructures to retrieve, extract and harmonise metadata entries for each blue data infrastructure into a common Blue Cloud level 1 metadata catalogue;
- **Blue Cloud data sources**, comprising blue data infrastructures, that are gathering and managing catalogues and data collections from multiple data and data product originators; the Blue-Cloud VRE is also considered as Blue Cloud data source, concerning publishable data products as resulting from the demonstrator Virtual Labs.
- **Marine-ID service,** operated by IFREMER, for registration and authentication of users to the Blue Cloud Data Discovery and Access service. Users only have to register once to receive their login details;
- **Data cache**, operated by EUDAT, for temporary storage of data packages, consisting of data sets, retrieved from the Blue Cloud data sources, plus associated metadata, as retrieved from the Blue Cloud data brokerage, and following the instructions as received from the Blue Cloud data brokerage. External users can download these data sets, after receiving information

from the Blue Cloud data brokerage, while the VRE can also be triggered to retrieve data packages for ingestion into the catalogue and data pool of the Blue Cloud VRE;

- **Blue Cloud Data brokerage service,** operated by MARIS. This service performs the master role in the Blue Cloud Data Discovery and Access service, interacting with the other modules. Regularly, it retrieves the latest Blue Cloud level 1 metadata catalogue from the Blue Cloud metadata brokerage, and ingests this into the discovery interface, whereby users can query the catalogue at level 1. The common level 1 metadata catalogue includes sufficient metadata for each blue data source to allow the first level queries at collection level with a few selection criteria and this way to identify which of the blue data infrastructures holds interesting data sets. The Blue Cloud level 1 metadata catalogue should also contain sufficient additional metadata to allow more specific searching at level 2 for those blue data infrastructures that only have data collections and other data products, but no service at granule level. While for other blue data infrastructures, supporting deeper searching at level 2 – granule level -, customised search profiles have been formulated, which allow the data broker to interacvt with the provided web services and APIs of the blue data infrastructures. The Blue Cloud Data brokerage service also contains a shopping mechanism with basket and ledger, by which users (external users and VRE) and blue data infrastructures can be informed about shopping transactions and their status in time. It interacts with the Blue Cloud Data Cache to give it precise instructions about retrieving data sets from the blue data infrastructures and to insert these for temporary storage, and to bundle these as downloadable data packages for each shopping order. It interacts with the Marine-ID service as users need to login to submit shopping baskets and to have access to the transaction ledger. It interacts with registered users and VRE to inform and instruct them about data packages that are ready for downloading by users or retrieval for ingestion by the VRE. Finally, it also interacts with the Blue Cloud Data Cache to receive information about the actual downloading by users and retrieval for ingestion by the VRE in order to update the ledger;
- **User interfaces,** operated by MARIS, to interact with users for discovery and shopping transactions at level 2, and to provide access to the transaction ledger for users and blue data infrastructures.

Note: In figure 2.2, the Blue Cloud VRE is given with simplified graphics, only to underpin the exchange with the Blue Cloud Data Discovery and Access service. Much more detail about the Blue Cloud VRE will be given in the next chapter.

2.3.1 Blue Cloud metadata brokerage:

For the metadata brokerage at the first level of data collections, CNR-IIA has advanced and deployed an internal service, namely a Blue-Cloud discovery broker service based on DAB technology. This middleware harvests metadata at collection level from each of the blue data infrastructures (BDIs), using their indicated web services or APIs. The DAB service transforms the harvested XML files from each of the BDIs into a common ISO Blue-Cloud collection profile, which is then published by the DAB service by means of a Blue-Cloud CSW service with a common XML profile for each BDI. See image below.

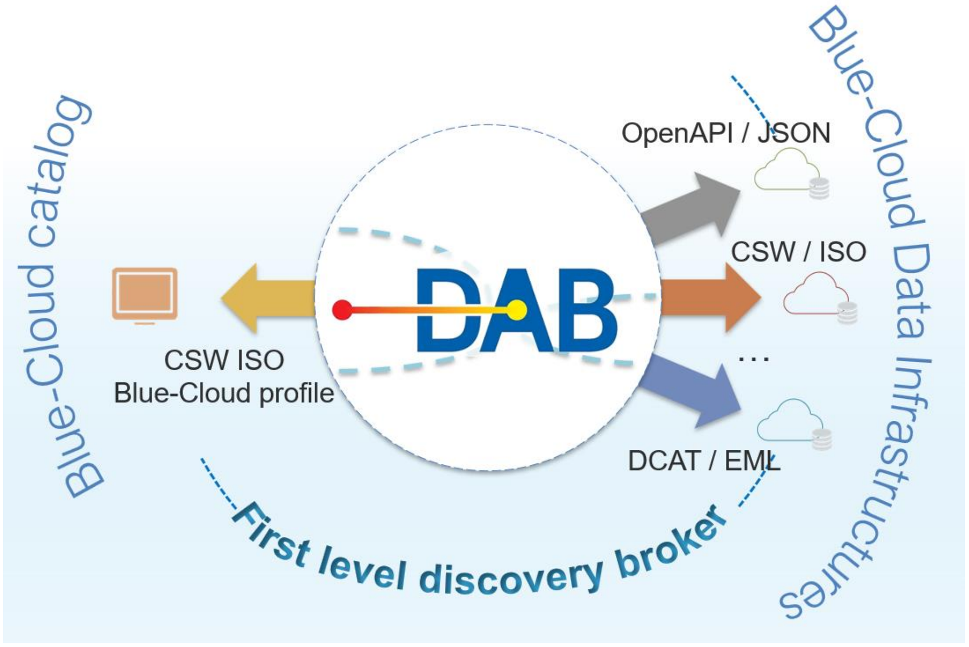


Figure 2.3: Blue-Cloud first level discovery broker component harmonizes the protocols and data models published by different heterogeneous BDIs to a harmonized CSW service based on ISO 19115.

The returned records are expressed according to the Blue-Cloud collection metadata profile, an ISO 19115 based metadata profile encoded using the recent ISO 19115-3:2016 XML schema implementation. In total 13 metadata elements from ISO 19115 are considered as the common elements of the profile, as they are deemed to be the more useful for discovery of Blue-Cloud collections. The common Blue-Cloud metadata elements are:

- IDENTIFIER: Blue-Cloud unique and persistent code for the metadata record
- TITLE: a characteristic, and often unique, name by which the collection is known
- ABSTRACT: a short description of the collection
- KEYWORD: a commonly used word, formalised word or phrase used to describe the subject
- BOUNDING_BOX: extent of the resource in the geographic space given as a bounding box
- TEMPORAL_EXTENT: time period covered by the content of the collection
- PARAMETER: name of the attribute described by the measurement value
- INSTRUMENT: measuring instrument used to acquire the data
- PLATFORM: platform from which the data were taken
- ORGANIZATION: organization associated with the collection
- DATESTAMP: the latest update date of the metadata description
- REVISION_DATE: the latest update date of the data
- RESOURCE_LINKS: download links where available and useful

The DAB service of CNR-IIA regularly harvests and thus updates the output of the Blue-Cloud CSW ISO v. 2.0.2 service per BDI. CSW is a well-known standard web service of the Open Geospatial Consortium (OGC), recommended by many initiatives for sharing metadata on the web**.** Next, MARIS harvests these common formatted XML entries on a regular basis from each of the Blue-Cloud CSW services and integrates these into a SQL database which is then indexed with Elastic Search, using

Logstash as fast connector between the SQL database and the non-SQL Elastic Search database. This processing makes full free text searching very efficient and fast. Moreover, it facilitates building facets for level 2 queries for those DBIs which only have a collection / data products level. This way, the first step of the Blue-Cloud query process is powered, which has been integrated by MARIS in the interface of the Blue-Cloud Data Discovery & Access service. And the common metadata base also serves the second level of the Blue-Cloud query process and the retrieval of data download links, but then only for the BDIs with one level of data, namely the SeaDataNet data products, the EMODnet Chemistry data products, and the EurOBIS – EMODnet Biology data collections. All has been set up as an automatic process without human intervention, driving daily updating from the connected BDIs and synchronisation from the DAB CSW services to the indexed Blue-Cloud catalogue service as part of the Blue-Cloud Data Discovery and Access service.

2.3.2 Data Broker and Shopping mechanism

Following the technical documentation, collated in D2.2, and further analyses and contacts with the operators of the blue data infrastructures, MARIS has progressed with integrating each BDI as part of the data brokerage service, arranging the 2nd query level and direct download links. The preferred way forward is that use can be made of web services and APIs at the BDIs to support building query profiles as a combination of facets and free search, providing results in a paging mode, and facilitating to browse detail pages per resulting record, and finally to retrieve the dedicated data links which are required for the shopping mechanism. And again, all these functions in automated and dynamic machine-to-machine interactions between the Blue-Cloud Data Discovery & Access service and the web services or APIs of each BDI. In practice, deploying this preferred concept is not feasible for each BDI as their web services are not (yet) fit and could not be adapted on short-term. In those cases, alternatives are followed, such as automatic direct harvesting of full metadata from a BDI and feeding these to the SQL db - Elastic Search db chain for building locally the facets, which then power the search. There is also quite some complexity, as there are several protocols being used, differing between the BDIs. This implicates that for each BDI a customised plug-in is being developed and deployed, also taking into account performance. In addition, hurdles had to be overcome that some of the BDIs do not provide direct machine-to-machine download links by https or ftp, but make use of HTML web forms. These had to be by-passed which required further communication with the BDI operators and adaptations from their side, which altogether took more time than earlier envisaged.

The following table gives an overview of the web services or APIs of each BDI for which the data broker service has set up customized interfaces.

Blue Data Infrastructure	Type of web service / API for level 2	Remarks
SeaDataNet CDI service	Dedicated API (Swagger documented)	
SeaDataNet Data Products service	DAB CSW	Using Blue-Cloud common level 1 catalogue + solution to

		by-pass web forms in download links
EMODnet Chemistry Products service	DAB CSW	Using Blue-Cloud common level 1 catalogue + solution to by-pass web forms in download links
EurOBIS – EMODnet Biology data collections service	DAB CSW	Using Blue-Cloud common level 1 catalogue + solution to construct download links from additional web services
ELIXIR-ENA data service	Dedicated API	
EcoTaxa data service	Dedicated API (OpenAPI)	
ICOS-Marine data service	SPARQL service / ERDDAP	
ICOS-SOCAT data service	ERDDAP	
Euro-Argo - Argo GDAC data services	Dedicated API	Solution to find FTP folders for download links

The shopping mechanism has been adopted and adapted from the SeaDataNet CDI service. It consists of:

- Shopping basket, which can be filled by users as a form, adding records from search results
- Marine-ID register, which holds account details for each user such as email, account name and password; shopping baskets can only be submitted by registered users
- Transaction ledger, which holds information about all submitted shopping baskets and their status of processing
- MyBlueCloud, dashboard for users to check order processing status and to download ready download packages; to be expanded with functionality for BDI operators to check Blue-Cloud orders made for their BDIs.
- E-mails to users to confirm their submitted orders and to alert users when orders are completed and ready for downloading.

2.3.3 Delivery component

EUDAT is in charge of the delivery service component of the Blue-Cloud Data Discovery and Access Service. This component is a temporary storage layer that is leveraged by the shopping basket interface to provide requested data to the final users. It exposes a dedicated API accessed from both the shopping basket interface for orders requests and from the final users for orders downloads. Once the user has filled the basket with requested data, the shopping system forwards the request to the data delivery component by providing a list of URLs in json format that are expected to be fetched from each of the BDIs.

Since the operation of downloading can involve potentially thousands of files, taking a long time, an asynchronous architecture is needed. For that reason, a shopping request is forwarded to a task worker that will download each file from the corresponding BDI onto a local filesystem. Once all files are downloaded, they are zipped together into one or more archives to ease the subsequent download. Multiple archives can be created to prevent the creation of final files larger than a threshold (< 2 GB). The shopping basket is notified when the download process is completed and the order is ready for the download. By contacting the API again, the shopping basket will retrieve a list of URLs that will be provided to the user through its MyBlueCloud dashboard for actual downloading. The URL embeds an identification token to authorize the download, which ensures that download URLs can only be obtained from the shopping basket interface to prevent any data leakage.

Several of the modules in the Blue Cloud Data Discovery and Access service are based upon the experience and services that MARIS, IFREMER and EUDAT have developed and are operating for the SeaDataNet CDI service as a result of the EU SeaDataCloud project. Several services have been adapted or upgraded to be fit for the Blue Cloud situation.

Data Cache API endpoints are written in Python by adopting the Flask microframework and served through a nginx reverse proxy, also providing a HTTP over TLS connection. Both user credentials and session tokens are stored into a dedicated PostgreSQL database. Asynchronous jobs are implemented in Python by using the Celery task queue, backed with a results database implemented with Redis. The communication between Flask APIs and the Celery tasks is ensured by a message broken system based on RabbitMQ.

The plan is that retrieved data will be accessed by two different paths. Next to the direct download by users (see description earlier), it is also planned to enable transfer to the VRE data pool. The latter is required as VRE users might want to use the downloaded data for further processing on the powerful D4Science VRE premises. This will take place in a very similar way as the download by users described above, except that the download will be carried out by the VRE. The experiences in SeaDataCloud have shown that pulling/downloading data is much more efficient and less error-prone than pushing/uploading the data, so the planned workflow will be:

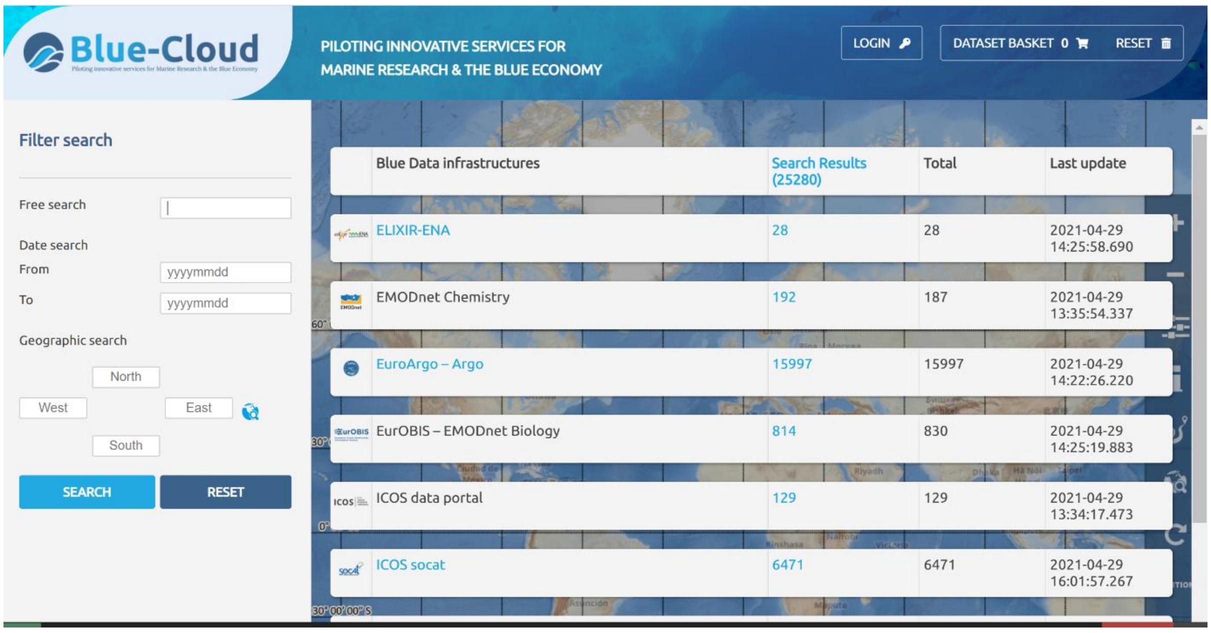
- The EUDAT API receives a request for transferring a batch of data to the VRE data pool (request from data broker to EUDAT API).
- The EUDAT component notifies the VRE that a data batch is available for pull (asynchronous request from EUDAT to VRE API, including download link and user name).
- The VRE downloads the data using the specified link (request from VRE to EUDAT API).
- Then, the data can be deleted or kept for further use (e.g. later downloads or transfers). This will depend on policies as well as on technical considerations and is not decided yet.

To realize this workflow, a component will have to be developed and added by CNR-ISTI to the VRE that can handle requests to pull data. As both CNR-ISTI and EUDAT's participating data centres DKRZ, CINECA and CSC are part of the European research network GÉANT, this transfer will benefit from the very fast network backbone between major European research centres. Note: this functionality has not yet been deployed, but this development will be undertaken soon after the launch of the Blue-Cloud Data Discovery and Access service.

2.3.4 DDA – User Interface

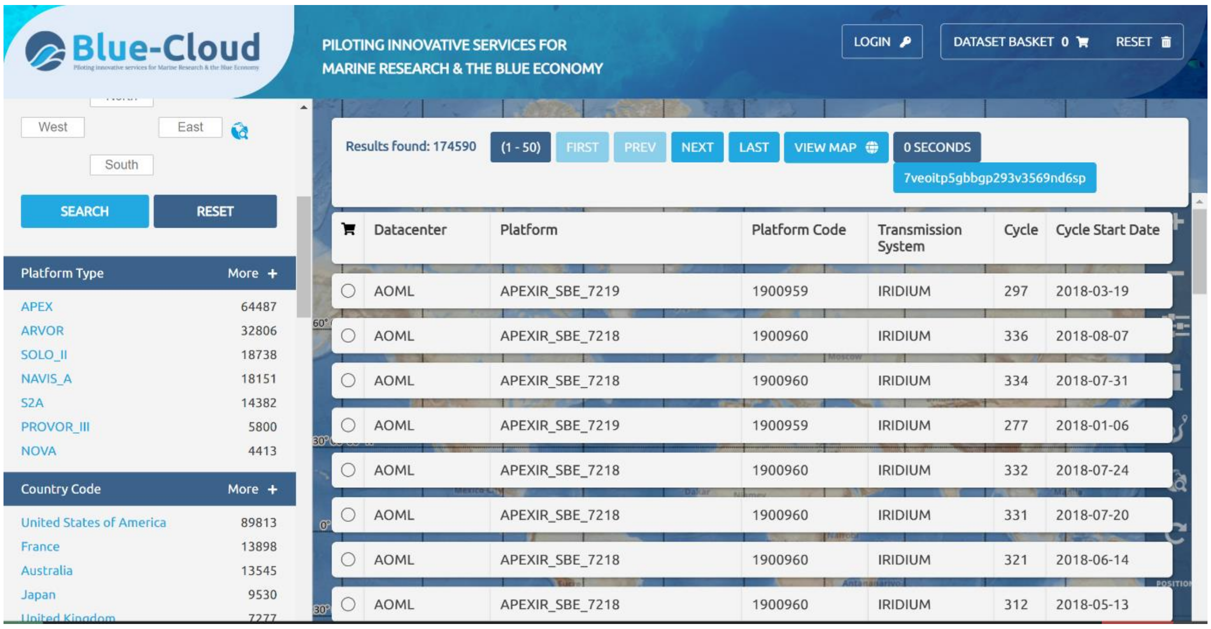
The Blue Cloud Data Discovery and Access service provides a common interface for discovery and retrieval of data collections from the federated blue data infrastructures. The GUI also includes facilities for mapping and viewing the locations of data sets, as this will be part of the query dialogue. Moreover, the GUI includes the query mechanism as a two-step approach, whereby the first step has a focus on identifying interesting data collections and products, while the second step facilitates drilling down and subsetting within the identified collections and products in order to get more specific data. For the second step, geographic and temporal criteria are instrumental, next to additional criteria which are specific per blue data infrastructure. Finally, users are able to download and store the retrieved data collections on their own machines or in a data pool as part of the Blue Cloud VRE.

The following screens are giving illustrations of the Blue-Cloud Data Discovery and Acces service.



Blue Data infrastructures	Search Results (25280)	Total	Last update
ELIXIR-ENA	28	28	2021-04-29 14:25:58.690
EMODnet Chemistry	192	187	2021-04-29 13:35:54.337
EuroArgo – Argo	15997	15997	2021-04-29 14:22:26.220
EurOBIS – EMODnet Biology	814	830	2021-04-29 14:25:19.883
ICOS data portal	129	129	2021-04-29 13:34:17.473
ICOS socat	6471	6471	2021-04-29 16:01:57.267

Figure: Impression of Blue-Cloud Data Discovery & Access service – 1st level search on data collections



Platform Type	More +
APEX	64487
ARVOR	32806
SOLO_II	18738
NAVIS_A	18151
S2A	14382
PROVOR_III	5800
NOVA	4413

Country Code	More +
United States of America	89813
France	13898
Australia	13545
Japan	9530
United Kingdom	7277

Results found: 174590

Datacenter	Platform	Platform Code	Transmission System	Cycle	Cycle Start Date
AOML	APEXIR_SBE_7219	1900959	IRIDIUM	297	2018-03-19
AOML	APEXIR_SBE_7218	1900960	IRIDIUM	336	2018-08-07
AOML	APEXIR_SBE_7218	1900960	IRIDIUM	334	2018-07-31
AOML	APEXIR_SBE_7219	1900959	IRIDIUM	277	2018-01-06
AOML	APEXIR_SBE_7218	1900960	IRIDIUM	332	2018-07-24
AOML	APEXIR_SBE_7218	1900960	IRIDIUM	331	2018-07-20
AOML	APEXIR_SBE_7218	1900960	IRIDIUM	321	2018-06-14
AOML	APEXIR_SBE_7218	1900960	IRIDIUM	312	2018-05-13

Figure: Impression of Blue-Cloud Data Discovery & Access service – 2nd level search on Argo data granules

2.4 Integrating of Blue Cloud data discovery and access service in EOSC

DKRZ and MARIS have agreed that the 1st level catalogue records of the Blue Cloud Data Discovery and Access Service, currently circa 25.000 records, will be populated into the EOSC metadata catalogue service. The latter service is based upon the EUDAT B2FIND service. For the population and synchronisation, MARIS is setting up an API which DKRZ can use in an automated service to harvest the Blue-Cloud metadata records as JSON files. These files are then to be transformed by the DKRZ service, following a mapping which has been determined by DKRZ. The Blue-Cloud metadata describes the data collections and will include deep links to the Blue-Cloud Data Discovery and Access Service, so that users of EOSC can identify interesting Blue-Cloud data collections and then jump to the Blue-Cloud service for down drilling and actual data ordering. This exchange will soon be deployed, once the Beta version of the Blue Cloud Data Discovery and Access Service has been launched, planned in middle of June 2021. The mapping and exchange are documented in **D2.5 - Interfacing Blue Cloud Data Discovery and Access with EOSC** -, which has been released end M20.

2.5 Authentication and authorization aspects

The Blue-Cloud Data Discovery and Access service makes use of user registration by means of the Marine-ID service which is well known in the marine data community and also used in SeaDataNet and CORIOLIS. The Marine-ID registration is necessary for the shopping and downloading process as this will happen in delayed mode. Moreover, it will give insights in who is using the services.

As all the communication with the individual users (except for the actual data download) occurs between the user and the Data Brokerage service, the requests to the EUDAT API will not need to authenticate the user on whose behalf a request happens. Since the Data Brokerage service must authenticate the users anyway, using the Marine-ID service, repeating this step on the backend is not necessary. Similarly, the authorization happens at the Data Brokerage service, as it knows best which users are allowed to access which data. The EUDAT API authenticates the Data Brokerage service (to make sure that only legitimate requests are made to the data backend) and assumes that the data broker is authorized to access any part of the data. This reduces complexity, avoids redundancy and thus inconsistency in the permissions management.

The user will be informed by e-mail by the Data Brokerage service that his/her request has been processed and that the data package is ready for downloading. The user then has to login with Marine-ID to his/her account at the Data Brokerage service to find the shopping request and the download option. At that moment, the Data Brokerage service will communicate with the EUDAT API to retrieve a temporary link (say valid for 6 hours) which will allow the user to do the actual download from the Data Cache at EUDAT. The download option for a shopping request will stay active in the user account at the Data Brokerage service for a longer period (say 15 days), but when using each time a new temporary download link will be requested by the Data Brokerage service from the EUDAT API and provided to the user. This set-up already functions very well in the new SeaDataNet CDI service.

2.6 Distribution of Blue Cloud VRE data products through Blue Cloud Data Discovery and Access service

As indicated in D1.2 - Data Management Plan –, the Blue Cloud project aims to deploy the FAIR principles for data management in Blue Cloud, making data findable, accessible, interoperable and re-usable (FAIR). This not only applies to data input, but also to the data products that researchers using and running the five Virtual Labs at the Blue-Cloud VRE will generate and would like to disseminate and publish.

The D4Science infrastructure (see also chapter 3) as basis for the Blue Cloud VRE already has a utility for building and maintaining provenance information about the processes as applied for generating specific data products in the Virtual Labs. Functionality includes storing information on data input, use and settings of algorithms, and data output into standard PROV records (the PROV standard[1] defines a data model, serializations, and definitions to support the interchange of provenance information on the Web). These provenance records support to document data products and provide very useful information about the data products for any potential use and re-use performed both by end-users and machine algorithms. They are also very useful for researchers that want to analyse and re-run the analytical processes, possibly changing input or settings for comparisons. Moreover, the D4Science infrastructure already has a catalogue service for all data sets and data products as managed for the Virtual Labs. This concerns two catalogues:

[1] PROV standard: https://www.w3.org/TR/prov-overview/

- a **CSW-compliant catalogue,** based on GeoNetwork technology, enabling users to browse and search for geospatial items by relying on the accompanying metadata;
- an **SDMX-compliant catalogue,** based on Fusion Registry technology – for searching statistical data by relying on their structural metadata;

which are joint in one **overall catalogue,** based on CKAN technology, which enables users to perform faceted search on the entire set of resources managed by the Virtual Labs. These existing D4Science services will provide the basis and will be adapted to serve as the so-called Blue Cloud VRE data catalogue and VRE data pool.

The VRE data catalogue and data pool will give users overview and access to all data sets as included in the VRE as input, but will contain also all data products generated in the Virtual Labs. It should be made possible that VRE researchers can label a subset of their data products for wider publication, which will allow to compile automatically a dedicated service to give metadata about and access to public VRE data products. This VRE products catalogue and products pool will be treated like one of the Blue Cloud data sources and connected to the Blue Cloud Data Discovery and Access service in a comparable way as the blue data infrastructures. The development and configuration of the VRE data catalogue and pool, including the public data product services, will take place in WP4. This will include developing of web services and/or API's for sharing product metadata and giving access to the data products.

The overarching VRE data catalogue and data pool are realised through a family of technologies leveraging cloud-based technologies to deliver high scalability, security, reliability, and availability. To any object stored in it, a unique and persistent identifier is generated and a unique and persistent web locator (PURL) is generated. Versioning is automatically enabled to guarantee persistence also when new versions are incrementally generated and stored.

2.7 Direct Blue Cloud VRE connectivity to selected blue data sources

As indicated earlier, the Blue Cloud Data Discovery and Access service will be a delayed mode service as it will work with retrieving selected data sets from blue data sources, and thereafter providing these for downloading by external users as well as for retrieval and ingestion into the VRE data catalogue and data pool services. An important function is to provide external and VRE users a common interface for discovery and access to a range of well-established and maintained blue data sources. The delayed mode will not hamper most of the VRE demonstrators, as several have a preparatory phase in which they gather and organise their data input, followed by processing and analytical steps. However, in case of demonstrator 3 – environmental indicators – there is a more operational need for fast and regular updated access to specific data sets, in particular from WEkEO (bundling CMEMS, C3S, and Sentinel data and products).

For these kinds of operational purposes, it should also be made possible in the Blue Cloud architecture to establish and manage direct connections from the Virtual Labs to blue data infrastructures. These connections might be preconfigured with settings, underpinning the data requirements of the demonstrator. Also, technologies should be explored for optimising the transfer, e.g. by streaming, parallelisation of data transfer from source to VRE, pre-processing at the source for reducing transfer volumes, and deploying applications as Docker containers at the source platform for running applications close to the data, remotely steered from the VRE.

The following Chapter 3 will go deeper in the current architecture and services of the D4Science infrastructure that will provide the basis for the Blue Cloud VRE. While Chapter 4 will highlight a number of integration issues which are relevant in the case of direct connectivity as discussed in this paragraph.

3 Architecture of Blue Cloud Virtual Research Environment (VRE)

The Blue Cloud Virtual Research Environment (VRE) will facilitate collaborative research using a variety of data sets and analytical tools, complemented by generic services such as sub-setting, pre-processing, harmonizing, publishing and visualization. Within the Blue Cloud project, a number of Demonstrators will be developed. Each Demonstrator will enact a family of analytical workflows (or pipelines) which consist of a series of applications and make use of selected datasets as input. Virtual Labs will be configured within the Blue Cloud VRE, each implementing a Demonstrator. For each Virtual Lab group accounts of researchers should be configured. The multi-disciplinary datasets can be retrieved from the blue data infrastructures by means of the Blue Cloud data discovery and access service, or can be retrieved and ingested by users from other data portals and (own) resources.

The Blue Cloud VRE will be based upon the existing **D4Science e-infrastructure** as developed and managed by CNR-ISTI. This e-infrastructure already hosts multiple Virtual Labs and offers a variety of services, which can be adopted for the Blue Cloud. The D4Science e-infrastructure also has proven solutions for connecting to external computing platforms and means for orchestrating distributed services, which will be instrumental for smart connections to the other e-infrastructures in the Blue-Cloud system.

The Blue Cloud demonstrators will be developed as Virtual Labs embedded in the D4Science VRE e-infrastructure and supported by data input from the Blue Cloud Data Discovery and Access service and other data resources, and possible additional computing services. The demonstrators are being worked out in WP3 for their scientific workflows and technical set-up, thereby considering the present D4Science VRE infrastructure and services as basis. For this process, there is close cooperation between WP3 and WP4, as the demonstrators might require adaption of existing services and development of additional services. This has resulted so far in Deliverable D3.1 - Demonstrator general technical requirements which gives information from the perspective of the demonstrator scientific teams concerning the input, output, and workflow processes that they envision for their Virtual Labs. A second Deliverable D3.2 – Demonstrator Implementation Guidelines was prepared by CNR-ISTI as manager of the D4Science e-infrastructure and as WP4 leader, providing guidance on how to use the D4Science infrastructure and its VRE for configuring Virtual Labs.

The further detailing of each of the demonstrators and analysing the impact of the confrontation between demonstrator requirements and present VRE provisions are currently ongoing and have not yet resulted in firm conclusions. Therefore, there is no insight yet whether the demonstrators might require upgrading of existing functionality or development of additional services. For that reason, the functionalities and architecture of the current D4Science e-infrastructure will be described in detail.

3.1 D4Science e-infrastructure – general overview

The D4Science architecture consists of a hardware layer and a service layer. The hardware layer is organized as a dynamic pool of virtual machines, supporting computation and storage, while the services layer is organized into e-infrastructure middleware, storage, and end user services. The hardware layer consists of an OpenStack installation, supporting the deployment of services in the upper layer by provision of computational and storage resources. The service layer, illustrated in Figure 3.1, consists of five service frameworks, which can be summarized as follows:

- ***Enabling Framework***: the enabling framework includes services required to support the operation of all services and the VREs supported by such services. As such it includes: a *resource registry* service, to which all e-infrastructure resources (data sources, services, computational nodes, etc.) can be dynamically (de)registered and discovered by user and other services; *Authentication and Authorization* services, as well as *Auditing* Services, capable of both granting and tracking access and usage actions from users; and a VRE manager, capable of deploying in the collaborative framework VREs inclusive of a selected number of “applications”, generally intended as sets of interacting services. This framework has been enhanced in several components and extended to include an orchestrator service to manage complex management workflows;
- ***Storage Framework***: the storage framework includes services for efficient, advanced, and on-demand management of digital data, encoded as: files in a distributed file system, collection of metadata records, and time series in spatial databases; such services are used by all other services in the architecture, exception made for the enabling framework;
- ***Analytics Framework***: the analytics framework includes the services required for running methods provided by scientists taking advantage, in transparent way, of the power of the underlying computation cloud (e.g. parallel computation) and of a plethora of standard statistics methods, provided out of the box to compute over given input data. This framework has been enhanced in several components and extended to include support for computational notebooks;
- ***Collaborative framework***: the collaborative framework supports all VREs deployed by the scientists and for each of them provides *social networking* services, *user management* services, *shared workspace* services, and WebUI access to the information cloud and to the analytics framework, via *analytics laboratory services.*
- ***Publishing framework:*** *the publishing framework includes services for documenting (by rich metadata) and publishing research artifacts (datasets, notebooks, processes, as well as any community-defined artifact) produced by the VRE and its VLabs thus to promote their FAIRness [5].*

The *Content Cloud Framework* instead will not be exploited by Blue-Cloud and it will not be reported in this document.

- *Content Cloud Framework*: the content cloud framework includes all services required to collect, transform, harmonize, and provide via APIs of different kinds all metadata records of interest to the D4Science community and provided by data sources managed by the organizations in the D4Science consortium. The data collection and provision activity are ruled by workflows, configured by data curators (e.g. transformation rules) and orchestrated by a local enabling layer, in order to keep the content cloud up to date with respect to the content available in the aggregated data sources;

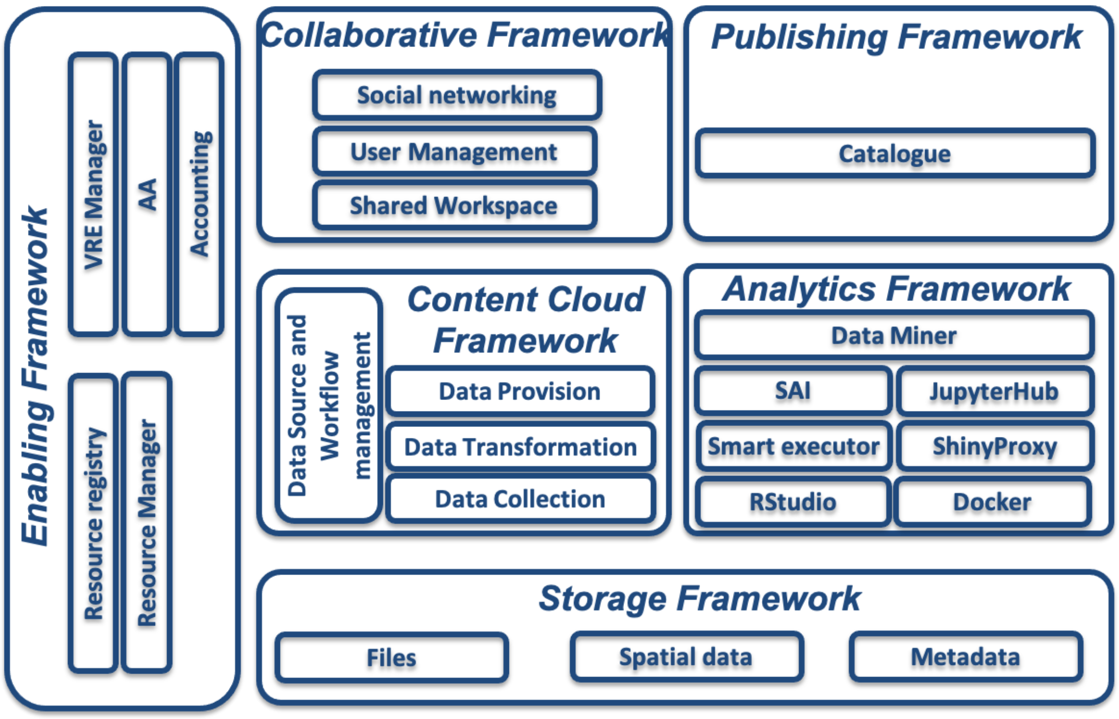


Figure 3.1: High-level architecture of the D4Science infrastructure

3.2 D4Science Hardware Layer

3.2.1 Enabling Technology

The following well-known technologies have been selected to manage the D4Science hardware resources:

a. Ceph, http://www.ceph.com, has been selected as block storage since it is Amazon S3 compatible and OpenStack Swift compatible, it is completely distributed, and it may even use disposable server hardware;

b. Openstack, http://www.openstack.org, has been selected as cloud-computing software platform. It uses Ceph as storage;

The ***Ceph Storage*** offers object, block, and file storage under a unified system. It has been designed to provide excellent performance, reliability and scalability. It supports rapid provisioning of massively scalable cloud storage and enables computation intensive workloads. It provides access to the storage via applications written in Java, Python, Ruby, C, etc. It scales to Petabytes and it offers linear scaling with linear performance increase.

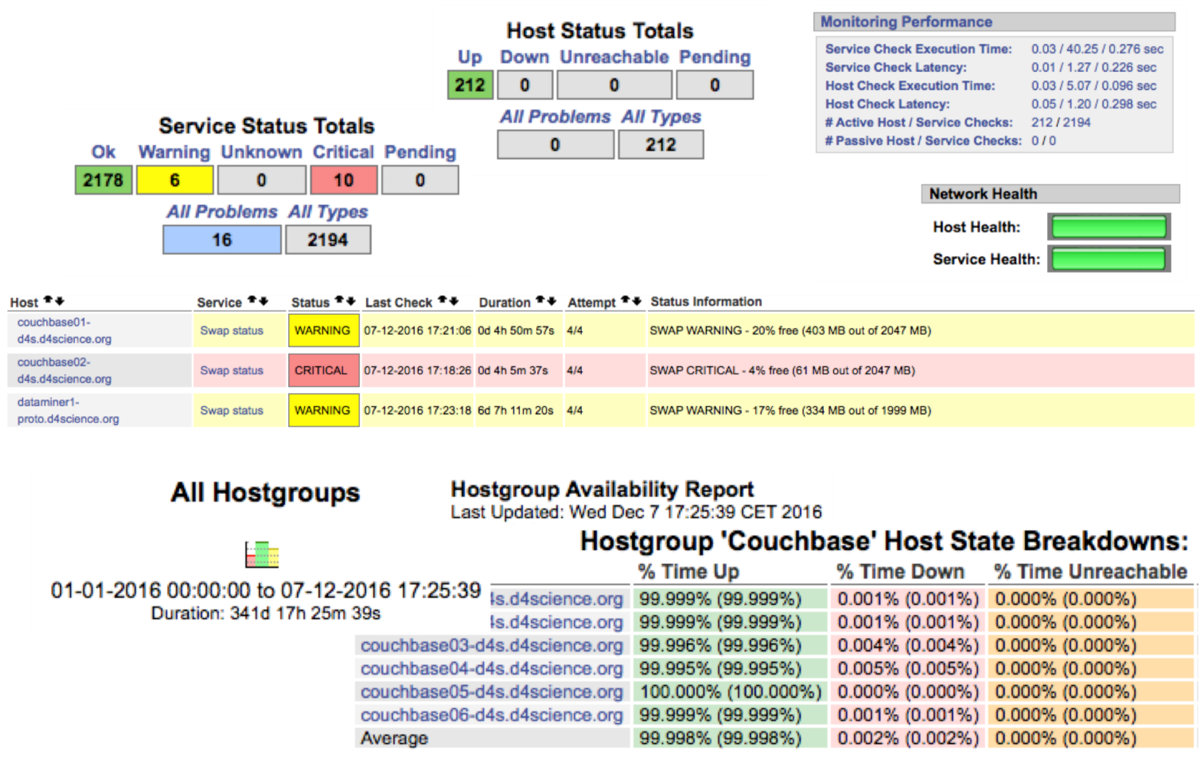
The Openstack, open-source cloud computing platform, provides Infrastructure-as-a-Service (IaaS). OpenStack lets the D4Science Enabling Framework deploy virtual machines and other instances that handle different tasks on the fly. It makes horizontal scaling affordable, which means that services that benefit from running concurrently can easily serve more or fewer tasks – issued either by users or by other services - on the fly by just spinning up more service instances.

3.2.2 Supporting Technology

3.2.2.1 Monitoring and Alerting System

The D4Science Infrastructure is currently counting 212 servers. This does mean neither that all of them are exploited at the same time nor that all of them have to be active concurrently to deliver specific service capabilities. Servers are allocated dynamically in accordance with the Cloud-computing approach and are activated/deactivated in response to load, failures, changes in policies and deployment strategies. This complexity requires proper monitoring infrastructure to check the servers and the services running on the servers and to proper alert when failures are identified. The D4Science exploits two well-known technologies to perform this task: Nagios and Prometheus.

Nagios is an enterprise-class monitoring and alerting solution that provides extended insight of the infrastructure enabling quickly identification and resolution of problems before they may affect critical business processes. It provides monitoring of all mission-critical infrastructure components including applications, services, operating systems, network protocols, systems metrics, and network infrastructure. Nagios provides a central view of operations, network, and business processes running on the infrastructure. Powerful dashboards provide at-a-glance access to powerful monitoring information and third-party data. Views provide users with quick access to the information they find most useful. Spot problems easily with advanced data visualization reports. Moreover, alerts are sent to infrastructure managers and the D4Science quality assurance task force via email or mobile text messages, providing them with outage details so they can start resolving issues immediately. Finally, multiple APIs provide for simple integration with in-house and third-party applications. In particular, for well-known technologies exploited in the D4Science e-infrastructure, e.g. MongoDB, Cassandra, Couchbase, PostgreSQL, etc, existing add-ons have been installed to extend monitoring and native alerting functionality; for technologies developed both by D4Science and by the exploited framework, i.e. gCube and D-Net, specific add-ons have been designed, implemented, and installed to extend monitoring and native alerting functionality in order to have a fully-complete and always up-to-date image of the status of the D4Science e-infrastructure. Overall, 2194 service checks have been added and continuously executed to the monitoring and alerting infrastructure.



Host Status Totals

Up	Down	Unreachable	Pending
212	0	0	0

All Problems	All Types
0	212

Monitoring Performance

Service Check Execution Time:	0.03 / 40.25 / 0.276 sec
Service Check Latency:	0.01 / 1.27 / 0.226 sec
Host Check Execution Time:	0.03 / 5.07 / 0.096 sec
Host Check Latency:	0.05 / 1.20 / 0.298 sec
# Active Host / Service Checks:	212 / 2194
# Passive Host / Service Checks:	0 / 0

Service Status Totals

Ok	Warning	Unknown	Critical	Pending
2178	6	0	10	0

All Problems	All Types
16	2194

Network Health

Host Health:	🟩
Service Health:	🟩

Host	Service	Status	Last Check	Duration	Attempt	Status Information
couchbase01-d4s.d4science.org	Swap status	WARNING	07-12-2016 17:21:06	0d 4h 50m 57s	4/4	SWAP WARNING - 20% free (403 MB out of 2047 MB)
couchbase02-d4s.d4science.org	Swap status	CRITICAL	07-12-2016 17:18:26	0d 4h 5m 37s	4/4	SWAP CRITICAL - 4% free (61 MB out of 2047 MB)
dataminer1-proto.d4science.org	Swap status	WARNING	07-12-2016 17:23:18	6d 7h 11m 20s	4/4	SWAP WARNING - 17% free (334 MB out of 1999 MB)

All Hostgroups

01-01-2016 00:00:00 to 07-12-2016 17:25:39
Duration: 341d 17h 25m 39s

Hostgroup Availability Report
Last Updated: Wed Dec 7 17:25:39 CET 2016

Hostgroup 'Couchbase' Host State Breakdowns:

	% Time Up	% Time Down	% Time Unreachable
ɪs.d4science.org	99.999% (99.999%)	0.001% (0.001%)	0.000% (0.000%)
ɪs.d4science.org	99.999% (99.999%)	0.001% (0.001%)	0.000% (0.000%)
couchbase03-d4s.d4science.org	99.996% (99.996%)	0.004% (0.004%)	0.000% (0.000%)
couchbase04-d4s.d4science.org	99.995% (99.995%)	0.005% (0.005%)	0.000% (0.000%)
couchbase05-d4s.d4science.org	100.000% (100.000%)	0.000% (0.000%)	0.000% (0.000%)
couchbase06-d4s.d4science.org	99.999% (99.999%)	0.001% (0.001%)	0.000% (0.000%)
Average	99.998% (99.998%)	0.002% (0.002%)	0.000% (0.000%)

Figure 3.2: Nagios Status Report and Availability Report for the Auditing Cluster

Prometheus is an open-source system monitoring and alerting toolkit originally built at SoundCloud[2]. It is a standalone open source project and maintained independently of any company. Prometheus's main features are:

- a multi-dimensional data model with time series data identified by metric name and key/value pairs;
- time series collection happens via a pull model over HTTP;
- PromQL, a flexible query language to leverage this dimensionality;
- no reliance on distributed storage; single server nodes are autonomous;
- pushing time series is supported via an intermediary gateway;
- targets are discovered via service discovery or static configuration;
- multiple modes of graphing and dashboarding support.

The multiple modes of graphing and dashboarding support feature has been exploited by adopting Grafana[3], which allowed us to query, visualise, alert on and understand Prometheus data on metrics.

Grafana is able to virtually define dashboards as a set of servers that collectively perform a specific task. In the D4Science we defined a catch-all dashboard to include all servers and then specific virtual clusters to monitor the performance and the exploitation of physical resources for the key enabling software frameworks exploited in the infrastructure and reported in Section 2.2 and subsequent sections.

[2] http://soundcloud.com/
[3] https://grafana.com/grafana

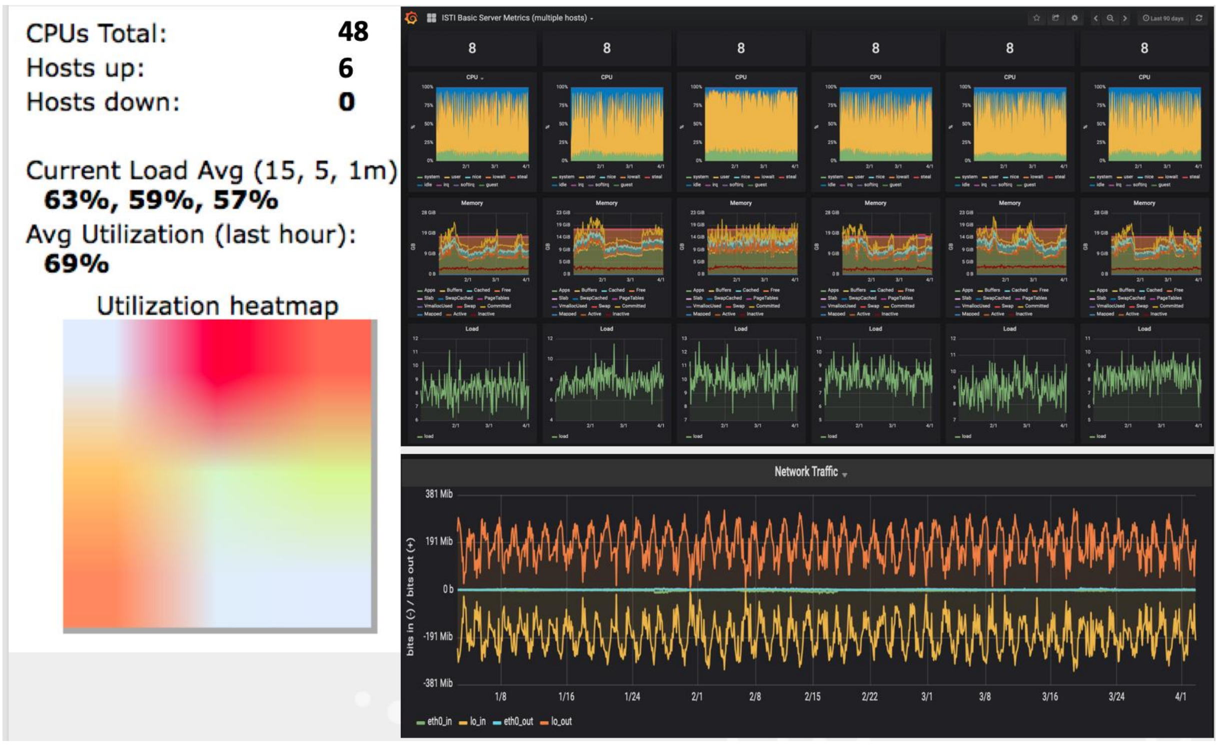


Figure 3.3: Prometheus Aggregated View via Grafana for the Auditing Cluster

3.2.3 Provisioning System

The D4Science is currently counting 212 servers and one of its core ambitions in designing it was the reduction of the deployment, operation, and maintenance costs. To achieve this ambition a key aspect was to automatize the configuration and management of servers, combining multi-servers software deployment, supporting ad hoc task execution, and configuration management.

Ansible is a free-software platform allowing to configure servers according to *idempotence*. Idempotency is basically based on the description of what state is required on a server and Ansible figures out how to get to that state. This approach is opposite to other approaches that require to specify what to run on a server and how to run it. This allows to drastically reduce the costs of operations since it becomes possible to run Ansible plays over and over and it does the right thing according to the status of the server instead of repeating commands and configurations. Ansible is really useful for repeatedly setting up servers in the Cloud which need to be set up the same way.

In order to exploit Ansible in the D4Science e-infrastructure, it was needed to define a number of resources and configuration scripts that than are exploited by Ansible to perform the activities

- inventories - list of servers to configure and maintain
- playbooks - collection of plays, or simply a collection of roles for a 1-play playbook
- plays - a collection of roles
- roles - generally, one service (like PostgreSQL or NGINX)
- tasks - a command that Ansible runs via its modules, like a task for installing a package via apt-get

- handlers - like tasks that get called when other tasks request them via notifications. Typically used to restart services.
- host vars - variables that apply to one collection of hosts
- modules - provided by Ansible to do things like configure MySQL (mysql module), install via apt-get (apt module), copy over files (file module), add users (user module).

Overall, to manage the D4Science 197 roles have been defined.

3.3 D4Science Enabling Framework

3.3.1 Overview

The Enabling Framework is realized by a combination of services and libraries powered by the gCube System open-source project. Those services promote the optimal exploitation of the resources available in the D4Science Cloud Infrastructure and the integration of technology external to it. They insulate as much as possible the management of the infrastructure from the data and the data management services that are hosted in or accessible through the infrastructure itself.

The motto at the heart of the management facilities is *less dependencies for more management* meaning that the requirements posed to resources (even independent resources) to be managed are minimal, close to zero in some cases. All the implemented solutions are prioritized in order to pursue this goal.

Towards new directions of openness and interoperability called by our growing community, management facilities move along:

- adoption of standards
- support for new software platforms by implementing a zero-dependency approach to software management.

The Enabling framework is composed by four main systems: Resource Management System, Information System, Security System, and the MicroService Orchestrator System. These are complex ICT systems that exploit tailored persistence technologies managed via web services.

The Resource Management System supports the creation of a Virtual Research Environment and its exploitation via the registration, management, and utilization of the resources assigned to it.

The Information System supports the registration, discovery, and access of the resources profile.

The Security System ensures the correct exploitation, auditing, and Auditing of the resources under the policies defined at registration time and customized at VRE definition time. It is orthogonal to all services operating in the infrastructure and its components are deployed on all computing nodes.

The MicroService Orchestrator System allows for a declarative definition of workflows which are then executed by an engine. Decoupling orchestration logic of complex management tasks from the internals of single services enables a more scalable and manageable approach to complex procedures, facilitates tracking, monitoring and inspection of service interactions and finally provides a non opinionated location for concentrating cross service logic.

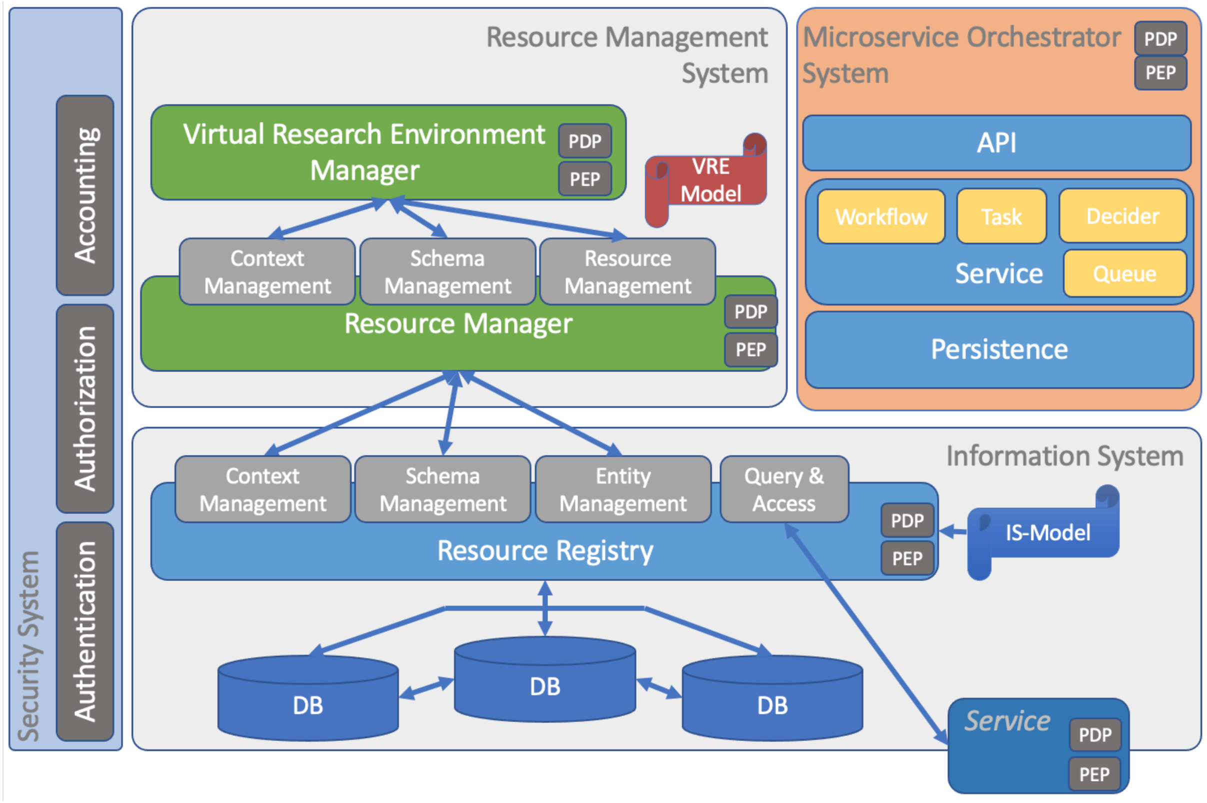


Figure 3.4: Enabling Framework Architecture

3.3.2 Key Features

Extensible notion of resource	a resource model which is open to modular extensions at runtime by arbitrary third parties
Transparent software resource management	nearly zero-dependency requested to managed resources for being part of the infrastructure
Environment propagation	operational information among services are transparently propagated over a range of protocols (SOAP, HTTP/S, and more)
Dynamic Deployment and Optimal Resource (re)Allocation	remote deployment and (re-)configuration of resources across the infrastructure
Resource lifetime management	complete running of the entire lifetime of resources ranging from creation and publication to discovery, access and consumption
Self-elastic management	dynamic resource provisioning to meet peaks and lows in demand
Interoperability, openness and integration at software level	third-parties software can be added to the infrastructure at runtime

Support to standards	crucial functionalities are accessible via recognized standards in order to enhance interoperability

3.3.3 Subsystems

3.3.3.1 Resource Registry

The gCube Resource Registry is the core subsystem connecting producers and consumers of resources. It acts as a registry of the infrastructure by offering global and partial views of its resources and their current status and notification instruments.

The approach provided by the Resource Registry is of great support for the dynamic allocation of resources and the interoperability solutions offered by the Resource Manager system. The feedback obtained during the first reporting period has been used to improve the quality of the design, the APIs of both services and clients, the design of the Graphical User Interfaces (GUIs), and the REST APIs (to strictly adhere to REST principles). Furthermore, the client's APIs has been simplified and enriched: two new Java clients have been released: Resource Registry Context Client and Resource Registry Schema Client which now makes a total of four Java Clients:

- Resource Registry Context Client;
- Resource Registry Schema Client;
- Resource Registry Publisher;
- Resource Registry Client.

Key Features

Resource Publication, Access and Discovery	The Resource Registry is functionally complete offering Java and WEB APIs to register new resources, to discover, and access them.
Consistency with the new Resource Model	The Resource Registry grants publication and access to resources compliant with the Resource Model
Production level QoS - Responsiveness	Each query served in milliseconds; thousands of queries served each hour
Production level QoS - Scalability	Infrastructures with more than 100K of resources successfully powered
Production level QoS - Permanent and Uninterrupted Functioning	The Resource Registry instances have been continuously up for more than one year without human intervention
Flexible deployment scenarios	The Resource Registry components can be deployed in several ways, to best fit the needs of the infrastructure or a specific community

Architecture

The design of the Resource Registry supports distribution and replication wherever it is possible while abstracting clients from the deployment scenario. It exploits HAProxy for proxing requests to the deployed instances of the Resource Registry web service. **HAProxy** is a free, very fast and reliable solution offering high availability and load balancing for very high traffic web applications. Over the years it has become the de-facto standard open-source load balancer and it is now shipped with most mainstream Linux distributions. For these reasons, it is deployed by default in the D4Science Cloud Infrastructure.

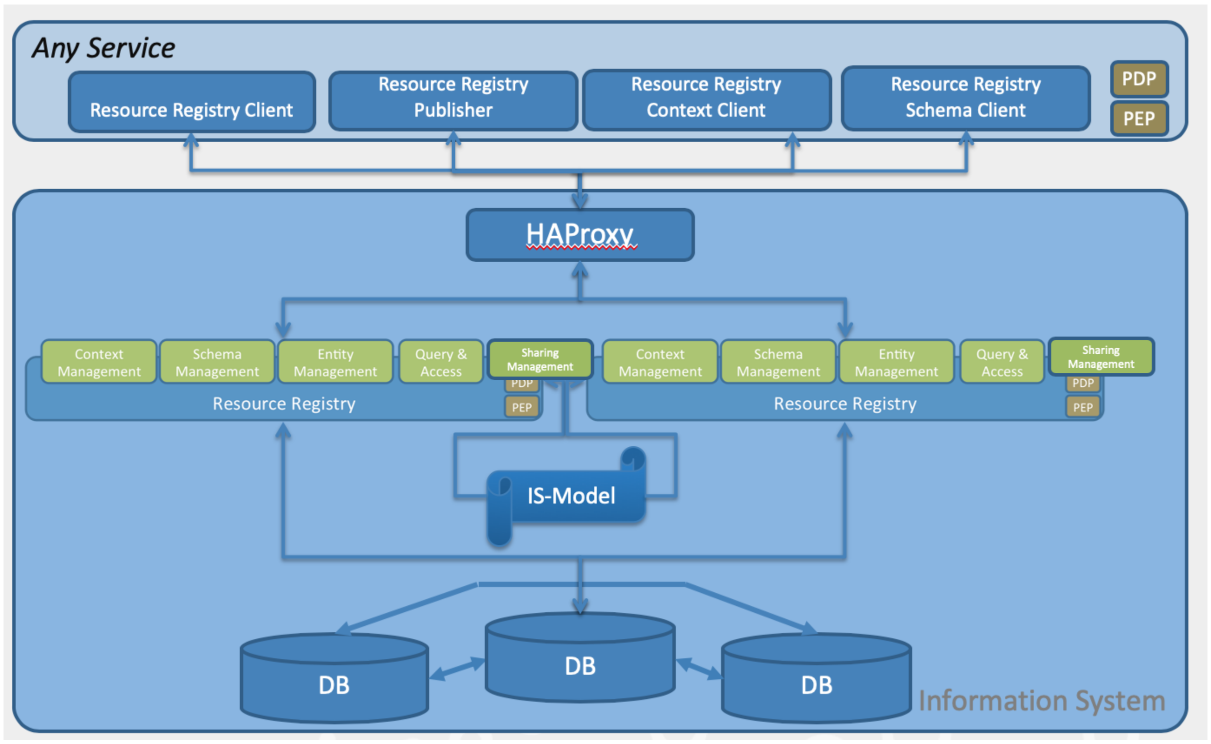


Figure 3.5: Resource Registry Architecture

The Resource Registry web service has now 5 port-types, each responsible for:

- **Context Management**: manage hierarchical contexts;
- **Types Management**: manages the definition of entities and relations types and their schema. This choice allows for easy extension and support modification to the resource model. This is the key factor for the sustainability of the service and infrastructure that have to last for several years
- **Instances Management**: manage instances of registered Entity and Relation type;
- **Sharing Management**: manages instances sharing across different contexts;
- **Query & Access**: query instances and get the schema definition of registered types.

Every port-type is exposed with a REST APIs. Query & Access is the only port-type that can be used by every client and it is documented at: https://dev.d4science.org/swagger/registry/. The other four port-types require a specific authorization that are assigned only to the Resource Manager.

The Resource Registry web service is stateless making it possible to replicate it horizontally.

3.3.3.2 Resource Manager

The Resource Manager is responsible for providing Resources compliant with the gCube-Model. In fact, this service is the only one entitled to perform operations on the Resource Registry. It does so by exposing three port types:

1. Context Management enables Resource Registry context management by checking if the requester has the proper role/rights to do the requested action.
2. Schema Management enables schema management on Resource Registry by checking if the requester has the proper role/rights to do it;
3. Resource Management: enables to manage Resource instances by checking if:
   - the requester has the proper role/rights to do the requested action;
   - the action can be performed looking at the policies attached to the entities and relation instances;
   - the action involves other entities or relations.

When all these checks are performed, and if and only if the action is feasible, the Resource Manager translates the incoming request in one or more outgoing requests to the Resource Registry service.

Key Features

Resource Publication, Access and Discovery	The Resource Manager offers Java and WEB APIs to register new resource types and instances.
Consistency with the gCube Model	The Resource Registry grants publication and access to resources compliant with the gCube Model at Resource level.

Architecture

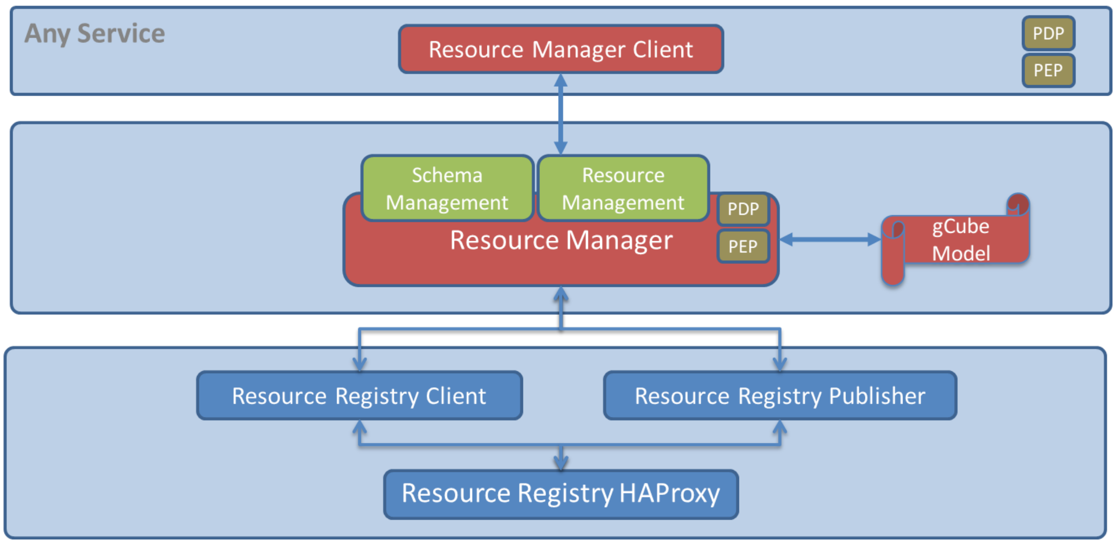


Figure 3.6: Resource Manager Architecture

As depicted in Figure 3.6: Resource Manager Architecture, the Resource Manager uses the Resource Registry Client to query the Resource registry and get the actual knowledge of the infrastructure.

When the Resource Manager receives a request, once performed the proper checks, it uses the Resource Registry publisher to make it effective.

Both Resource Registry Client and Publisher interact with one of the instances of Resource Registry through HA-Proxy.

3.3.3.3 Virtual Research Environment Manager

VRE Manager is responsible for providing context guarantees based on the gCube-Model.

The VRE Manager operates on the D4Science Cloud Infrastructure by using components of:

- the enabling technologies such as Resource Manager;
- supporting technologies such as Provisioning System.

The VRE Manager contacts the Resource Registry to get a current view of the infrastructure; uses the provisioning system to deploy/undeploy services and data; and asks the Resource Manager to update the infrastructure state consistently.

Key Features

Context Management	The VRE Manager offers Java and WEB APIs to create, edit, and delete security context, i.e. Virtual Research Environment.
Consistency with the gCube Model	The VRE Manager grants publication and access to resources compliant with the gCube Model at context level.

Architecture

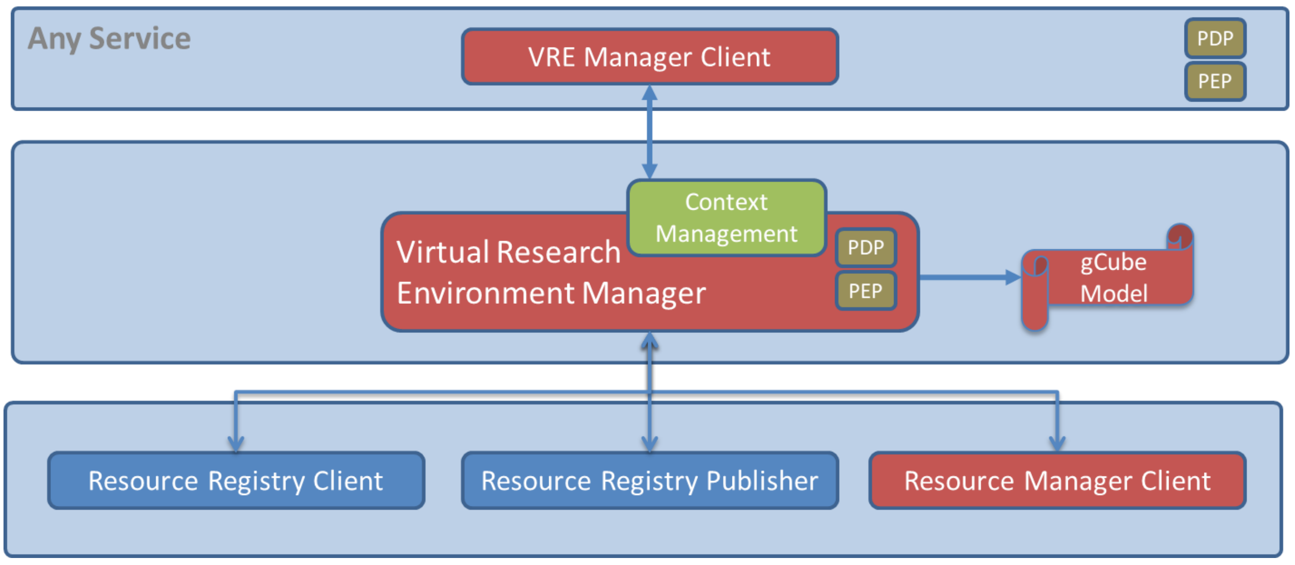


Figure 3.7: VRE Manager Architecture

As shown in Figure 3.7: VRE Manager Architecture, the VRE Manager uses the Resource Registry Client to query the Resource registry and get the actual knowledge of the infrastructure resources. By exploiting this information, the VRE Manager provides the support for the creation of VRE. It creates a new security context and registers it in the Resource Registry. Then it creates a secure symmetric key to enable encrypted conversion in the newly created security context. Finally, it interacts with the Resource Manager to allocate infrastructure resources to the newly created security context.

During the VRE lifetime, when the VRE Manager receives requests for VRE modifications, once performed the proper checks, it interacts with the Resource Manager to either edit, modify, or delete a Virtual Research Environment.

3.3.3.4 Authentication and Authorization

The goal of the Policy-oriented Security Facilities is to protect D4Science Cloud Infrastructure resources from unauthorized accesses.

Service Oriented Authorization and Authentication is a security framework providing ''security services'' as web services, according to ''Security as a Service'' ('''SecaaS''') research topic. It is based on standard protocols and technologies, providing:

- an open and extensible architecture
- interoperability with external infrastructures and domains, obtaining, if required, also so-called ''Identity Federation''
- total isolation from the enabling framework and technologies: zero dependencies in both the directions

This framework is compliant with the Attribute-based access control (ABAC) that defines an access control paradigm whereby access rights are granted to users through the use of policies which combine attributes together.

ABAC defines access control based on attributes that describe:

- the requesting entity (either the user or the service),
- the targeted resource (either the service or the resource),
- the desired action or scope (read, write, delete, execute),
- and environmental or contextual information (either the VRE or the VO where the operation is executed).

ABAC is a logical access control model that is distinguishable because it controls access to objects by evaluating rules against the attributes of the entities (requesting entity or target resource) actions and the environment relevant to a request. ABAC relies upon the evaluation of attributes of the requesting entity, attributes of the targeted resource, environment conditions, and a formal relationship or access control rule defining the allowable operations for entity-resource attribute and environment condition combinations.

The Authorization framework is compliant with the XACML reference architecture. XACML is the OASIS standard for fine-grained authorization management based on the concept of Attribute-based access control (ABAC), where access control decisions are made based on attributes associated with relevant entities while operating in a given operational context, a natural evolution from Role Based Access Control (RBAC).

Key Features

Security as a Service	Authentication and Authorization provided by web services called by resource management modules
Flexible authentication model	The user is not requested to have personal digital certificates
Attribute-based Access Control	A generic way to manage access: access control decisions are based on one or more *attributes*
Support to different categories of attributes	User related attributes (e.g. roles) and environment related attributes (e.g. context)
Modularity	Composed by different modules: each module has a well-defined scope and provides well-defined services
Support to standards	All the operations delivered by the facilities are built atop of recognized standards
High performance	The design and architectural choices have been made paying great attention to performances
Resource Usage Tracking	Administrators and users can monitor applications resources usage

Architecture

The activities performed in the period aimed at the full adoption of state of the art industry standards for authentication and authorization. In particular, the implementation now fully adopts OIDC (OpenID Connect) for authentication and UMA (User Managed Authorization) for authorization flows.

Both protocols are specializations of the generic OAuth 2.0 specification.

A new IAM (Identity and Authorization Manager) has been adopted to enhance the gCube architecture.

Keycloak has been chosen as the implementation of the IAM. Keycloak is an industry ready, widely adopted open source implementation providing most of the models and workflows underpinning modern authentication and authorization management.

In order to better express the current implementation the following table lists all the useful terms and acronyms typically involved in authentication and authorization flows.

Concept	Acronym	Description
Resource Owner	RO	Owner of protected resources. May be human, software or system.

Concept	Acronym	Description
Resource Server	RS	The computing system providing access to protected resources.
Credentials	CRED	Any means of providing identity claims for humans or software.
Access Token	AT	Access token carrying a set of identity claims (names, email, roles, ...) certified by an IAM that is the issuer.
Requesting Party Token	RPT	A token enriched with explicit permission claims.
Protection API Token	PAT	A specific token provided directly to RO allowing for managing its protected resources.
Policy Enforcement Point	PEP	A software or system where authorization checks are enforced.
Policy Decision Point	PDP	The computing system or software where a decision about permission is taken
Policy Administration Point	PAP	A user interface or API where authorization policies for protected resources can be managed.
Policy Information Point	PIP	A computing system or software where information useful for authorization evaluation can be retrieved.

The following picture shows an abstract representation of the way D4Science authenticates a User who is accessing the platform.

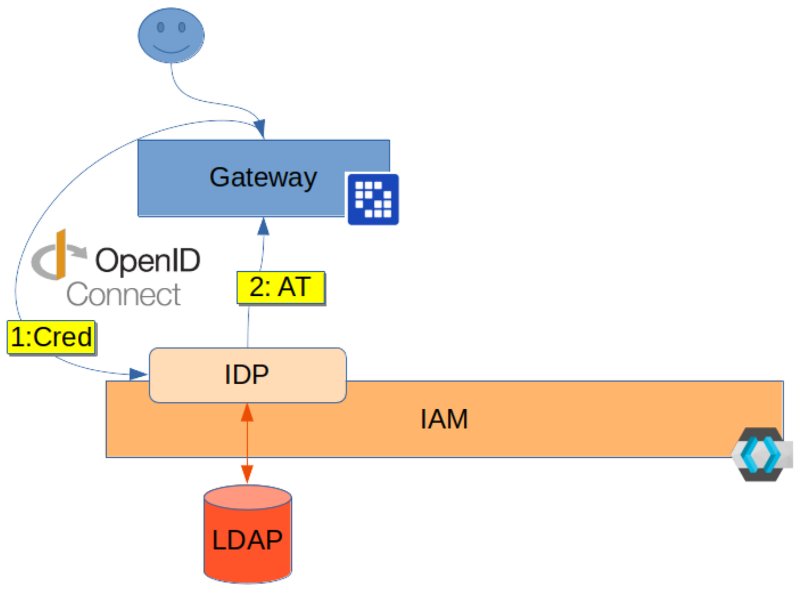


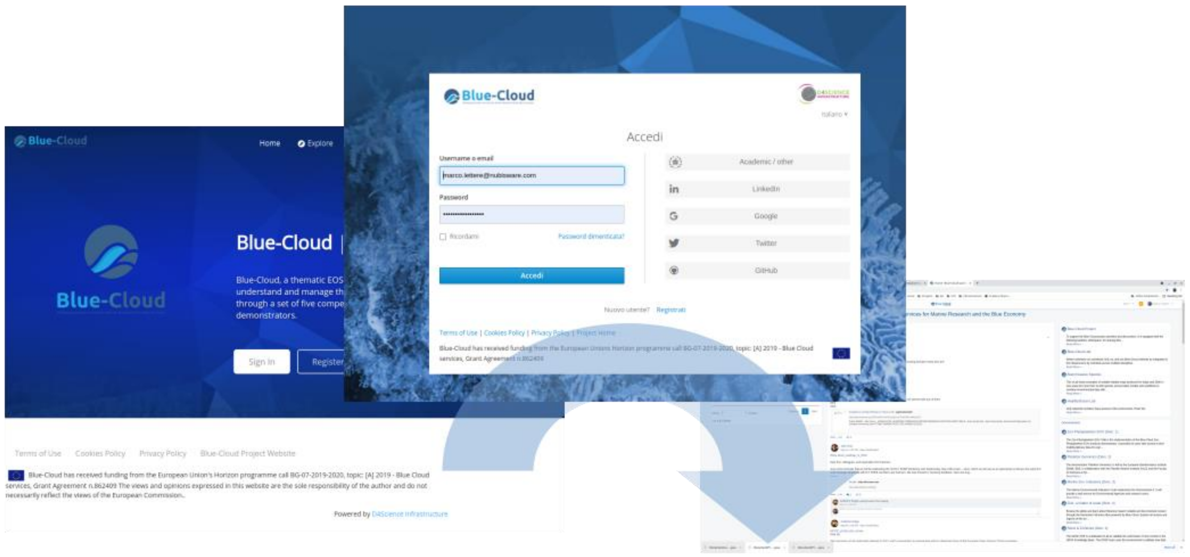
Figure 3.8: Logical view of login process

The user is enabled to access the D4Science platform through front-facing applications called Gateways.

In order to be authenticated the Gateway implements the authorization code grant flow defined by OAuth2. This allows for not having to share any credentials neither for users nor for the gateway service with software different from the IAM.

As shown in the following figure, user agents are redirected to proper login forms served by the IAM. If they are not already signed in on other gateways (SSO), users are asked for their credentials which typically consist of usernames and passwords. At the end of the workflow users are redirected back to the Gateway and they will have their credentials exchanged with a JWT Access token. This token instructs the gateway about the user’s identity and roles and it could be used to make authorized calls to backend services which do not require other than the User’s identity.

Thanks to the use of a full-fledged IAM software, Identity federation is a simple matter of configuration. Thus, social identities such as LinkedIn, GitHub, Google or Twitter are allowed to log into the infrastructure.


Blue-Cloud
Home
Explore
Blue-Cloud
Blue-Cloud, a thematic EOS understand and manage th through a set of five compe demonstrators.
Sign In
Register
Terms of Use
Cookies Policy
Privacy Policy
Blue-Cloud Project Website
Blue-Cloud has received funding from the European Union's Horizon programme call BG-07-2019-2020, topic: [A] 2019 - Blue Cloud services, Grant Agreement n.862409 The views and opinions expressed in this website are the sole responsibility of the author and do not necessarily reflect the views of the European Commission.
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Italiano
Accedi
Username o email
marco.lettere@nubisware.com
Password
Ricordami
Password dimenticata?
Accedi
Academic / other
LinkedIn
Google
Twitter
GitHub
Nuovo utente? Registrati
Terms of Use | Cookies Policy | Privacy Policy | Project Home
Blue-Cloud has received funding from the European Unions Horizon programme call BG-07-2019-2020, topic: [A] 2019 - Blue Cloud services, Grant Agreement n.862409

Figure 3.9: Login through authorization code grant flow

As an architectural choice, it has been decided to keep user identities stored inside LDAP servers in order to continue to share the information with third party services which do not yet support OAuth based interoperability.

Actually, the whole organizational model of D4Science is structured as a three-level tree rooted in the Root Virtual Organization (RootVO). All operations in D4Science occur inside a specific authorization context which are the Virtual Organizations (VO) and the Virtual Research Environments (VRE).

Even roles are assigned to users relative to VO and VRE. For instance, a user might be a simple Member of a VO while being VRE_Manager inside.

As shown in the next figure, in order for a user to be authorized to access the functionality that his or her roles grant inside a VO or VRE a first PEP is realized inside the gateway in the form of a menu of possible contexts which is dynamically built upon the role information transmitted inside the AT.

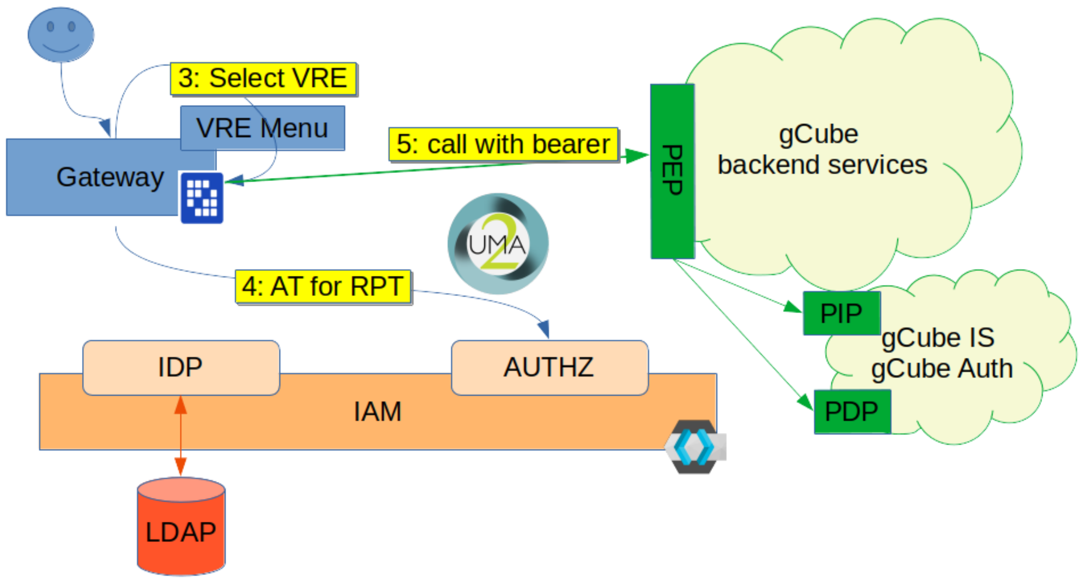


Figure 3.10: Authorization grant to access context (VO or VRE)

VO and VRE contexts are modelled as logical Resource Owner and Server of an abstract resource. For every context a permission is set up that allows access to its abstract resource for all users that have according roles in that context.

By interacting with the authorization services of Keycloak, according to the UMA 2 protocol specification, the gateway exchanges the user's AT (containing the user's certified identity) with a permission token, called RPT. The RPT carries specific permissions for the selected VO or VRE.

With this new token the gateway is allowed to call gCube backend services by adding it as a bearer token header.

Complex authorization patterns can be accomplished by interacting with PIP and PDP implemented in the gCube Information System and legacy Authorization Service.

The PEP is implemented for gCube's reference application containers called SmartGears. This enables it to intercept the AT or RPT passed in the calls and perform validation for all gCube services. Third-parties services and applications are instead protected with authorization proxies. This is particularly useful when no assumption can be made on the implementation technology.

Historical note

This paragraph reports about the original implementation of the gCube Authorization framework which has been superseded by the new implementation. It is kept because it documents components and workflows which are still alive for backward compatibility.

The gCube Authorization framework is a token-based authorization system. The token is a string generated on request by the Authorization service for identification purposes and associated with every entity interacting with the infrastructure (users or services).

The token is passed in every call and is automatically propagated in the lower layers.

The token can be passed to a service in 3 ways:

- using the HTTP-header: adding the value ("gcube-token","{your-token}") to the header parameters
- using the query-string: adding gcube-token={your-token} to the existing query-string
- logging via the default authentication widget shown by the browser using your username as username and your token as password.

The personal token can be retrieved using the token widget deployed on every environment of the portal.

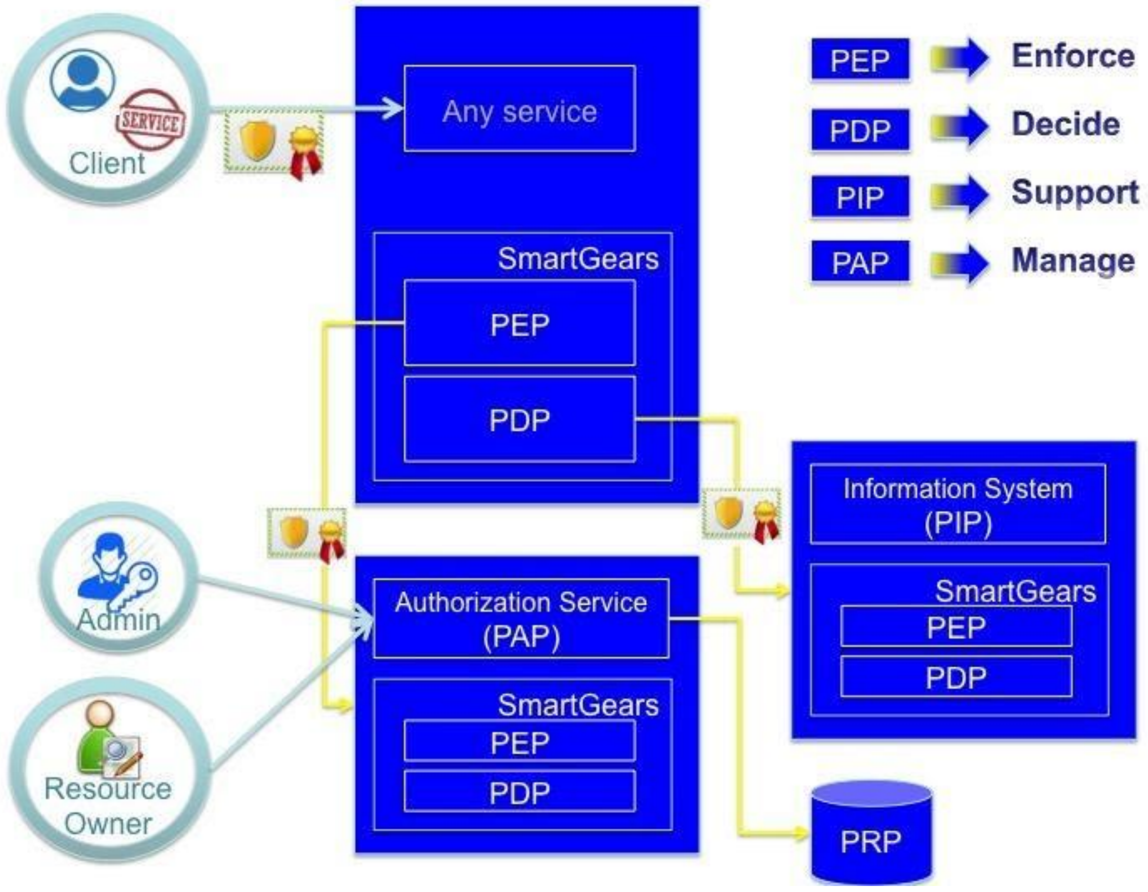


Figure 3.11: Authorization Architecture

The gCube Authorization Framework controls access to applications to allow or prevent the clients to perform various operations in the applications. This is controlled by the Authorization Service with the help of authorization policies. The purpose of authorization policies is to control clients' access. The authorization policies determine at runtime whether or not a particular action is denied.

All the policies are used to DENY to a client an operation in a specific context.

Two types of policy are supported:

- User2Service (U2S)
- Service2Service (S2S)

The U2S policies are used to deny to a user or a role the access to specific service or class of services. The S2S policies are used to deny to a service or a class of services the access to specific service or class of services. To allow access only to a few clients except restriction clauses can be added to the policies. For every policy, a specific ACTION, i.e. Access, Write, Delete, and Execute, can be specified (if supported from the service) otherwise all the ACTION will be denied.

3.3.3.5 Auditing

Auditing is defined as the recording, summarizing, and classifying of service invocations and other events, e.g. storage of data, systematically, in a simpler sense, is the procedure of communicating and translating raw data from the infrastructure operation to its managers and stakeholders.

Key Features

open and extensible Auditing model	the underlying Auditing model is flexible to adapt to diverse provider needs
highly modular and extensible architecture	the entire subsystem comprises a large number of components clearly separating the functional constituents
multiple options for storage	the subsystem can rely on an array of diverse solutions for actually storing records

Architecture

The gCube Auditing architecture is logically divided in four different layers:

- Consumer Layer
- Enabling layer
- Backend layer
- Storage layer

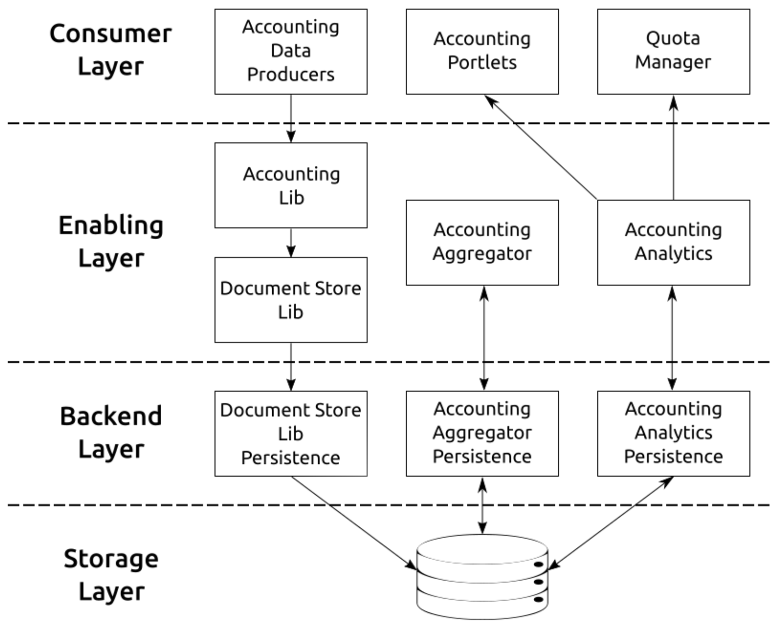


Figure 3.12: Auditing Architecture

All component respects a set of common rules adopted to ensure high-availability, fully-distributed operations, low-operation costs

Each enabling layer has its own correspondent back-end implementation;

Each back-end implementation is dynamically discovered at run-time. This allows to decouple the deployment of a different back-end from the development of the enabling layer. In other word each component on the enabling layer must not have any dependency over a certain back-end implementation.

Auditing Enabling Layer

The **Accounting Lib** collects, harmonizes and stores Auditing data. It is mainly based and developed exploiting the facilities provided by the Document Store Lib.

The **Accounting Analytics** exposes a common access point interface to query the collected Auditing data.

The **Accounting Aggregator** aggregates the collected Auditing data according to dynamically defined policies. The D4Science Auditing policies have been defined to incrementally aggregate past Auditing data without loss of information

Auditing Storage Layer

This layer is not developed by gCube. Rather it relies on technologies guaranteeing HA (High Availability).

In the current settings, it is implemented by relying on **CouchBase**. Other supported backend technologies are CouchDB and MongoDB.

In the reporting the storage layer was enhanced to use TimeScaleDB, a relational database for time-series data that relies on the rock-solid reliability of PostgreSQL. It offers native optimisations for time-series and guarantees up to 100x faster queries than PostgreSQL, InfluxDB, and MongoDB. Clearly, it also supports horizontal scalability that represents a prerequisite for the exploitation in D4Science.

Auditing Backend Layer

Each component in this layer has been explicitly developed over a certain storage technology. They rely on the Resource Registry to discover the information needed to connect to the underling storage. In other words, any component does not have hard-coded connection information or a local configuration file. This approach allows retrieval of the storage connection information by specifying the underlying storage technology and the enabling component to use.

The first filter allows switching to different storage backends at runtime and it supports the co-existence of different storage backends – particularly useful to migrate from one storage type to another without any downtime.

The second filter allows keeping separated connection information for each component. This allows supporting tailored access policies for each component, e.g. write-only for Auditing-lib connection and read-only for Auditing-analytics.

The **document-store-lib-BACKEND** supports the connection to and the storage of Auditing data to the technology selected as persistence layer. It has been extended to support the fourth underlying technologies TimescaleDB: , document-store-lib-couchbase, document-store-lib-mongodb; document-store-lib-timescaledb;

The **Accounting-analytics-persistence-BACKEND** supports the connection to and the discovery and access of Auditing data to the technology selected as persistence layer. It has been extended to support the fourth underlying technologies: Auditing-analytics-persistence-couchdb, Auditing-analytics-persistence-couchbase; Auditing-analytics-persistence-mongodb; Auditing-analytics-persistence-timescaledb;

The **Accounting-aggregator-persistence-BACKEND** supports the connection to and the aggregation of Auditing data to the technology selected as persistence layer. It has been implemented to support the four underlying technologies: Auditing-aggregator-persistence-couchdb, Auditing-aggregator-persistence-couchbase; Auditing-aggregator-persistence-mongodb; Auditing-aggregator-persistence-timescaledb.

Auditing Consumer Layer

Each component in this layer allows either producing or consuming Auditing information. It does include also graphical interfaces designed for managers, i.e. **Accounting Portlet, Accounting Dashboard (new), and Accounting Datastudio (new)**.

3.3.3.6 MicroService Orchestrator System

The continuous growth of the gCube platform in terms of complexity and size has highlighted the necessity to better govern complex service interactions.

As an example, use case consider user management.

In previous implementations of the gCube framework, source of truth for user identity and roles was the Liferay based portal application. This approach made it simple to perform a whole set of administrative tasks that realized the workflows of user and community management. On the other hand, the deep coupling of back-office code with a specific software technology and version produced a vendor and version lock-in which has become unsustainable.

With the adoption of a dedicated service for user, group and authorization context management, the portal becomes a mere consumer of this information as do all other services in the gCube framework. Moreover, Keycloak provides a comprehensive set of REST APIs to enable remote, service-oriented operation.

Nevertheless, the whole set of graphical tools and widgets implemented in the portal to perform user management is still of fundamental value. Thus, the objective is to keep them operational and make them guide the back-office procedures that are now moved from Liferay to Keycloak.

In order to untangle user administration workflows and make them more future proof, it has been decided to introduce a micro service orchestrator.

An Orchestrator is a software that allows for a declarative, technology agnostic definition of workflows which are then executed by an engine. Decoupling orchestration logic from the internals of single services enables a more scalable and manageable approach to complex procedures, facilitates tracking, monitoring and inspection of service interactions and finally provides a non-opinionated location for concentrating cross service logic.

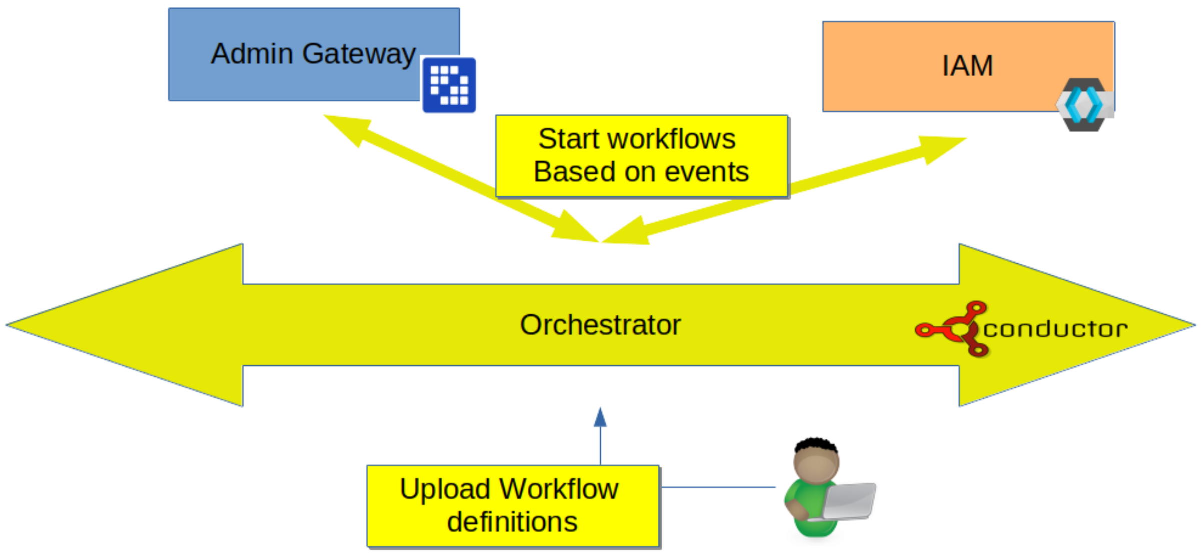


Figure 3.13: Orchestration of management tasks

Key features

Orchestration as a Service	Scalable, Distributed, REST based software for clear orchestration of complex interactions among micro services
Operational	Model driven, declarative yet operational specification of workflows definition
Independence	Technology and implementation independence
Auditing	Every process can be tracked, inspected and monitored
Replay	In case of error conditions workflows can be replayed exactly in the same way

Netflix OSS Conductor (Conductor) has been chosen as the implementation of the gCube orchestrator.

Conductor is a very operation oriented micro service orchestration software which favors configuration and code over design. It is designed as a distributed system from the ground up and supports several control structures such as fork-join, dynamic-fork-join, loop, termination, lambda, events.

Custom task definitions can be added by plugging worker process which can poll for availability of tasks from queues. Definitions of workflows is written in JSON and all administrative operations are performed through a proper REST API.

Components such as the Portal can eventually start a workflow by sending the required input operation trough a simple REST call.

Architecture

From an architectural viewpoint, Conductor is itself a set of micro services implementing: a pluggable persistence layer, and indexing system for queries based on Elasticsearch, the engine and an administrative graphical user interface.

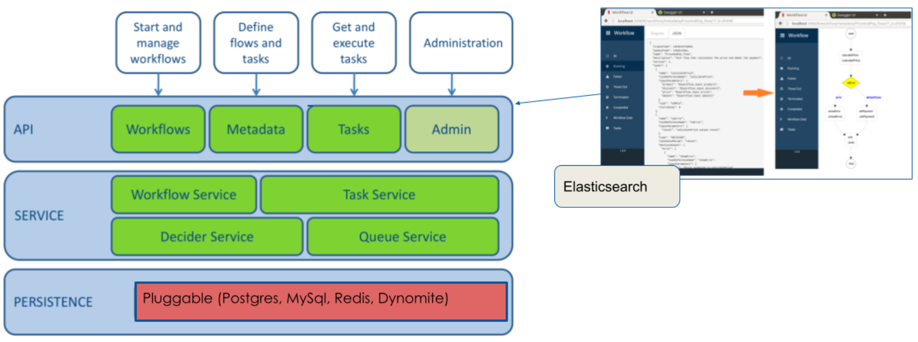


Figure 3.14: MicroService Orchestrator Architecture

The gCube infrastructure now hosts four deployments of the whole Conductor stack serving development, staging and production environments.

Several internal uses cases are now being addressed in order to fully exploit Conductor but most importantly, at the time of writing, the following user management workflows have been deployed to production:

- Addition and removal a user from a VRE or VO,
- Assignment or un-assignment a specific role to a user in a VRE or VO;
- Acceptance of invitation of a user to a VRE;
- Additions of VRE or VO;
- Additions and removal of new roles to all VOs and VREs;
- Deletions of user accounts.

All the management workflows, but the deletion of a user's account, are triggered by events sent by the Liferay portal. The delete user account is an operation that occurs directly on the Keycloak user interface. Thus, this workflow is triggered by Keycloak with a specific event.

The following picture shows and example of a completed instance of the workflow that adds a user as a member to a VRE. In the GUI offered by the Conductor deployment every task can be inspected and each input and output produced by every task can be monitored in order to understand where possible bugs may have arisen.

In case of errors, workflows can be update and replayed in the exact same conditions they are originating from without requiring extra logic in the initiator.

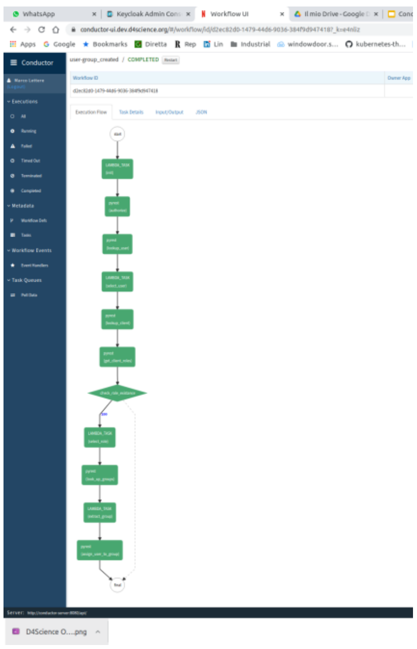


Figure 3.15 Workflow for the addition of a user to a VRE displayed in the conductor UI

3.4 D4Science Storage Framework

3.4.1 Overview

The Storage framework is realized by a combination of services and libraries powered by the gCube System open-source project. It is composed by two main systems: File-Based System and Spatial Data Repository System. These acts as main driver for clients that interface the storage resources managed by the system or accessible through facilities available within the system.

The File-Based System supports functions for **standards-based** and **structured access** and **storage of files** of arbitrary size.

The Spatial Data Repository System is composed by a number of different spatial data repositories for storing **spatial data** in different (standard) formats (e.g. NetCDF, vector data, raster data etc.)

3.4.2 Key Features

Standards compliancy	Support for standard communication protocols / interfaces and data / metadata formats.
Economy of scale	Services constituting one aggregative infrastructure may be hosted over servers maintained at different sites

Failover Management	Automatically transfers control to a duplicate computational node when faults or failures are detected
Support of geospatial dataset lifecycle	Support for generation, revision, publishing, access, visualization and sharing of geospatial data.
Support for analysis and processing	Support for high performance operations over datasets
Geo-referencing datasets	Provide analysis tools to create standard spatial representation of datasets

3.4.3 Subsystems

3.4.3.1 File-Based Store System

The File-Based Store system includes services providing clients functions for standards-based and structured access and storage of files of arbitrary size. This is a fundamental requirement for a wide range of system processes, including indexing, transfer, transformation, and presentation. Equally, it is a main driver for clients that interface the resources managed by the D4Science infrastructure or accessible through facilities available within the same infrastructure.

The File-Based System is composed by a service abstracting over the physical storage and capable of mounting several different store implementations, (by default clients can make use of the MongoDB store) presenting a unified interface to the clients and allowing them to download, upload, remove, add and list files or unstructured byte-streams (binary objects). The binary objects must have owners and owners may define access rights to files, allowing private, public, or shared (group-based) access.

All the operations of this service are provided through a standards-based, POSIX-like API which supports the organization and operations normally associated with local file systems whilst offering scalable and fault-tolerant remote storage

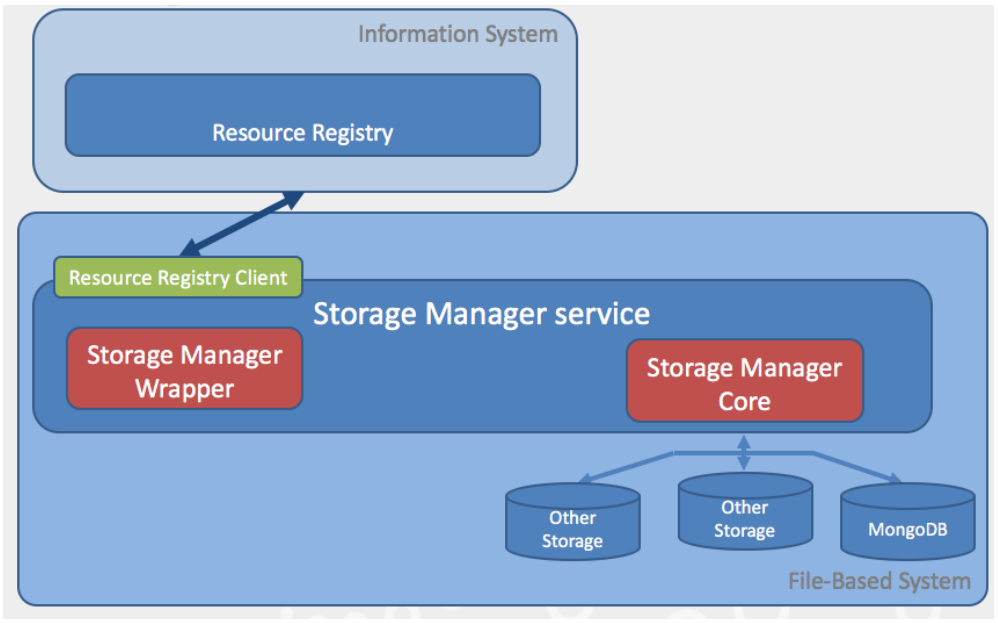


Figure 3.16: File-Based System Architecture

As shown in Figure 3.16: File-Based System Architecture the core of the Storage Manager service is a software component named Storage Manager Core that offers APIs allowing to abstracts over the physical storage. The Storage Manager Wrapper instead is a software component used to discover back-end information from the Resource Registry service of the D4Science Infrastructure. The separation between these two components is necessary to allow the usage of the service in different contexts other than the D4Science Infrastructure.

3.4.3.2 Spatial Data Repositories

The Spatial Data Repositories include services, technology, policies and practices designed in order to provide the following features:

- **Data Discovery**: The ability to browse, query and access metadata files about accessible geospatial datasets. This feature is obtained exploiting **GeoNetwork** webservice, the Open Source catalogue for geospatial metadata compliant with standards mandated by Open Geospatial Consortium (OGC).
- **External Repository Federation**: Transparently extend the Data Discovery capabilities by including output from registered external catalogues and repositories in order to give users global result from a single point.
- **Data Access & Storage:** Provide users and applications to access/store geospatial data in standard formats. Due to the heterogeneity of spatial data representation and formats, the following technologies have been adopted:
    - **PostGIS**: Geospatial extension of **PostgreSQL** relational DBMS;
    - **GeoServer**: Open Source application for management and dissemination of geospatial data through standards mandated by OGC;

  - **Thredds Data Server**: Unidata's Thematic Real-time Environmental Distributed Data Services (THREDDS) is a web server that provides data access for scientific geospatial dataset formats (i.e. NetCDF).
- **Data Processing**: The Data Processing framework includes services designed to perform analysis and transformations over geospatial datasets. The adoption of **52°North Web Processing Service** (WPS) grants users a standardized way to interact with Data Processing facilities.
- **Data Visualization**: Web application, named GeoExplorer, designed to render views of overlapped geospatial datasets on a specific Earth projection, with the ability to query / inspect and export selected data and rendered images.

The set of spatial data repositories and the comprehensive set of integrated technologies for their management, discovery, and exploitation is fully integrated with both infrastructure's enabling technology and layers in order to exploits provisioning, monitoring, Auditing, authentication and storage facilities of the infrastructure.

Key Features

Support of geospatial dataset lifecycle	Support for generation, revision, publishing, access, visualization and sharing of geospatial data.
Support for analysis and processing	Support for high performance operations over geospatial datasets
Dataset enrichment and harmonization	Provide tools to harmonize and add information on existing data
Georeferencing datasets	Provide analysis tools to create standard spatial representation of datasets
Standards compliancy	Support for standard communication protocols / interfaces and data / metadata formats.
External repository federation	Gather all available information in one single point.
Policies adoption assurance over third-party technologies	Configuration/orchestration of third party technologies in order to ensure access policy compliancy.
Horizontal scalability	Ability to expand / contract the SDI resource pool in order to accommodate heavier or lighter loads.

Architecture

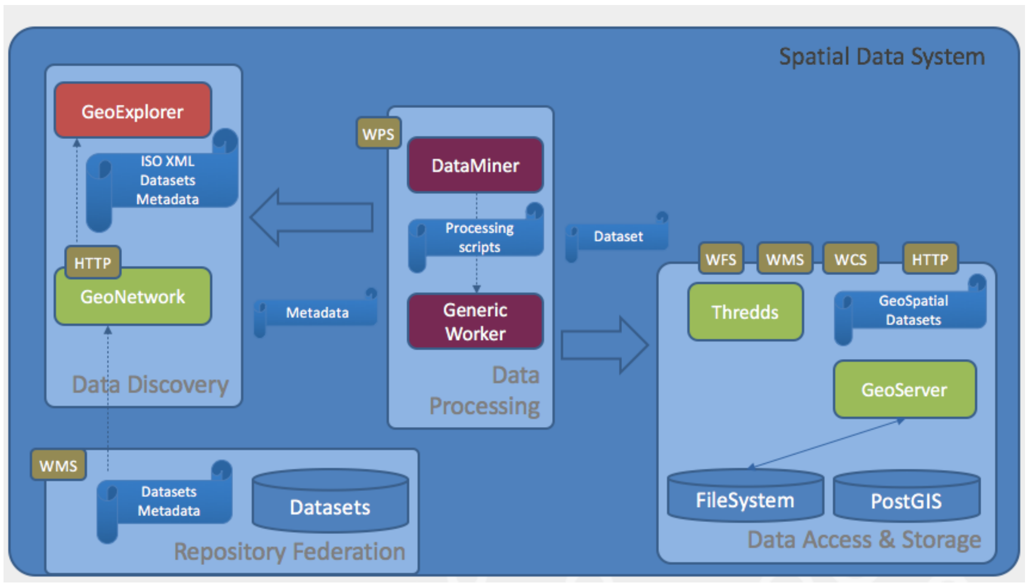


Figure 3.17: Spatial Data Repositories Architecture

The set of Spatial Data Repositories technologies selected and integrated are not only fully compliant with the Open Geospatial Consortium (OGC) standards, i.e. Web Map Service (WMS), Web Coverage Service (WCS), and Web Feature Service (WFS). Rather specific mediators and validators have been designed and implemented to respect the INSPIRE Directive, the EU initiative geared to help to make spatial or geographical information more accessible and interoperable for a wide range of purposes supporting sustainable development.

The Data Discovery components allows the discovery at runtime all available datasets independently of their locations and it is indifferent to the technology used to persist them. It also indifferent to the fact that the data are maintained by a repository managed by the D4Science Cloud Infrastructure or by an independent provider. The same applies also to the Data Processing components that first discovery the datasets to process and then are able to process them independently of the technology used to persist them and the provider entitled to manage them.

3.5 D4Science Analytics Framework

3.5.1 Overview

The Analytics Framework includes a set of features, services and methods for performing data processing and mining on information sets. These features face several aspects of data processing ranging from modeling to clustering, from identification of anomalies to detection of hidden series. This set of services and libraries is used by the e-infrastructure to manage data mining problems even from a computational complexity point of view. Algorithms are executed in parallel and possibly distributed fashion, using the same e-infrastructure nodes as working nodes. Furthermore, Services performing Data Mining operations are deployed according to a distributed architecture, in order to balance the load of those procedures requiring local resources.

3.5.2 Key Features

Parallel Processing	Support for the execution of algorithms on multi-cores computational nodes
Distributed Processing	Transparent distribution of the execution on sets of computational nodes
Failover Management	Automatically transfers control to a duplicate computational node when faults or failures are detected
State-of-the-art data mining algorithms	General purpose algorithms (e.g. Clustering, Principal Component Analysis, Artificial Neural Networks, Maximum Entropy, etc.) supplied as-a-service
Data trends generation and analysis	Identification of trends; inspection of time series to automatically identify anomalies; basic signal processing techniques to explore periodicities in trends

3.5.3 Subsystems

3.5.3.1 Data Miner System

The Data Miner System's goal is to offer a unique access for performing data mining or statistical operations on heterogeneous data. These data can reside on the client side in the form of CSV files or they can be remotely hosted, as SDMX documents or, furthermore, they can be stored in a database.

The Data Miner System is composed by a service, namely Data Miner service, able to take such inputs and execute the operation requested by a client interface, by invoking the most suited computational infrastructure, choosing among a set of available possibilities: executions can run on multi-core machines, or on different computational infrastructures, like Windows Azure, CompSs and other options.

Algorithms are implemented as plug-ins which makes the injection mechanism of new functionalities easy to deploy.

Key Features

Openness	Interaction with external software supporting Standard protocols
Parallel Processing	Support for the execution of algorithms on multi-cores computational nodes
Distributed Processing	Transparent distribution of the execution on sets of computational nodes
State-of-the-art data mining algorithms	General purpose algorithms (e.g. Clustering, Principal Component Analysis, Artificial Neural Networks, Maximum Entropy, etc.) supplied as-a-service

Architecture

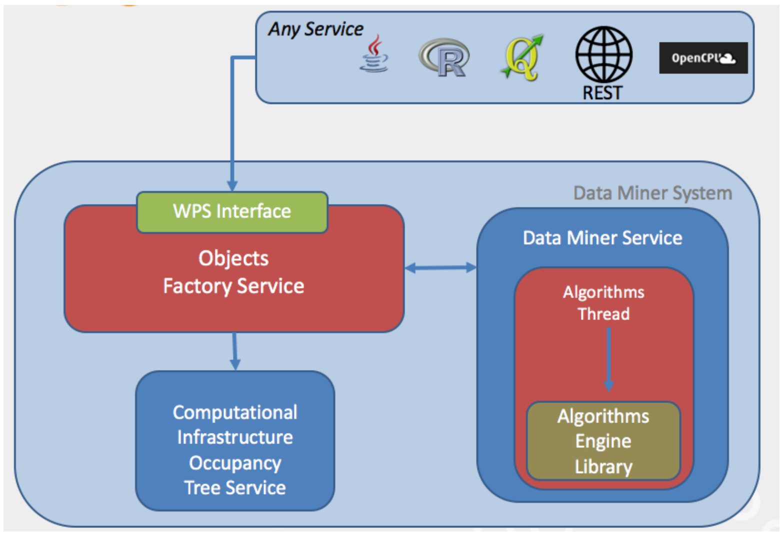


Figure 3.18: Data Miner System Architecture

According to Figure 3.18: Data Miner System Architecture, the Data Miner System comprises the following components:

- **Computational Infrastructure Occupancy Tree service**: a service which monitors the occupancy of the resources to choose among when launching an algorithm;
- **Data Miner Service**: a service executing all the computations asked by a single user\service. It is composed by two components:
  1. **Algorithms Thread**: an internal process which puts in connection the algorithm to execute with the most unloaded infrastructure resource which is able to execute it. Infrastructures are weighted even according to the computational speed; the internal logic will choose the fastest available;
  2. **Algorithms Engine Library**: a container for several data mining algorithms as well as evaluation procedures for the quality assessment of the modeling procedures. Algorithms follow a plug-in implementation and deploy;
- **Object Factory Service**: a service acting as a broker for Data Miner Service and a link between the users' computations and the Occupancy Tree service;

It is worth to notice that thanks to the support of HTTP-REST and WPS protocols the Data Miner System is capable of interacting with different external software supporting such standard (e.g. QGIS, OpenCPU) and different programming languages, in particular Javascript, R, Java.

3.5.3.2 Smart Executor System

The SmartExecutor service allows to execute "gCube Tasks" and monitor their execution status. Each instance of the SmartExecutor service can run the "gCube Tasks" related to the plugins available on such an instance.

Each instance of the SmartExecutor service publishes descriptive information about the co-deployed plugins.

Key Features

Repetitive Tasks	Task can be scheduled to be periodically repeated.
Tasks take over	Task can be taken in charge from new instances in case of instance failure or instance overload.

Architecture

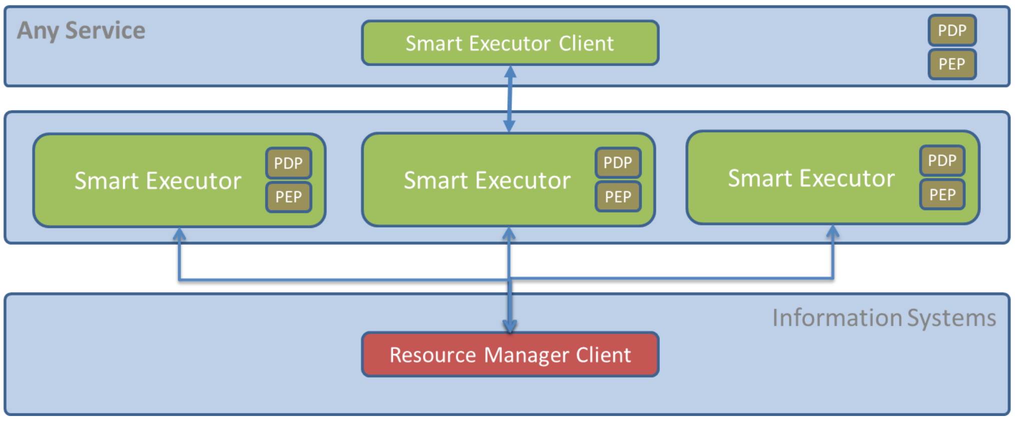


Figure 3.19: Smart Executor System Architecture

Clients may interact with the SmartExecutor service through a library (SmartExecutor Client) of high-level facilities to simplify the discovery of available plugins in those instances. Each client can request to execute a "gCube Tasks" or getting information about the state of their execution.

The SmartExecutor service allows tasks execution through the use of co-deployed plugins. The service allows to pass inputs parameter to the plugin requested to run.

The execution is invoked every time it matches the scheduling parameters. The way to schedule the plugin execution is indicated by scheduling parameter. There are two different way to schedule an execution:

- **run and die**: the plugin is launched just for one time and after this execution it won't be repeated;
- **scheduled**: the plugin repeats its execution over time according to a delay interval or to a “cron” expression.

SmartExecutor instances could take care of a scheduled run when the node where it was previously allocated crashes or is overloaded. To achieve this goal a scheduled task description is registered in the Information System through the Resource Manager.

3.6 D4Science Collaborative Framework

3.6.1 Overview

The Collaborative Framework is realized through a combination of software components (services and libraries) powered by the gCube System. Three main subsystems characterise the Collaborative Framework:

- Social Networking System
- Shared workspace System
- User Management System

These systems provide consumers with a homogenous abstraction layer over different external technologies enabling to operation of the framework. The external technologies involved comprises, Apache Cassandra, Apache Jackrabbit, Elastic Search, MongoDB, and Liferay Portal. In particular, the Social Networking System exploits an Apache Cassandra cluster and an Elastic Search cluster, the Shared Workspace System exploits an Apache Jackrabbit repository (metadata) and a MongoDB cluster (payload) for its backend, the User Management System exploits Liferay Portal for its backend and to allow users to login for personalized services or views.

3.6.2 Key Features

Collaboration	You can share posts and have multiple discussions on the VRE homepage, adding comments and files in line with the discussion.
Folder Sharing	Folder sharing enables the reuse of content and the ease of creating multiple VREs for different audiences with shared content.
Custom Notifications	Important and personalized alerts appear in each user's notification area, and custom applications can add their own notifications.
Responsive Design support	Web Applications are based on Twitter Bootstrap, making it possible to create responsive pages that look great regardless of device.
Economy of scale	Services constituting one aggregative infrastructure may be hosted over servers maintained at different sites

3.6.3 Subsystems

3.6.3.1 Social Networking System

Social Networking System comprising services conceptually close to the common ones promoted by social networks – e.g., posting news, commenting on posted news, likes, private messages and notifications; It is composed by 2 main services, the Social Networking Service and the Social Indexer Service.

The Social Networking Service logic relies on the Social Networking Model, this Model is used also for the efficient storage of the Social Networking Data (Posts, Comments, Notifications etc.) in the underlying Apache Cassandra Cluster. This Cluster is queried by means of a Java client.

Architecture

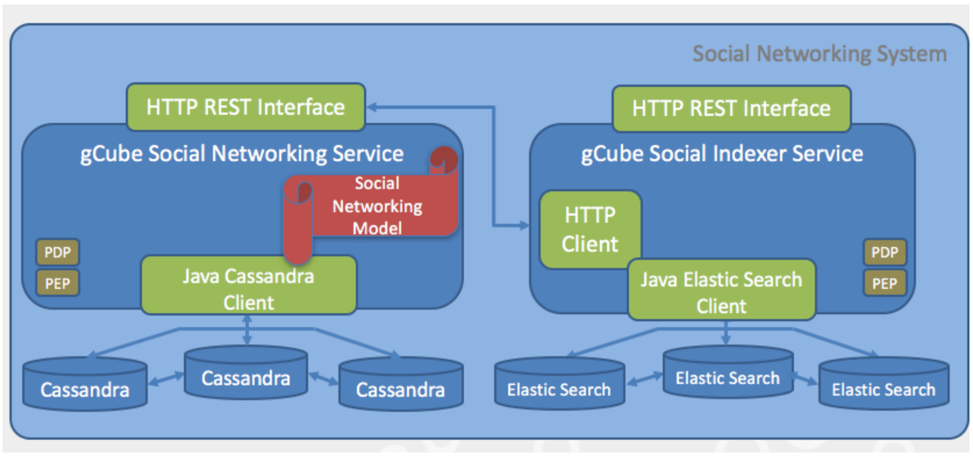


Figure 3.20 Social Networking System Architecture

The Social Networking Service exposes an HTTP REST Interface for the external, and non, services of the infrastructure. The Social Indexer Service uses such interface for the retrieval of the Social Networking Data to index by means of an Elastic Search Cluster. The Social Indexer Service exposes an HTTP REST Interface for the external, and non, services of the infrastructure needing to perform search operations over the Social Networking Data.

Both Services rely on the Policy Decision Point (PDP) and the Policy Enforcement Point (PEP) to intercepts user's access request and evaluate these requests against authorization policies of the Authorization System of the Infrastructure.

3.6.3.2 Shared Workspace System

The Shared Workspace System provides a remote (Cloud) folder-based file system, supporting sharing of folders and different item types (ranging from binary files to information objects representing, for instance, tabular data, workflows, distribution maps, statistical algorithms).

Architecture

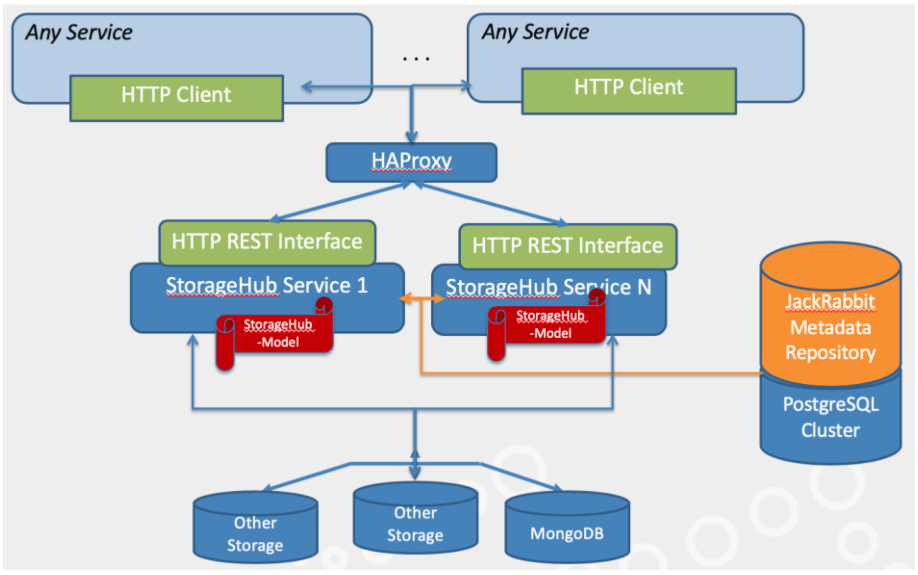


Figure 3.21: Shared Workspace System Architecture

With respect to the last reporting period the Shared Workspace System was heavily redesigned with the aim of increasing its scalability and overall performance. It consists of one gCube service, named StorageHub Service, relying on 2 different storage technologies to store the metadata of the items being stored, namely Apache Jackrabbit as metadata repository and PostgreSQL as Apache Jackrabbit Bach-end Database. The StorageHub Service is replicable and a HAProxy on top is used for proxying requests to the deployed instances of it. One other distinguish feature of the StorageHub Service is that the actual payload of the items can be stored on a number of in house and commercial storage technologies, for instance in a MongoDB Cluster, but also on other types, including Cloud Storages solutions (e.g. Amazon S3). An additional backed has been added to manage large volume of data close to the analysis performed with notebooks. This additional backend is named **Dataspace** and it is local to the Kubernetes cluster serving JupyterHub.

The StorageHub Service identifies a core set of capabilities to work on JackRabbit content. Together with its model, named StorageHub model, exposes content in the content repository as HTTP resources, fostering a RESTful style of application architecture. Home RESTFUL interface processes HTTP requests coming from clients. The following operations are supported:

- retrieve content;
- create content;
- modify existing content;
- remove existing content;
- move existing content to a new location;
- copy existing content to a new location;

3.6.3.3 User Management System

Users are the fundamental entity managed by this System. As a matter of fact, User is an entity that can sign into the portal and do something. Users are assigned a Role and a Role is what defines the user's privileges. The User Management System provides functionality to manage personal profiles and users in the D4Science Virtual Research Environments, supporting user groups (for the purpose of group specific privileges) and roles for application specific needs related to the user's role within a given VRE.

3.7 D4Science Publishing Framework

3.7.1 Overview

The publishing framework is conceived to make it possible for providers to document (by rich metadata) any research outcome and publish it (make it "public" / "known") thus to possible implement the FAIR principles. In fact, the framework caters for both providers willing to advertise research artifacts and consumers willing to discover existing artifacts and access them.

3.7.2 Key Features

Configurable metadata	Metadata accompanying items cater for common metadata (e.g. title, description, license) and additional metadata specified by community defined profiles.
Automatic Classification directives	Additional metadata might be annotated with classification directives organising catalogue items in groups.
Powerful search and browse	A rich search experience is offered allowing for quick 'Google-style' keyword search as well as faceting by tags and browsing between related items. Quick view on available items, in which formats and with which licence, straight from the search results. All metadata fields are searchable.
Geospatial support	Items can be annotated with their spatial extent and made searchable by spatial queries.
Federation oriented	Published items are made available by both a REST API and known standard and protocols (DCAT, OAI-PMH) enacting others to systematically access and collect them. Items can be systematically collected from existing data sources by standard-based harvesters (DCAT, OAI-PMH, CSW) and ad-hoc harvesters.

3.7.3 Subsystems

3.7.3.1 The Catalogue System

The Catalogue System provides its users with facilities for documenting and publishing items as well as searching and browsing across the published items to access them. Catalogue items have a unique and actionable identifier, are characterised by rich metadata, and are accompanied with a list of resources, i.e., pointers to the payloads of the item.

Architecture

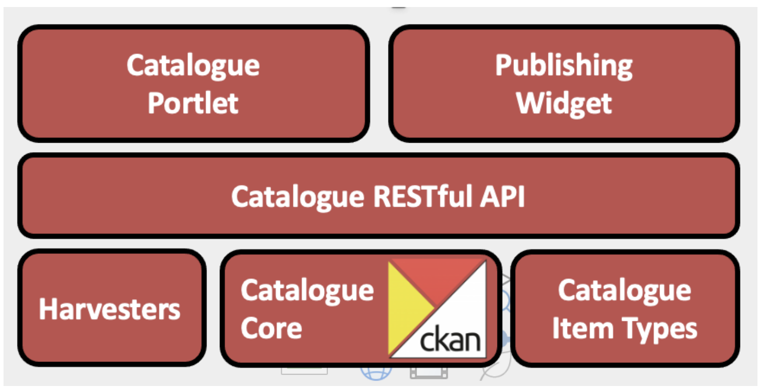


Figure 3.22: Resource Registry Architecture

The central part of the Catalogue System is based on the on open-source technology for data catalogues (CKAN ckan.org). It has been extended to (a) be integrated with D4Science services and (b) support a rich, community-defined, and extensible set of catalogue item typologies.

Catalogue item types (aka profiles) are specifications of additional metadata fields to be added to the common metadata characterising every catalogue item. Each profile is stored into the Resource Registry and consists of a list of fields each having a name, a mandatory directive (whether the field is mandatory or optional, a type (e.g., string, number, spatial extent), a max occur directive to specify whether the field can be instantiated one time only or many times), a default value, a descriptive note helping to understand the intended meaning of the field, a controlled vocabulary (if any) of allowed values to use to compile the field, and a validator (if any) to check the inserted value adherence to specific validation rules.

On top of this there is a RESTful Service (gCat) to programmatically interact with the D4Science Catalogue System Core component according to the model briefly discussed above. This API provide authorised users with facilities for managing Items, Resources, Profiles, Namespaces, Licenses, Groups, Organizations, and Users.

The Catalogue Portlet and the Publishing Widget realise the graphical user interface of the overall system. In particular, the Catalogue Portlet implements the component for searching and browsing catalogue contents while the Publishing Widget implements the component supporting the publishing phase, i.e., the writing of metadata and the adding of the resources to assemble an item.

3.8 D4Science Third-Party Frameworks

3.8.1 NLPHub

NLPHub is a distributed system that orchestrates and combines several state-of-the-art text mining services that recognize spatiotemporal events, keywords, and a large set of named entities. NLPHub integrates: (i) the Stanford CoreNLP software for English, German, French, and Spanish; (ii) the Italian NLP Tool (Tint) for Italian; (iii) Apache OpenNLP toolkit that includes methods for language detection, tokenization, part-of-speech tagging, morphological parsing, and named entity recognition; (iv) ItaliaNLP that includes methods for part-of-speech tagging, tokenization, morphological parsing, lemmatization, named entity recognition, clustering, words similarity assessment, and sentiment analysis; (v) NewsReader event recognizer; (vi) Keywords NEW that produces tag clouds of words and nouns. For all of them the access is offered as-a-service.

An orchestrator algorithm (AMERGE), implemented as a DataMiner process, receives a user-provided input text, along with the indication of the text language (optionally), and a set of annotations to extract (selected among those supported for that language).

NLPHub is exploitable with anonymous access only via its graphical user interface. By exploiting the user interface, a user may upload a text file and obtain an annotated text. Programmatic exploitation of the NLPHub is possible only by joining a VRE offering it as a service.

3.8.2 ShareLatex Application

ShareLaTeX is an online LaTeX editor that allows real-time collaboration and online compiling of projects to PDF format. In comparison to other LaTeX editors, ShareLaTeX is a server-based application, which is accessed through a web browser. On July 20, 2017, ShareLaTeX was acquired by Overleaf. Overleaf plans to continue ShareLaTeX under the brand Overleaf v2 which was in beta testing up until the 4th of September 2018. The provision of the ShareLaTeX service is therefore limited to the availability of the open source license and it will be guaranteed by D4Science.org until Overleaf will not change it.

3.8.3 RShiny Application

The Shiny application is delivered by the user to the D4Science.org as a complete Shiny Application on the Docker Registry[4].

The user is responsible to build the standard Docker image as described in the ShinyProxy documentation by writing the docker file, building the docker image and providing the configuration for ShinyProxy.

D4Science.org makes accessible the Shiny Application on the D4Science infrastructure by ensuring its operation and orchestration in a cluster. The cluster is composed by multiple Docker hosts which run in parallel mode and act as managers and workers.

3.8.4 RStudio Application

The RStudio allows to perform online statistical analyses with the R software for statistical computing. The user is responsible to implement proper R scripts as described in the RStudio documentation.

The D4Science Infrastructure makes accessible the RStudio Application on the D4Science infrastructure by ensuring its operation and orchestration in a cluster. The cluster is composed by multiple hosts, each of which is assigned in exclusive mode to a user for an entire online session. At the end of the session, all the content stored in that host may be removed by D4Science Infrastructure. All the data, scripts, and other resources that the user needs to persist have to be stored into the Workspace that is accessible through the RStudio Application.

[4] https://hub.docker.com

3.8.5 JupyterHub

JupyterHub is a web-based interactive development environment for Jupyter notebooks, code, and data. It allows users to configure and arrange the user interface to support a wide range of workflows in data science, scientific computing, and machine learning.

The Blue-Cloud VRE makes the JupyterHub accessible on the D4Science infrastructure ensuring its operation and orchestration in a cluster, which is made by multiple hosts assigned exclusively to a user for an entire online session. Currently, the cluster supports 80 users (at 8 GB RAM; Cores per user: 4/8; Memory per user (GB): 8/16/32; Storage per user (GB): 10GB; Allocation type: pledged).

JupyterHub uses ephemeral storage as local storage. The content locally stored is removed at the end of each session. All the data, scripts, and other resources that the user needs to persist must be stored either in the Workspace to enabling controlled sharing and publication of such resources, or in the Dataspace to share those resources in the virtual laboratory and reuse across sessions.

3.9 D4Science Software Methods Provision and Integration

The data processing platform (named DataMiner) is an open-source computational system based on the gCube system. This platform is fully integrated with the D4Science e-Infrastructure, and has been conceived to meet the Open Science paradigm requirements, thus to promote collaborative experimentation and open publication of scientific findings, while tackling Big Data challenges. DataMiner is able to interoperate with the services of the D4Science e-Infrastructure, and uses the Web Processing Service (WPS) standard to publish the hosted processes. Further, it saves the computational provenance of an executed experiment using the Prov-O standard. DataMiner implements a Cloud computing Map-Reduce approach and is able to process Big Data and save outputs onto a collaborative experimentation space. This space allows users to share computational information with other colleagues. This service was conceived to execute processes provided by communities of practice in several domains, leveraging integration effort at the same time. The DataMiner deployment is fully automatic through ANSIBLE scripts and is spread across different machines providers, including the Italian Garr network.

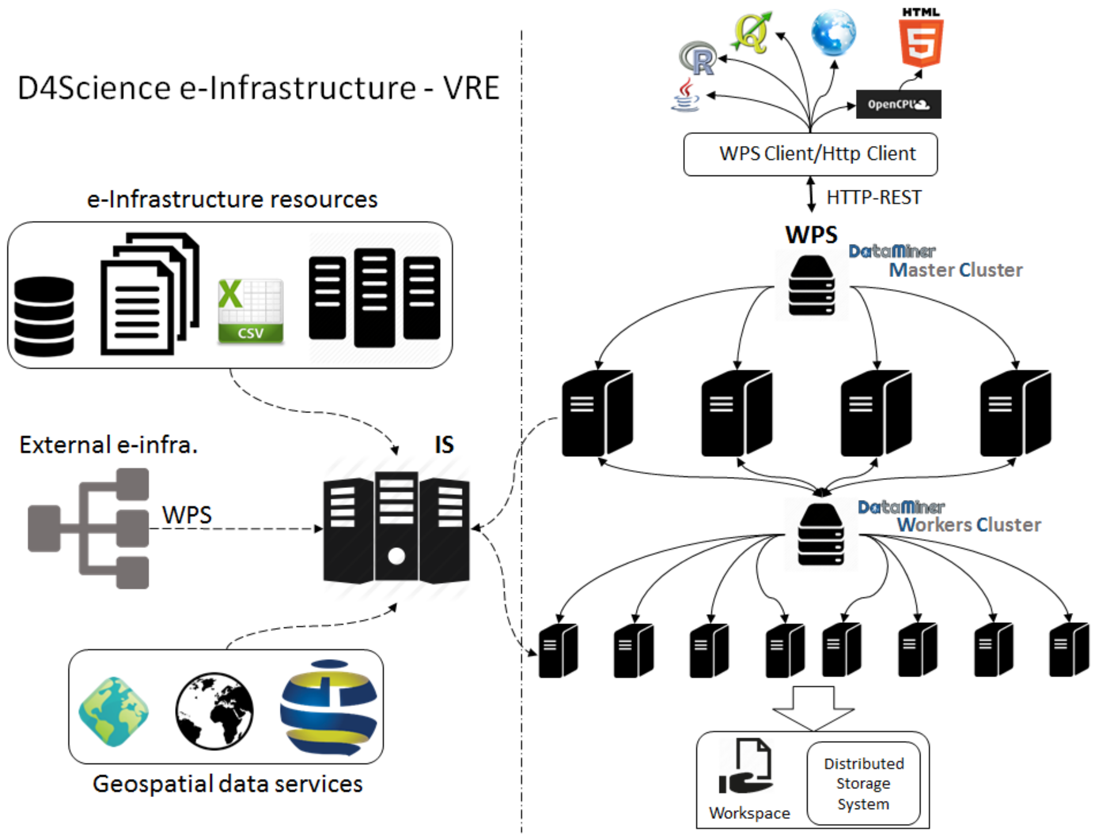


Figure 3.23: Architecture of the DataMiner data processing system

The DataMiner (DM) [4] architecture is made up of two sets of machines (clusters) that operate in a Virtual Research Environment [3]: Master and Worker cluster. In a typical deployment scenario, the Master cluster is made up of a number of powerful machines (e.g. Ubuntu 18 x86 64 with 16 virtual CPUs, 32 GB of random-access memory, 100 GB of disk) managed by a load balancer that distributes the requests uniformly to the machines. Each machine is endowed with a DM service that communicates with the D4Science Information System (IS), i.e. the central registry of the e-Infrastructure resources, to notify its presence and capabilities. The balancer is indexed on the IS and is the main access point to interact with the DMs. The machines of the Worker cluster have the same computational power and serve Map-Reduce computations. DM is based on the 52North WPS implementation, but extends it to meet D4Science e-Infrastructure requirements. It is developed with Java and the Web service runs on an Apache Tomcat instance endowed with gCube system libraries. Further, it offers a development framework to integrate new algorithms and interact with the e-infrastructure.

Using the WPS standard in a Cloud computing system allows a number of thin clients to use the processes. The DataMiner services use the security services of the D4Science e-Infrastructure and require a user token to be provided for each operation. This token is passed via basic HTTPS-access authentication, which is supported by most WPS and HTTP(S) clients. The token identifies both a user and a Virtual Research Environment and this information is used by DM to query the IS about the capabilities to be offered in that VRE, i.e. the processes the user will be able to invoke with that authorization.

The DataMiner computations can take inputs from the D4Science Workspace. Inputs can also come from Workspace folders shared among several users. This fosters collaborative experimentation already at the input selection phase. Inputs can also come from external repositories, because a file can be provided either as a HTTP link or embedded in a WPS execution request. The outputs of the computations are written onto the D4Science Distributed Storage System and are immediately returned to a client at the end of the computation. Afterwards, an independent thread also writes this information on the Workspace. Indeed, after a completed computation, a Workspace folder is created which contains the input, the output, the parameters of the computation, and a provenance document summarizing this information. This folder can be shared with other people and used to execute the process again. Thus, the complete information about the execution can be shared and reused.

DataMiner can also import processes from other WPS services. If a WPS service is indexed on the IS for a certain VRE, its processes descriptions are automatically harvested, imported, and published among the DM capabilities for that VRE. During a computation, DM acts as a bridge towards the external WPS systems. Nevertheless, DM adds provenance management, authorization, and collaborative experimentation to the remote services.

3.8.1 Functional specifications

DataMiner satisfies functional specifications related to the processing of a large variety of data types (including geospatial data) in the wide context of Big Data processing and Open Science. Indeed, several computational systems exist, also used by e-Infrastructures, that typically parallelise the computation on several available cores/processors or machines of the e-Infrastructure. Nevertheless, DataMiner also satisfies new requirements requested by new Science paradigms, which include:

- Publishing local-machine processes, provided by a community of practice (e.g. scripts, compiled programs etc.), as-a-Service;
- Managing several programming languages;
- Interoperate with other services of an e-Infrastructure, possibly through a standard representation of the processes and of their parameters;
- Saving the "provenance" of an executed experiment, i.e. the set of input/output data, parameters, and metadata that would allow to reproduce and repeat the experiment;
- Supporting data and parameters sharing through collaborative experimental spaces;
- Being economically sustainable, e.g. easy to install and deploy on several partners machines;
- Supporting security and Auditing facilities;
- Managing and analysing Big Data;
- Designing and executing Workflows that combine different processes published as services.

DataMiner was conceived to satisfy the reported requirements. One major advantage is that all the DM services publish their capabilities using a standard, which enhances the interoperability with other external services and software, with respect to using custom clients. Further, the DM clusters are managed by fast load balancers that are able to dynamically add machines and to ignore them when offline. Since the Worker nodes are exact replicas of the Master nodes, the Worker cluster can be used directly from clients and fosters alternative usages of the Cloud computing system. For example, external users of D4Science (authorised with proper tokens) may also implement their own Cloud computations by invoking the Worker cluster in custom workflows. Another DM feature is that it can interact with data preparation and harmonisation services. This speeds up the typical time-consuming phase of data preparation for an experiment. Further, providing a shared experimentation area allows reusing the results of processes and also fosters multidisciplinary experiments. Users could also be services or external machines (e.g. sensors) that produce experimental data at different frequencies and time scales, while other processes analyse these data and take decisions. The same facilities are automatically offered to desktop software supporting WPS. Further, generating and storing provenance information improves the possibility to repeat and reproduce an experiment executed by other scientists. Finally, since processes and service installation is fully automatic through ANSIBLE scripts, it is easy to deploy DataMiner on a number of machines providers. The hosted processes currently hosted by DataMiner are written with the R, Java, Fortran, Linux-compiled, .Net, Octave, KNIME, and Python programming languages and have been provided by developers with heterogeneous expertise (e.g. biologists, mathematicians, agronomists, physicists, data analysts etc.).

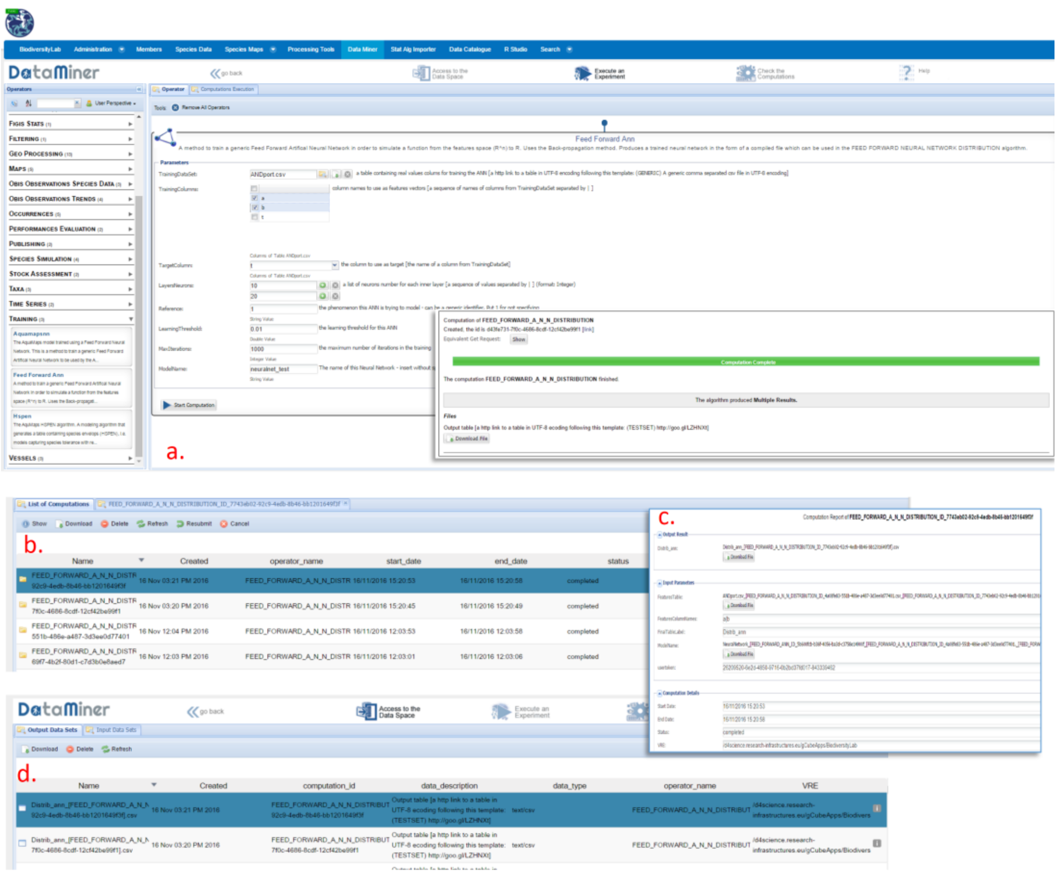
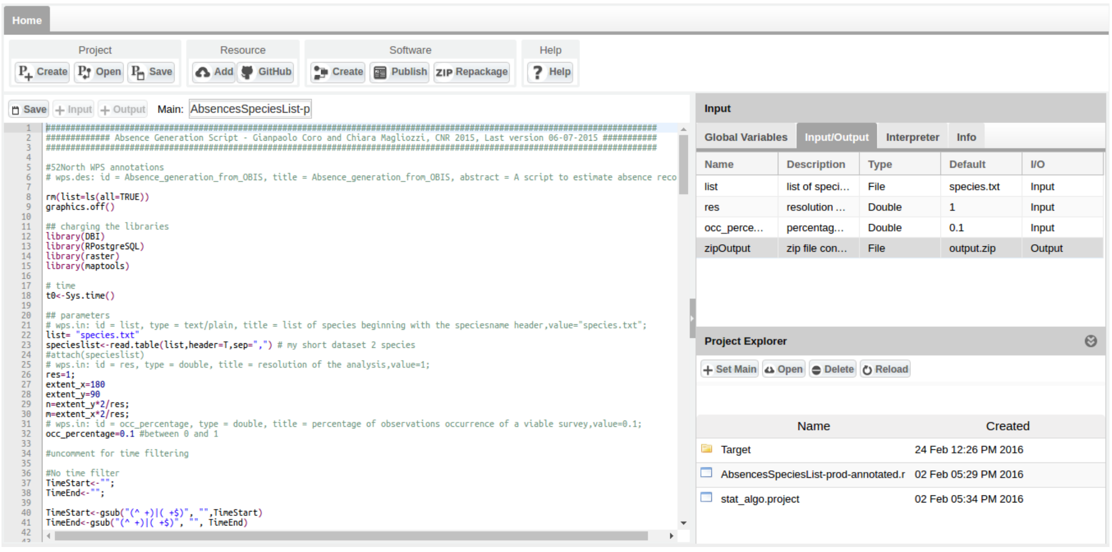


Figure 3.24: Interface of the gCube DataMiner system

DataMiner offers a Web GUI to the users of a VRE. On the left panel (a), the GUI presents the list of capabilities available in the VRE, which are semantically categorised (the category is indicated by the process provider). For each capability, the interface calls the WPS *DescribeProcess* operation to get the descriptions of the inputs and outputs. When a user selects a process, in the right panel the GUI on-the-fly generates different fields corresponding to the inputs. Input data can be selected from the Workspace (the button associated to the input opens the Workspace selection interface). The "Start Computation" button sends the request to the DM Master cluster, which is managed as explained in the previous section. The usage and the complexity of the Cloud computations are completely hidden to the user, but the type of the computation is reported as a metadata in the provenance file. In the end, a view of the Workspace folders produced by the computations is given in the "Check the Computations" area (b), where a summary sheet of the provenance of the experiment can be obtained ("Show" button, c). From the same panel, the computation can be also re-submitted. In this case, the Web interface reads the Prov-O XML information associated to a computation and rebuilds a computation request with the same parameters. The computation folders may also include computations executed and shared by other users. Finally, the "Access to the Data Space" button allows the user to obtain a list of the overall input and output datasets involved in the executed computations (d), with provenance information attached that refers to the computation that used the dataset.

3.8.2 Software and Algorithms Integration



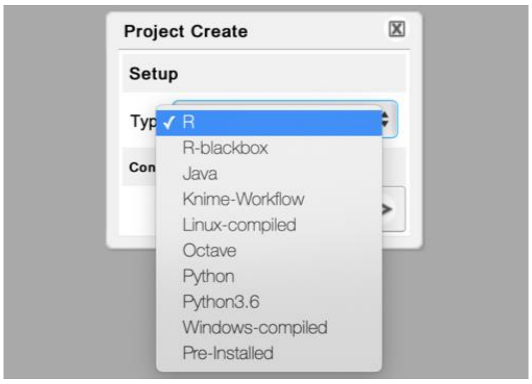
```
###########################################################################################################
############# Absence Generation Script - Gianpaolo Coro and Chiara Magliozzi, CNR 2015, Last version 06-07-2015 ###########
###########################################################################################################

#52North WPS annotations
# wps.des: id = Absence_generation_from_OBIS, title = Absence_generation_from_OBIS, abstract = A script to estimate absence reco

rm(list=ls(all=TRUE))
graphics.off()

## charging the libraries
library(DBI)
library(RPostgreSQL)
library(raster)
library(maptools)

# time
t0<-Sys.time()

## parameters
# wps.in: id = list, type = text/plain, title = list of species beginning with the speciesname header,value="species.txt";
list= "species.txt"
specieslist<-read.table(list,header=T,sep=",") # my short dataset 2 species
#attach(specieslist)
# wps.in: id = res, type = double, title = resolution of the analysis,value=1;
res=1;
extent_x=180
extent_y=90
n=extent_y*2/res;
m=extent_x*2/res;
# wps.in: id = occ_percentage, type = double, title = percentage of observations occurrence of a viable survey,value=0.1;
occ_percentage=0.1 #between 0 and 1

#uncomment for time filtering

#No time filter
TimeStart<-"";
TimeEnd<-"";

TimeStart<-gsub("(^ +)|( +$)", "",TimeStart)
TimeEnd<-gsub("(^ +)|( +$)", "", TimeEnd)
```

Name	Description	Type	Default	I/O
list	list of speci...	File	species.txt	Input
res	resolution ...	Double	1	Input
occ_perce...	percentag...	Double	0.1	Input
zipOutput	zip file con...	File	output.zip	Output

Name	Created
Target	24 Feb 12:26 PM 2016
AbsencesSpeciesList-prod-annotated.r	02 Feb 05:29 PM 2016
stat_algo.project	02 Feb 05:34 PM 2016

Figure 3.25: Interface to import an R process on DataMiner

Prototype scripting is the basis of most models in environmental sciences. Scientists making prototype scripts (e.g. using R and Matlab) often need to share results and make their models used also by other scientists on new data. To this aim, one way is to publish scripts as-a-Service, possibly under a recognized standard (e.g. WPS). The Statistical Algorithms Importer (SAI[5]) is an interface that allows scientists to easily and quickly import scripts onto DataMiner. DataMiner in turn publishes these scripts as-a-Service and manages multi-tenancy and concurrency. Additionally, it allows scientists to update their scripts without following long software re-deploying procedures each time. In summary, SAI produces processes that run on the DataMiner Cloud computing platform and are accessible via the WPS standard.



The SAI interface for R scripts resembles the R Studio environment, a popular IDE for R scripts, in order to make it friendly to script providers, whereas the interface for software written in other programming languages does not allow to edit the main script. However, SAI provides support for scripts implemented in several languages as shown in the following picture.

The *Project* button allows creating, opening and saving a working session. A user uploads a set of files and data on the workspace area (lower-right panel). Upload can be done by dragging and dropping local desktop files. As next step, the user indicates the “main script”, i.e. the script that will be executed on DataMiner and that will use the other scripts and files.

For R scripts integration, after selecting the main script, the left-side editor panel visualises it with R syntax highlighting and allows modifying it.

Afterwards, the user indicates the input and output of the script by highlighting variable definitions in the script and pressing the *+Input* (or *+Output*) button. In the case of other programming languages than R, the Input and Output variables should be manually specified directly in the Input / Output panel.

For R scripts, SAI also supports WPS4R annotations inside the script to automatically generate inputs and outputs. Other tabs in this interface area allow setting global variables and adding metadata to the process. In particular, the *Interpreter* tab allows indicating the R interpreter version and the packages required by the script and the *Info* tab allows indicating the name of the algorithm and its description. In the *Info* tab, the user can also specify the algorithm’s name and category.

[5] Described in Coro, G., Panichi, G., & Pagano, P. (2016). A Web application to publish R scripts as-a-Service on a Cloud computing platform. Bollettino di Geofisica Teorica ed Applicata, 57, 51-53. With a user guide available at https://wiki.gcube-system.org/gcube/Statistical_Algorithms_Importer

Once the metadata and the variables information has been fulfilled, the user can create one DataMiner as-a-Service version of the script by pressing the *Create* button in the Software panel. The term “software”, in this case indicates a Java program that implements an as-a-Service version of the user-provided scripts. The Java software contains instructions to automatically download the scripts and the other required resources on the server that will execute it, configure the environment, execute the main script and return the result to the user. The computations are orchestrated by the DataMiner computing platform that ensures the program has one instance for each request and user. The servers will manage concurrent requests by several users and execute code in a closed sandbox folder, to avoid damage caused by malicious code.

Based on the SAI Input / Output definitions written in the generated Java program, DataMiner automatically creates a Web GUI. By pressing the *Publish* button, the application notifies DataMiner that a new process should be deployed. DataMiner will not own the source code, which is downloaded on-the-fly by the computing machines and deleted after the execution.

This approach meets the policy requirements of those users who do not want to share their code. The *Repackage* button re-creates the software so that the computational platform will be using the new version of the script. The repackaging function allows a user to modify the script and to immediately have the new code running on the computing system. This approach separates the script updating and deployment phases, making the script producer completely independent on e-Infrastructure deployment and maintenance issues. However, deployment is necessary again whenever Input / Output or algorithm’s metadata are changed.

To summarise, the SAI Web application relies on the D4Science e-Infrastructure and enables a software (R, Java, Fortran, Linux-compiled, .Net, Octave, KNIME, Python), provided by a community of practice working in a VRE, with as-a-Service features. SAI reduces integration time with respect to direct Java code writing. Additionally, it adds (i) multi-tenancy and concurrent access, (ii) scope and access management through Virtual Research Environments, (iii) output storage on a distributed, high-availability file system, (iv) graphical user interface, (v) WPS interface, (vi) data sharing and publication of results, (vii) provenance management and (viii) Auditing facilities.

3.10 D4Science Tools Provision and Integration

The tools provision and integration of software deployed as service follows:

3.10.1 SmartGears

SmartGears is a set of Java libraries that turn Servlet-based containers and applications into gCube resources, transparently.

In this section, we introduce SmartGears[6] and explain how it is an improvement over existing gCube solutions. The discussion is relevant to node and infrastructure managers, who perform and maintain SmartGears installations, and to developers, who package or write software for a gCube infrastructure.

[6] More details about SmartGears can be found in the set of dedicated wiki pages at the address: https://wiki.gcube-system.org/gcube/SmartGears.

A piece of software is an infrastructure resource (the so-called Software as Resource, SaR) if we can manage it in the D4Science infrastructure. This means that we can do a number of things with the software, including:

- discover where it is deployed in the infrastructure, so as to use it without hard coded knowledge of its location. For this, we need to describe each and every software deployment, and publish these descriptions, or profiles, in the infrastructure;
- monitor and change the status of its deployments, so as to take actions when they are not in an operational status (e.g. redeploy the software, or at least prevent discovery and usage of the deployments). For this, we need to track their current status, report it in the profiles we publish, and republish the profiles when the status changes;
- dedicate its deployments to certain groups of users, in the sense that only users in those groups can use them. We can change the sharing policies of individual deployments at any time, i.e. share them across more or less groups. We can also grant different privileges to different types of users within given groups.

Publication, *discovery*, *lifecycle management*, *controlled sharing* are the pillars of the resource management. Yet relying on humans to compile deployment profiles, publish them in the infrastructure, keep track and change the status of deployments, or enforce sharing policies is all but practical. In some cases, it is downright impossible. We need instead automated solutions that live alongside each and every deployment and help us turn it into a resource we can manage. SmartGears is one such solution.

We focus on software that can be used over the network, such as distributed applications and network services. Software deployments then correspond to software endpoints.

Typically, software endpoints run within containers and, in D4Science, containers can be resources in their own right, the so-called gCube Hosting Nodes (gHNs).

Managing gHNs is a way to manage multiple endpoints simultaneously (e.g. to deactivate a gHN means to deactivate a set of endpoints at once). Equally, it is a way to manage underlying hardware resources (e.g. dedicate a gHN to selected groups of users).

This is a notion of "Container-as-Resource" (CaR), and it raises the same requirements as SaR, including publication and discovery, lifecycle management, and controlled sharing. SmartGears helps us meet these requirements too, i.e. turns containers as well as the endpoints therein into gCube resources.

SmartGears is not a development framework. Rather, SmartGears is invisible to the software, not part of its stack at all. As a result, any software can run in the infrastructure: SaR becomes a nature that software acquires at runtime.

Indeed, SmartGears has few requirements of the software. All we ask of software is that it is based on the Servlet specifications, which define the hooks that we need to track its lifecycle and its use. The software is thus a Web Application and may more specifically be a Soap service, a Rest service, or a generic Web Application. It may adopt different standards and technologies (e.g. JAX-RPC, JAX-

WS, JAX-RS, but also Dependency Injection technologies, persistence technologies, etc.). And of course, it may run in any container that is Servlet-compliant (Web Containers, Application Servers).

Finally, the evolution of SmartGears is inconsequential for the software: most of the APIs of SmartGears remain private to SmartGears.

Containers and applications need a minimal set of requirements before SmartGears can turn them into gCube resources:

- containers must comply with version 3 of the Servlet specifications;
- applications must include at least one gcube-app.xml configuration file alongside their deployment descriptor (i.e. under /WEB-INF);

In addition:

- node managers must define a GHN_HOME environment variable that resolves to a location where SmartGears can find a container.xml configuration file.

Starting from version 3, the Servlet specifications allow SmartGears to intercept relevant events in the lifecycle of individual applications whilst being shared across all applications, in line with the deployment scheme of SmartGears. In particular, the specifications introduce a ServletContextInitializer interface that SmartGears implements to be notified of application startup. The specifications also allow programmatic registration of filters and servlets, which SmartGears uses to transparently manage applications without the need of additional configuration in their web.xml descriptor.

Configuration is thus limited to WEB-INF/gcube-app.xml and $GHN_HOME/container.xml, which provide the configuration of, respectively, the application and the container as gCube resources. Details about their contents are available in the gCube Wiki Appendices.

Smartgears is distributed as a tarball that contains the libraries, scripts, and configuration files required to install Smartgears in a given container, and to maintain the installation over time. Instructions on how to download, install and maintain Smartgears are available in the SmartGears Web Hosting Node (wHN) Installation.

3.10.2 OAuth2.0

By means of the OAuth 2.0 protocol (authorised) third party applications can operate on a user's behalf over the D4Science infrastructure (while protecting the member's credentials). For more information about the OAuth authorization framework please visit the official OAuth site[7]. For technical details also see the OAuth 2.0 RFC[8]. In the following, the steps needed to authorize third party applications to operate on a user's behalf and the D4Science infrastructure are explained.

This exploitation case makes it possible to integrate in the infrastructure services, tools, and applications that are not deployed on SmartGears powered containers.

[7] https://oauth.net/2/
[8] https://tools.ietf.org/html/rfc6749%7C

More details about how the OAuth 2.0 service work can be exploited in D4Science can be found in the set of dedicated wiki pages at the address:

https://wiki.gcube-system.org/gcube/OAuth2.0

3.11 D4Science Exploitation Models

D4Science offers access to services delivered and managed via tailored Virtual Research Environment. Each VRE can have different access policies that can be selected at any time during the operation of the VRE:

- *private access*: the VRE is private and a user can access it only by invitation issued by the VRE Manager. Upon acceptance of the user of the invitation, the user becomes member of the VRE with a user role;
- *restricted access*: a user registered to the gateway and with a valid identity can request access to the VRE. The VRE Manager can approve or reject any user request. In case of approval, the user becomes member of the VRE with a user role;
- *public access*: a user registered to the gateway and with a valid identity can become member of the VRE by simply accessing it. The VRE Manager is just notified.

Furthermore, four different roles are supported by default and additional ones can be defined as per request of the Customer:

- *VRE Manager*: this kind of user manages user registration/deregistration to the VRE and assign/remove roles by accessing the Administration dashboard;
- *User*: any user with this role can access the VRE data and share private data with other selected members of the VRE;
- *Processor* (Optional): any user with this role can register its own process and execute a process by accessing the Method Engine service;
- *Editor*: the users with this role can publish data to all members of the VRE by exploiting the Catalogue service.

Tailored exploitation models have been designed for a single user, a group of users, and for community of users. The main characteristics of each of them are reported in the following table.

As-a-User

Description	You need a workspace where you can store, access, and optionally share files and datasets. You wish to follow the activities performed by the other users of a large community and to join one of the existing applications offered by the existing VREs.
Reserved Resources	Zero. Storage and computational jobs queues are shared with other users.

Resources Highlights	Your data is kept private until you share it. However, the computational resources are shared with other users and assigned to you only when needed.
How	Register on one of the available Gateways and join one of the existing public Virtual Research Environment.
Type of engagement	You are a single user requiring immediate access to data and tailored applications.
Cost	Free to use according to the Terms of Use.

As-a-Group

Description	You need to create a dedicated environment with specific applications and manage the users by authorizing them to join. Only authorized users will have access to the data used and generated by the newly created applications. You may exploit any of the capabilities and you may add your specific applications and data.
Reserved Resources	From Zero to the resources assigned to manage your private applications.
Resources Highlights	Your data is kept private until you share it with other user of the newly created application. However, the computational resources are shared with other users and assigned to you only when needed.
How	Register on one of the available Gateways, join the gCubeApps community and ask the gCubeApps VO Manager to become a VRE Designer. Then, design your specific new VRE that will be subject to approval by the VO Manager. On average, a new application is created in less than 24 hours.
Type of engagement	You manage a small set (up to hundreds) of users focusing on a specific scientific topic requiring a common infrastructure to store, maintain, and process data.
Cost	Free to use according to the Terms of Use and without installing any custom and private service.

As-a-Community

Description	You need to manage a community for a medium/long period and you want to offer members an integrated storage and computational platform for the execution of daily tasks. You may exploit any of the available capabilities and you may add your specific applications and data. Data and applications are kept private to your community and confidentiality and security are guaranteed by encryption.
Reserved Resources	A minimum equivalent Amazon m3.xlarge – 15 GiB of memory, 13 EC2 Compute Units (8 virtual cores with 3.25 EC2 Compute Units each), EBS storage only, 64-bit platform - is assigned to the community. According to the applications selected in the Application Bundles that have to be offered to the community, the minimum configuration can grow up to 2 m3.2xlarge – 30 GiB of memory, 26 EC2 Compute

	Units (16 virtual cores with 3.25 EC2 Compute Units each), EBS storage only, 64-bit platform – resources that are reserved to the community. Additional resources can be assigned on-demand to scale up distributed computations and up to the negotiated quota as established in the negotiated phase between the Community Manager and the iMarine Infrastructure Manager.
Resources Highlights	Your data is kept private until you or any other authorized user shares it with either other users of the newly created applications or with the wider community. Only the members of the community use the computational resources assigned to it and the data is moved and stored according to an encryption key that is specific to the community.
How	Contact D4Science through the contact-point and report the description of the community, the average number of users, the scientific applications you wish to host in D4Science, and any additional information useful for a proper analysis of your request.
Type of engagement	You manage a medium/large set of users focusing on many scientific topics ranging from the analysis of statistical and biodiversity data to the management of geo-referenced data. The community needs a common infrastructure to store, maintain, and process data through the creation of focused applications (VREs), each of which is focusing on a specific scientific goal.
Cost	Negotiated. It depends on the QoS and the number of users of the community.

3.12 D4Science APIs: Useful Links

- Developers web site: to get information about a set of commonly used APIs:
  - https://dev.d4science.org/,
- Profile & Social Networking API: to get profile and user information or boost your content's reach by making it easy for people to share it on Virtual Research Environments (VREs)
  - https://dev.d4science.org/swagger/social-networking/
- Workspace (Storage Hub) API: to learn how to browse, upload and download user's workspace files and folders:
  - https://gcube.wiki.gcube-system.org/gcube/StorageHub_REST_API
- Metadata Catalogue (gCat) API: to learn how to publish and search collections of metadata for items including data, services, and related information objects:
  - https://wiki.gcube-system.org/gcube/GCat_Service
- Information System API: to learn how to interact with resources hosted in the Infrastructure and its Virtual Research Environments (VREs):
  - https://dev.d4science.org/swagger/registry/
- New Methods/Algorithms for DataMiner: to learn how to implement custom Methods and Algorithms for DataMiner:
  - https://wiki.gcube-system.org/gcube/Category:Statistical_Algorithms_Importer
- Supported languages for new Methods/Algorithms for DataMiner:

  - https://wiki.gcube-system.org/gcube/Statistical_Algorithms_Importer:_Create_Project
- DataMiner online interfaces
  - Web: https://wiki.gcube-system.org/gcube/DataMiner_Manager)
  - Web Processing service: https://www.opengeospatial.org/standards/wps
- DataMiner overview:
  - https://wiki.gcube-system.org/gcube/Data_Mining_Facilities.
- authorisation framework.
  - https://dev.d4science.org/authorization/
  - https://wiki.gcube-system.org/gcube/Authorization_Framework.
- Spatial Data Infrastructure capabilities
  - https://gcube.wiki.gcube-system.org/gcube/SDI-Service
  - https://gcube.wiki.gcube-system.org/gcube/Spatial_Data_Storage_and_Publishing
  - https://gcube.wiki.gcube-system.org/gcube/Spatial_Data_Discovery_and_Access.

To communicate with D4Science and to get additional information about Docker, ShinyApps, and third-parties services

  - https://support.d4science.org/

4 Integration aspects

In this chapter a number of integration aspects are considered, which are relevant for the interactions between the 2 main Blue Cloud components and for further federation of computing resources and algorithms. The Blue Cloud VRE will have its basis at the D4Science infrastructure, as operated by CNR-ISTI. But it should be possible to connect to other services than data at blue infrastructures and to e-infrastructures as part of the VRE and its Virtual Labs and to perform analyses in workflows which are divided over multiple platforms, with the Virtual Lab at D4Science in the director role.

4.1 Link from Data Discovery and Access service to VRE Data Pool

As described in Chapter 2 there is a data exchange planned between the Blue Cloud Data Discovery and Access service and the Blue Cloud Virtual Research Environment (VRE). In paragraph 2.4 this bridge is already detailed from the perspective of the Blue Cloud Data Cache that is to be developed and operated by EUDAT.

In this paragraph the bridge is considered from the perspective of Blue Cloud VRE that is operated by CNR-ISTI.

The VRE Data Pool will be based on the D4Science Shared Workspace, hereafter shortly named Workspace. The workspace is at the core of the D4Science infrastructure since, abstracting over several technologies, it offers a single space where to manage data and products either uploaded, shared, or generated in the VRE.

The Shared Workspace System provides an easy-to-use interface and APIs on top of a distributed, fault-tolerant, replicated, and secure cloud storage.

The Workspace provides a cloud storage file sharing service, supporting:

- Sharing of folders and files of different item types (ranging from binary files to information objects representing, for instance, tabular data, distribution maps, algorithms/methods);
- Publication of the items contained in a directory on the Catalogue;
- Distribution of the items contained in a directory via the THREDDS Server as well as their continuous and automatic synchronization with a THREDDS collection;
- Persistence of any computation results/output. The results are automatically saved and accompanied by provenance information as well as by the input files used to launch the computation.

The VRE Data pool will be manifested as a directory in the Workspace and the user will be able to use it as any other directory. Thus, she will be able to share content saved in that directory, to publish data in the Catalogue, to start computation using those data, etc.

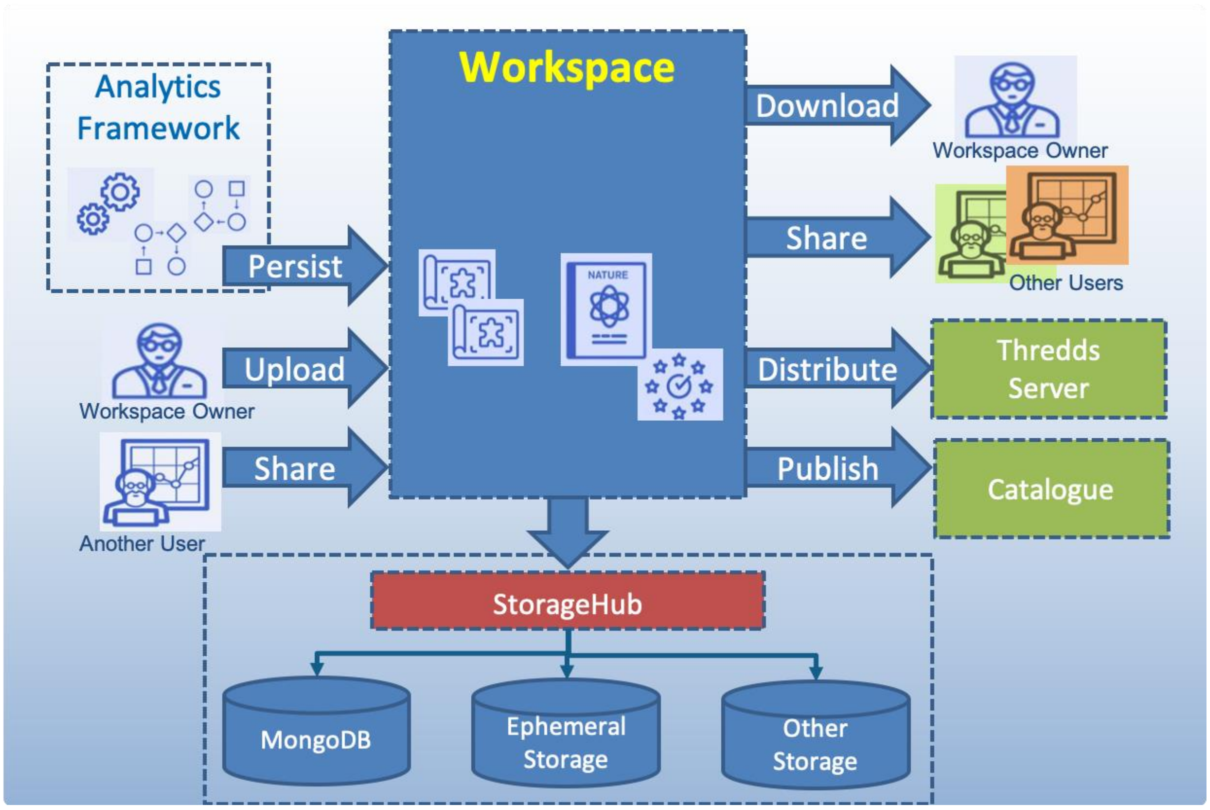


Figure 4.1: The Workspace

It is worth reporting that the Workspace uses versioning and versions automatically the stored items so that it is possible to refer and access any version of the item at any time using its persistent, unique, and web-accessible identifier (Persistent URL). This feature is exploited by the Analytics Framework to support reproducibility. The Analytics Platform generates a detailed provenance record for every analytics task executed by the platform, by reporting the Persistent URL to the version of the data specified as input parameters, the parameters of the execution, and any other metadata that would allow a user to reproduce and repeat the analytical task. This information is stored into the workspace and documented by a PROV-O-based accompanying record together with the data generated by the task.

The Workspace is accessible via the graphical user interface and via the StorageHub APIs (https://gcube.wiki.gcube-system.org/gcube/StorageHub_REST_API).

To exploit those APIs, a valid authorization token has to be used. In short, the APIs provide the following REST operations:

- **Retrieve WS**: to retrieve the user Workspace;
- **Folder Listing**: to list the content of a folder;
- **Retrieve VRE Folder**: to retrieve the VREFolder related to the token;
- **Find**: to find a file or a folder by name or pattern;
- **Delete**: to remove a file or a folder (including subfolders);
- **Download**: to download a file or a folder in ZIP format;
- **Get Public Link**: to get a public link of a file;

- **Create Folder**: to create a folder in the given parent folder;
- **Unzip**: to upload a zip file in a specific folder;
- **Upload file**: to upload a file in a folder.
- **Versions**: to get a specific version of a file.

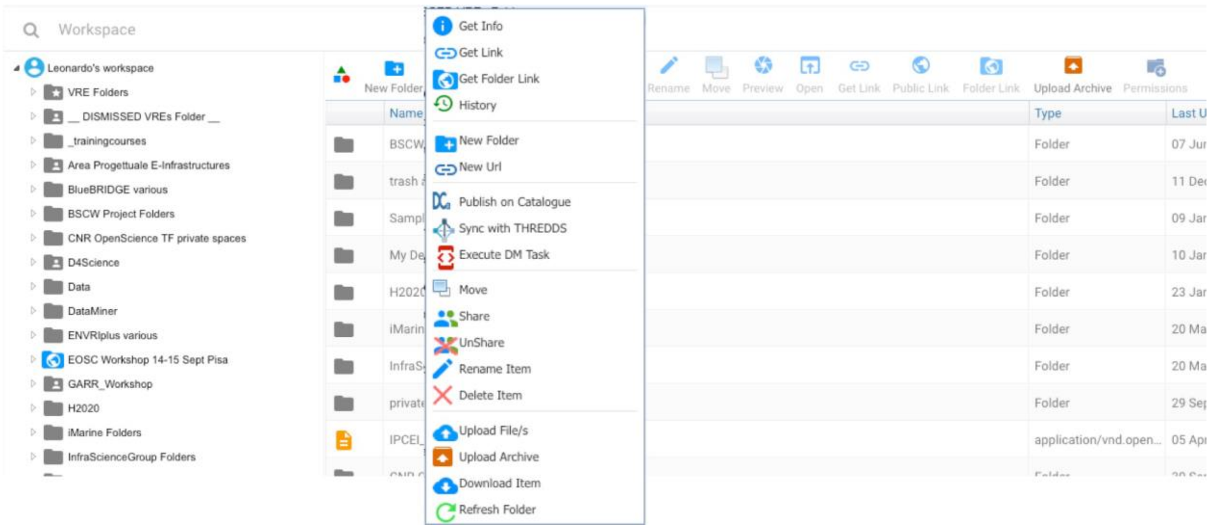


Figure 4.2: The Workspace Graphical User Interface

Authentication interoperability between systems

The D4Science token-based Authorization System is compliant with the Attribute-based access control (ABAC), which defines an access control paradigm whereby access rights are granted to users through the use of policies which combine attributes together. The D4Science token is a string generated on request by the Authorization service for identification purposes and associated with every entity belonging to D4Science (users or services). The token is passed in every call and is automatically propagated in the lower layers. It can be passed to a D4Science service in 3 ways:

- using the HTTP-header: adding the value ("gcube-token","{your-token}") to the header parameters;
- using the query-string: adding “gcube-token={your-token}” to the existing query-string;
- logging via the default WEB authentication shown by the browser using your username as username and your token as password.

A Blue Data Service is either a pre-existing service or a new one deployed and operated by an infrastructure different from D4Science that wishes to become interoperable with the Blue-Cloud VRE. Hence, any Blue Data Service needs to use a D4Science token to be able to identify the user identity, authorize the user request, and call any other D4Science service if needed.

There exist 2 types of D4Science tokens: User and Application token. The former is used by “humans” using the VRE whereas the latter is used by services/applications.

There are 3 possible approaches a Blue Data Service can adopt, they are depicted in the 3 scenarios present in Figure 4.3, each of these has pros and cons.

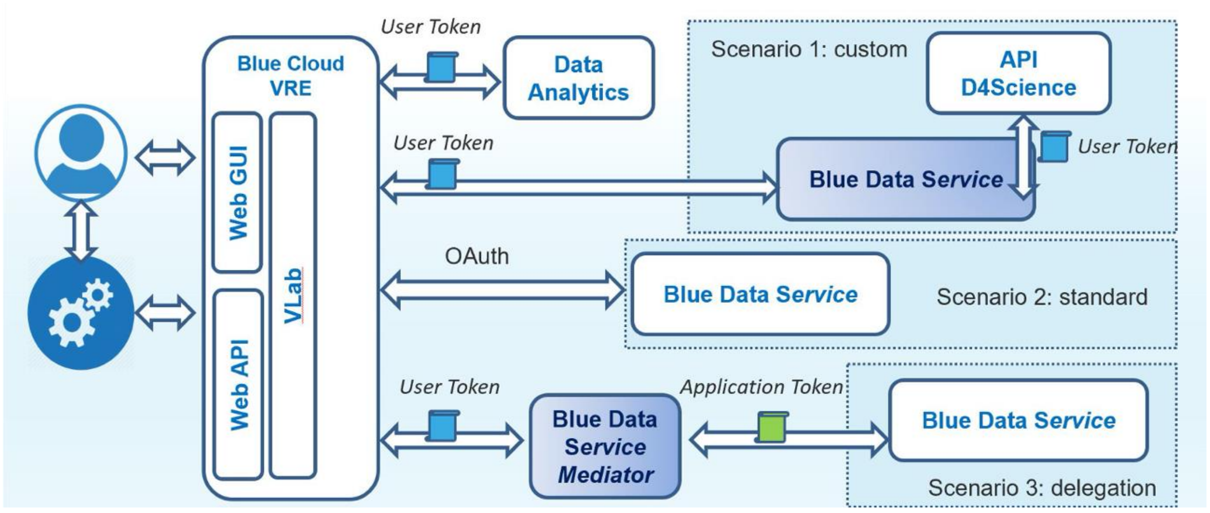


Figure 4.3: the supported Scenarios enabling interoperability across services

Pros and cons of each modality are:

1. **The custom modality:** requires that any Blue Data Service expects to receive a User Token as input parameter, this parameter can have any name (d4s-token in the example) and is added in the HTTP Query String whenever the Blue Data Service is called via HTTPS: eg https://mybluedataservice.eu/endpoint?d4s-token=**12345-abcd**
   In turn, the Blue Data Service uses this token to authenticate and resolve the user and the role associated by making a HTTP REST call to a given D4Science API[9] using the d4s-token received in the previous step.
   For instance, suppose that the token **12345-abcd** would belong to the user "Andrea Rossi" in the VLab named Blue-CloudLab, then the HTTPS REST call:

   https://api.d4science.org/rest/2/people/profile?gcube-token=**12345-abcd**

   Would return the following JSON:

```
{
 "success": true,
 "message": null,
 "result": {
  "roles": [VRE-Manager],
  "context": "/d4science.research-infrastructures.eu/D4OS/Blue-CloudLab",
  "avatar": "https://services.d4science.org/image?img_id=5567",
  "fullname": "Andrea Rossi",
  "username": "andrea.rossi"
```

[9] https://api.d4science.org/rest/2/people/profile

```
 }
}
```

PROS: Completely transparent to the end-users.
CONS: Blue Data Service needs to be slightly modified to become interoperable and this is not always possible.

See also API available at: https://dev.d4science.org

2. **The standard modality:** requires that any Blue Data Service is compliant with OAuth 2.0[10] and OpenID Connect. OAuth 2.0 is designed only for authorization, for granting access to data and features from one application to another. OpenID Connect[11] (OIDC) is a thin layer that sits on top of OAuth 2.0 that adds login and profile information about the person who is logged in. To this end each Blue Data Service is provided with a Client ID and a Client Secret, that only the Blue Data Service and the D4Science Authorization Server know. The user logs in on the Blue Data Service via her D4Science credentials, in turn, the Blue Data Service uses the access token returned by the OAuth/OpenID Connect flow to interact with any other D4Science service on behalf of the user.

   PROS: Blue Data Service may already be compliant with such standard and required no modification except for the configuration parameters.
   CONS: The user has to login a first time to exploit the Blue service;

3. **Delegation (Mediator) modality:** requires that any Blue Data Service is "proxied" by a specific mediator service (that may need to be implemented in some cases) capable of authorising the user request and mediate them by exploiting an application token, which in turn is used by the Blue Data Service to authorise the incoming request and may be used to call some, but not every, D4Science service. This modality is not recommended and could be used for specific (corner) cases.

   PROS: Easy to achieve for Blue data services not compliant with standards, few modifications required.
   CONS: Blue-Cloud Management costs, Blue Data Services authorise the VRE and not the users.

[10] https://www.oauth.com/

[11] https://openid.net/connect/

Blue Cloud System monitoring

Monitoring of the availability and performance of the Blue Cloud system and its components is needed to get insight in its performance.

In paragraph 3.2.2 it is already explained how Nagios is used in the D4Science infrastructure for monitoring availability (uptime) of the VRE and its services. It is reported that for technologies developed both by D4Science and by the exploited framework, i.e. gCube and D-Net, specific add-ons have been designed, implemented, and installed to extend monitoring and native alerting functionality in order to have a fully-complete and always up-to-date image of the status of the D4Science e-infrastructure.

In the Blue Cloud Architecture this set of add-ons will be extended to add any Blue Cloud service that will be exploited in the Blue Cloud VRE. To do so, it will be requested to any of these Blue Cloud services a web service endpoint that can be invoked to monitor the service availability and possibly another web service endpoint that can be invoked to monitor the service reliability.

In Chapter 3 about D4Science, in several paragraphs also auditing software components were described. This set of components allows to record, summarize and classify service invocations and other events, e.g. storage of data, access to the Workspace, usage of the Catalogue, etc.

The following set of indicators are currently collected and made available. This is done by means of two dashboards accessible for the Blue Cloud VRE managers: the Accounting Dashboard and the DataStudio Dashboard.

Accounting Dashboard

The **Accounting Dashboard** allows analysing the exploitation of the different services offered by the Blue Cloud VRE. This analysis can be performed either at Blue Cloud VRE level or at the level of each hosted Virtual Laboratory. Several measures and indicators can be monitored in this way across time. The data are aggregated by month. There are five measures: Accesses, Catalogue, Method Invocation, Social Interactions, and Users. Each measure then offers several indicators that are accessible both at Blue Cloud VRE level and Virtual Laboratory level.

The Accesses measure includes the following indicators:

- Access to any Virtual Laboratory;
- Access to the Workspace;
- Access to the Message;
- Access to Notification settings;
- Access to the User Profile;
- Access to the Catalogue.

The Catalogue measure includes the following indicators:

- Download of a manifestation associated with an item published in the catalogue;
- Access to the item metadata;
- Queries performed in the catalogue.

The Method Invocation measure includes just one indicator:

- Method invocation, i.e. number of jobs executed in the Blue-Cloud VRE.

The Social Interactions measure includes the following indicators:

- Posts
- Replies
- Likes

The User measure include just one indicator

- Users, i.e. number of users registered/unregistered to/from the Blue-Cloud VRE.

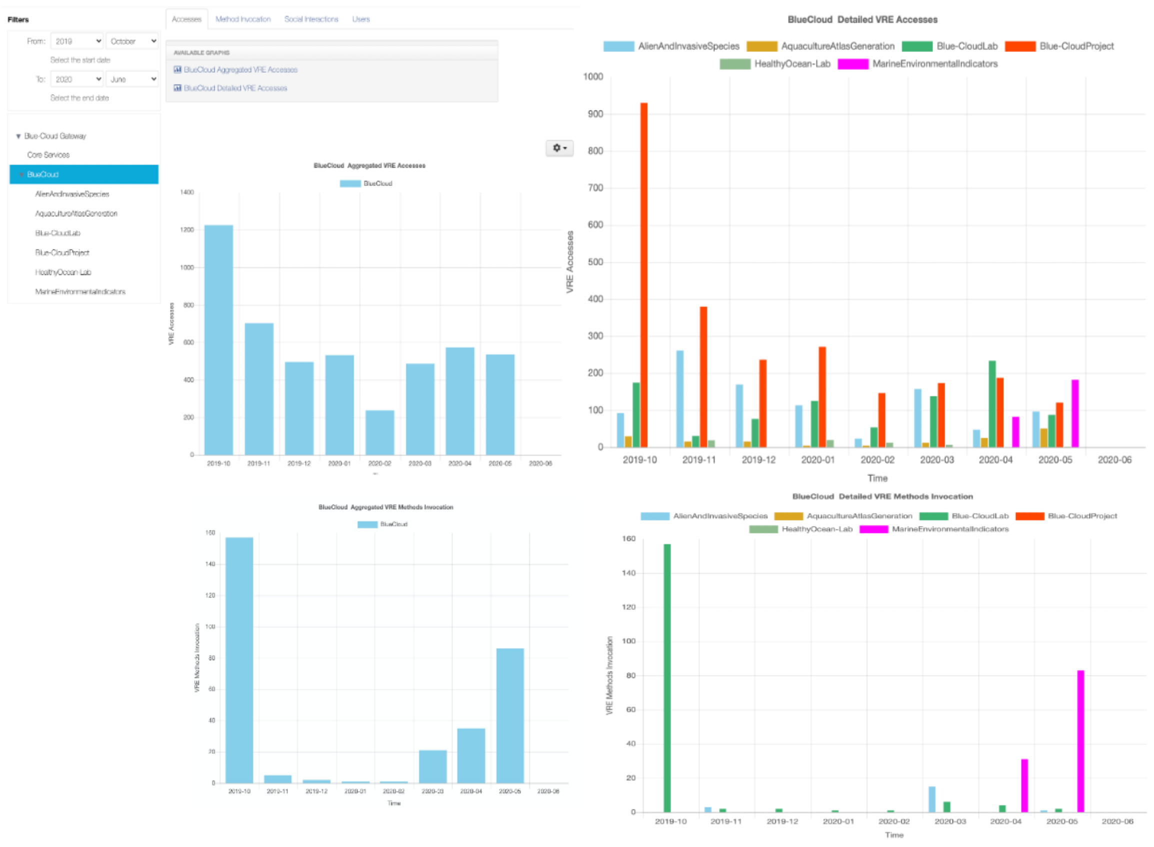


Figure 4.4: Accounting dashboard

The Accounting Dashboard can be extended with additional accounting data plugins. Each plugin has to define the measure and the indicators and it has to report data monthly aggregated. This mechanism will be exploited to add specific measures for the Blue Cloud services.

DataStudio Dashboard

The **DataStudio Dashboard** is realized exploiting Google Analytics and Google Data Studio. It can be used to analyse the exploitation of the Blue-Cloud VRE in terms of web accesses, geographically distribution of the accesses, web sessions and their average duration. Any Blue Cloud service may contribute to the DataStudio Dashboard by specifying the Google Accounting ID defined for Blue Cloud VRE.

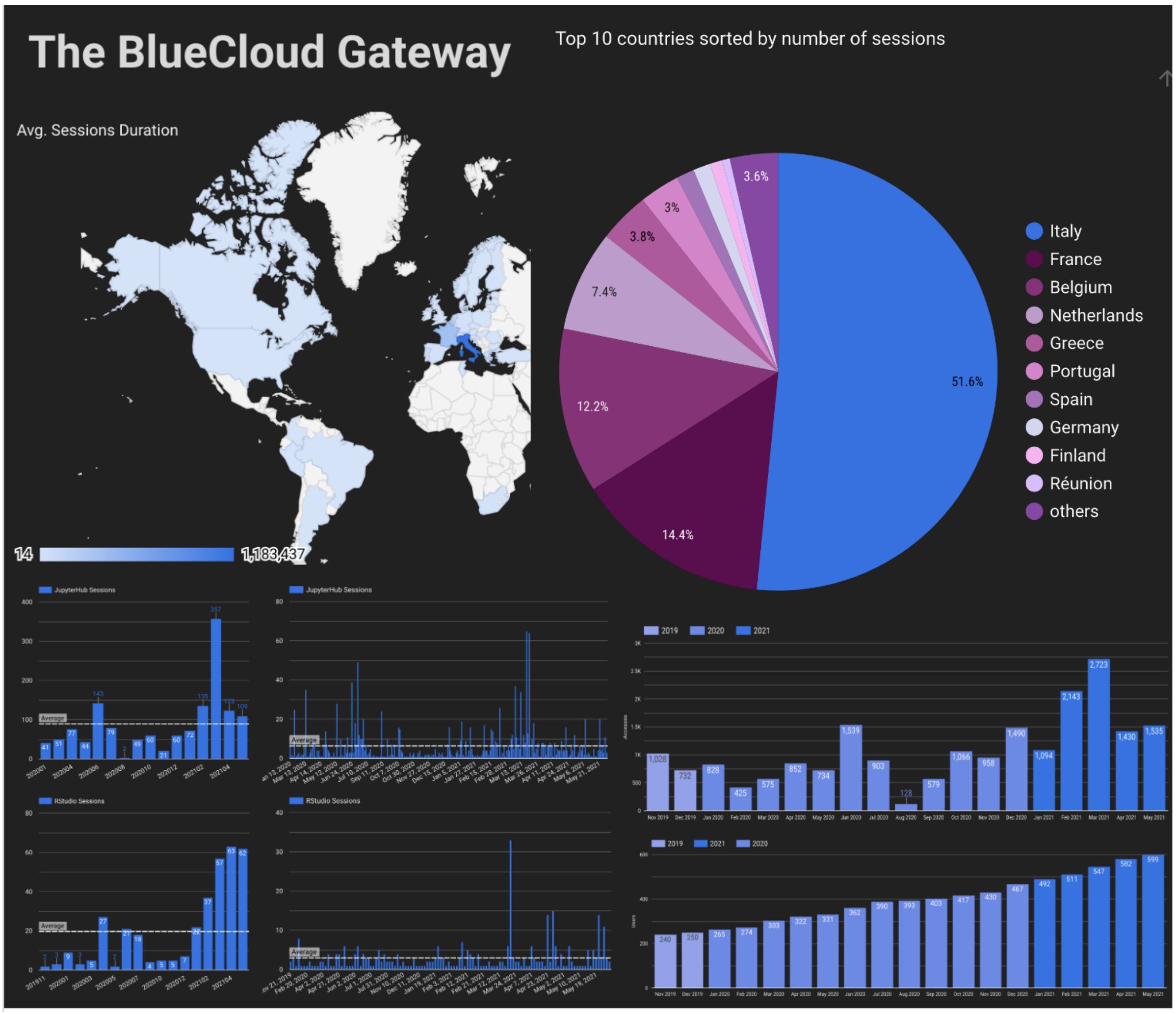


Figure 4.5: DataStudio dashboard

References

[1] Assante, M., Candela, L., Castelli, D., Cirillo, R., Coro, C., Frosini, L., Lelii, L., Mangiacrapa, F., Pagano, P., Panichi, G., Sinibaldi, F. (2019) **Enacting open science by D4Science**, Future Generation Computer System DOI: 10.1016/j.future.2019.05.063

[2] Assante, M., Candela, L., Castelli, D., Cirillo, R., Coro, G., Frosini, L., Lelii, L., Mangiacrapa, F., Marioli, V., Pagano, P., Panichi, G., Perciante, C., Sinibaldi, F. **The gCube System: Delivering Virtual Research Environments as-a-Service**. Future Generation Computer Systems (Vol. 95) DOI: 10.1016/j.future.2018.10.035

[3] Candela, L., Castelli, D., Pagano, P. (2013) **Virtual Research Environments: An Overview and a Research Agenda**. Data Science Journal, Vol. 12 DOI: 10.2481/dsj.GRDI-013

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[5] Wilkinson, M., Dumontier, M., Aalbersberg, I. et al. (2016) **The FAIR Guiding Principles for scientific data management and stewardship**. Sci Data 3, 160018 (2016). DOI: 10.1038/sdata.2016.18

Annex 1 EUDAT Collaborative Data Infrastructure

EUDAT has developed a service stack that forms the Collaborative Data Infrastructure (CDI). The services are as follows:

- B2SAFE, Replicate Research Data Safely.
- B2STAGE, Get Data to Computation.
- B2FIND, Find Research Data.
- B2SHARE, Store, Share and Publish Research Data.
- B2DROP, Sync and Exchange Research Data.

In addition, a set of EUDAT core operational services, essential for the management of the CDI have been defined as follows:

- B2ACCESS (identity and authorisation), easy-to-use and secure Authentication and Authorisation platform.
- B2HANDLE (Persistent IDentification (PID) management), a service to register persistent identifiers called Handles to data objects and retrieve data objects via these identifiers, serving a purpose similar to DOIs for papers.
- B2HOST, a Service Hosting Framework that allows communities to deploy and operate their own applications and data-oriented services on machines next to the data storage.

Most of these components are depicted in Figure 1 and described in more detail below

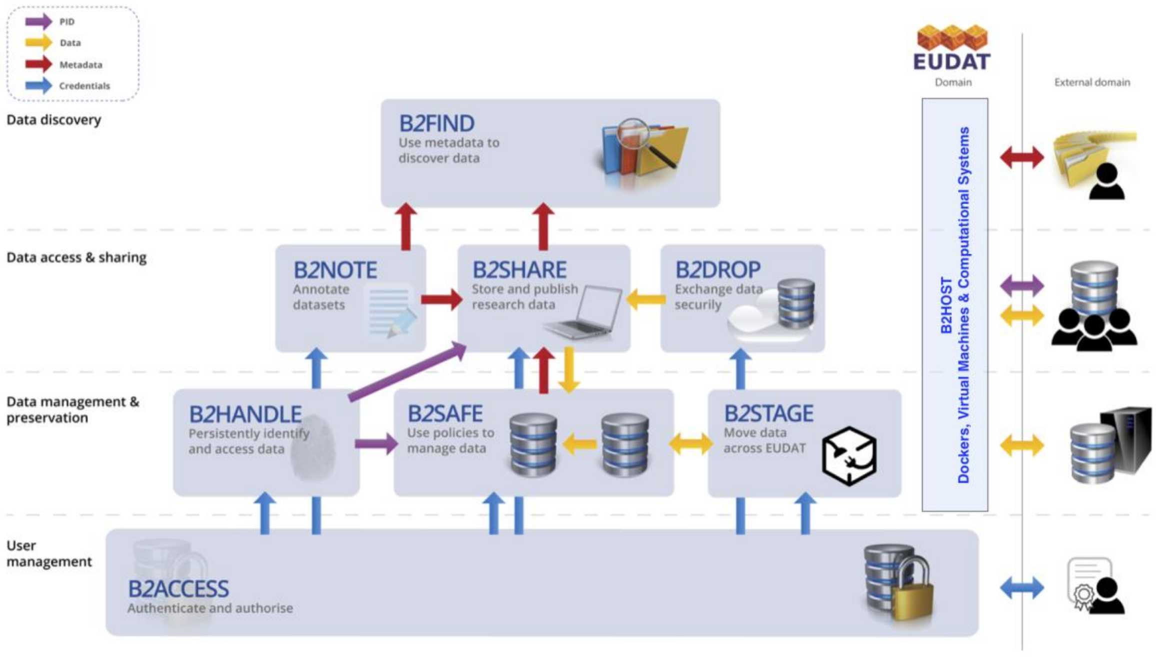
PID
Data
Metadata
Credentials
Data discovery
Data access & sharing
Data management & preservation
User management
B2FIND
Use metadata to discover data
B2NOTE
Annotate datasets
B2SHARE
Store and publish research data
B2DROP
Exchange data securily
B2HANDLE
Persistently identify and access data
B2SAFE
Use policies to manage data
B2STAGE
Move data across EUDAT
B2ACCESS
Authenticate and authorise
EUDAT
Domain
External domain
B2HOST
Dockers, Virtual Machines & Computational Systems

Figure 1: EUDAT Collaborative Data Infrastructure Services Suite & Architecture

B2ACCESS

B2ACCESS is an easy-to-use and secure Authentication and Authorization platform developed by EUDAT. B2ACCESS is versatile and can be integrated with a wide range of services. When integrated with a given service, the user may log in by using different authentication methods like, Home organisation identity provider, Google account, EUDAT ID.

EUDAT IDs are created by the B2ACCESS upon registration. Therefore, B2ACCESS is an Identity Provider for the users that do not have neither a Google account nor a Home Organisational Identity.

B2ACCESS offers also the tool for the managements of the EUDAT IDs and contain the following features:

- Support for personal certificates to support eduGAIN, Social Identities (Facebook, Google, Microsoft, Gitlab), ORCID and local accounts
- IdP support for SAML, OpenID, OAuth2, X.509
- SP support for SAML, OIDC, OAuth2, X.509
- Supports several methods of authentication via the users' primary identity providers (OpenID, SAML, OAuth2, X.509)
- Integrated services: B2SHARE, B2SAFE, B2STAGE, B2DROP, B2NOTE, GEF, SPMT, DPMT, Confluence wiki, Gitlab
- Allows group-, community- and service managers to specify authorisation decisions.

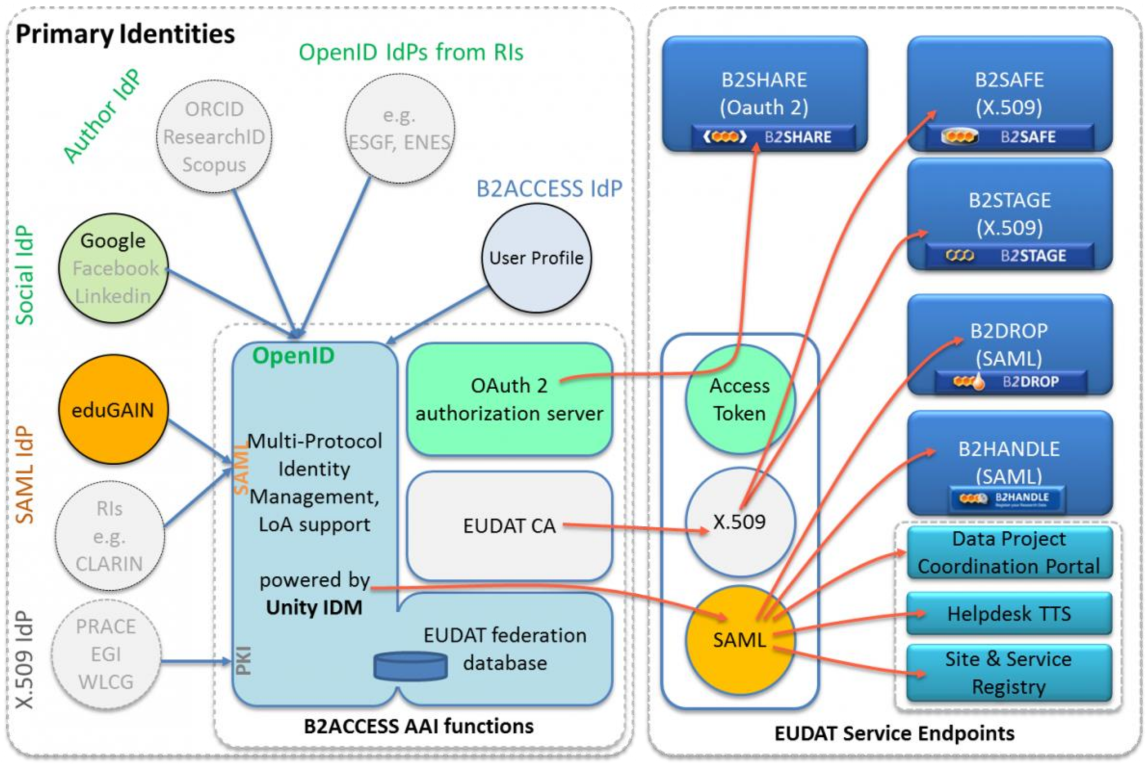

Figure 2: B2ACCESS Components & Architecture

B2SAFE

B2SAFE is a robust, safe and highly available service that allows both community and departmental repositories to implement in a trustworthy manner sets of data management policies across multiple administrative domains.

B2SAFE is a solution intended for:

- Provide an abstraction layer to virtualize large-scale data resources
- Guard against data loss in long-term archiving and preservation
- Optimize access for users from different regions
- Bring data closer to powerful computers for compute-intensive analysis

B2SAFE features:

- Based on the execution of auditable data policy rules and the use of persistent identifiers (PIDs)
- Respects the rights of the data owners to define the access rights for their data and to decide how and when it is made publicly referenceable
- Able to aggregate data from different disciplines into a storage system of trustworthy and capable data service providers
- Support for repository packages (e.g. DSPACE, FEDORA) and a lightweight HTTP-based solution
- Support metadata
- Optimize and extend policies to support data curation and provenance
- Support authorization on basis of community access rules
- Integration with other EUDAT services

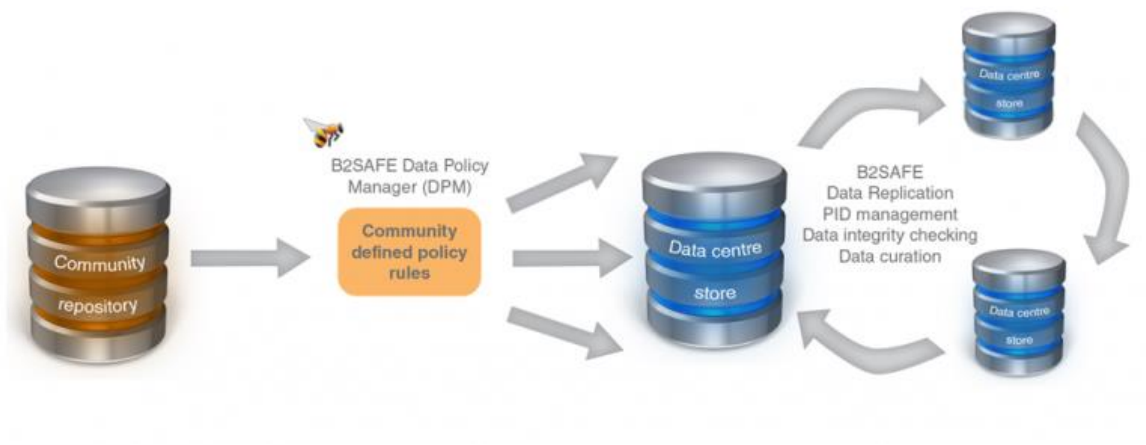

Figure 3: B2SAFE Process & Architecture

B2STAGE

B2STAGE is a reliable, efficient, light-weight and easy-to-use service to transfer research data sets between EUDAT storage resources and high-performance computing (HPC) workspaces.

The service allows users to:

- Transfer large data collections from EUDAT storages to external HPC facilities for processing
- In conjunction with B2SAFE, replicate community data sets, ingesting them onto EUDAT storage resources for long-term preservation
- Ingest computation results into the EUDAT infrastructure
- Access data through a RESTful HTTP interface

B2STAGE features:

- An extension of the B2SAFE and B2FIND services, which allow users to store, preserve and find data
- Data-staging script facilitates staging, ingestion and retrieval of persistent identifier (PID) information of transferred data
- users negotiate access to remote HPC services in parallel
- Collaboration with other infrastructures, such as the European Grid Infrastructure (EGI) and Partnership for Advanced Computing in Europe (PRACE)
- Support GridFTP protocol
- Furthermore, B2STAGE implements a set of Restful HTTP-APIs by adopting an extensible framework used as a basis for the development of community-tailored HTTP-APIs

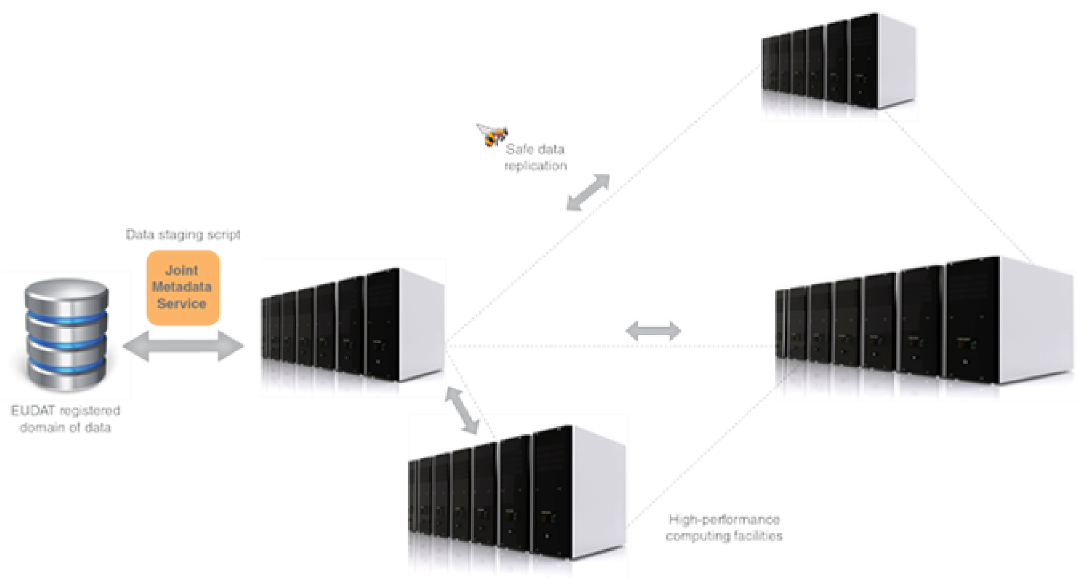
Safe data replication
Data staging script
Joint Metadata Service
EUDAT registered domain of data
High-performance computing facilities

Figure 4: B2STAGE Process

B2HANDLE

B2HANDLE enables EUDAT services and user communities to assign Persistent Identifiers (PIDs) to different kinds of managed objects stored in the EUDAT CDI.

PIDs are used in EUDAT to reliably identify and cite data objects over a long period of time and it is thus a vital part of long-term data management.

The underlying technology of B2HANDLE is based on the Handle System, which is a reliable, redundant and scalable system built on top of an open architecture. B2HANDLE is mostly transparent to the end-users, especially shielding them from the complexity of infrastructure details.

B2HANDLE is a distributed service, with the organisations hosting the service mirroring each other's Persistent Identifiers, thus ensuring the sustainability and reliability of PIDs in the EUDAT domain.

B2HANDLE Features include:

- Follows policies to register data and make it long term referable and citable
- Reliability through mutual PID mirroring
- Provides abstraction layer between a globally unique persistent identifier and physical location of data objects
- Machine readable via HTTP RESTful API

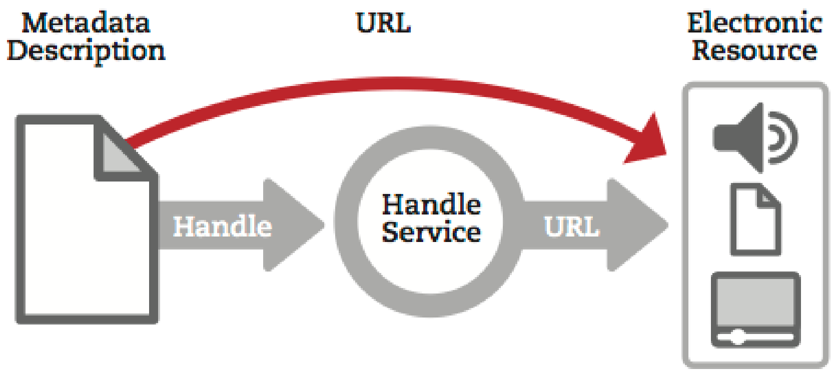

Figure 5: B2HANDLE System

B2SHARE

B2SHARE is a user-friendly, reliable and trustworthy way for researchers, scientific communities and citizen scientists to store, publish and share small-scale research data from diverse contexts.

A formidable solution to:

- Store registered research data (incl. software) and add domain meta data
- Preserve (small-scale) research data for long-term
- Share: allows data, results or ideas to be shared worldwide

B2SHARE features

- Integrated with the EUDAT collaborative data infrastructure
- Free upload and registration of stable research data
- Data assigned a permanent identifier, which can be retraced to the data owner
- Data owner defines access policy
- Community-specific metadata extensions and user interfaces
- Openly accessible and harvestable metadata
- Representational state transfer application programming interface (REST API) for integration with community sites
- Data integrity ensured by checksum during data ingest
- Professionally managed storage service – no need to worry about hardware or network
- Monitoring of availability and use

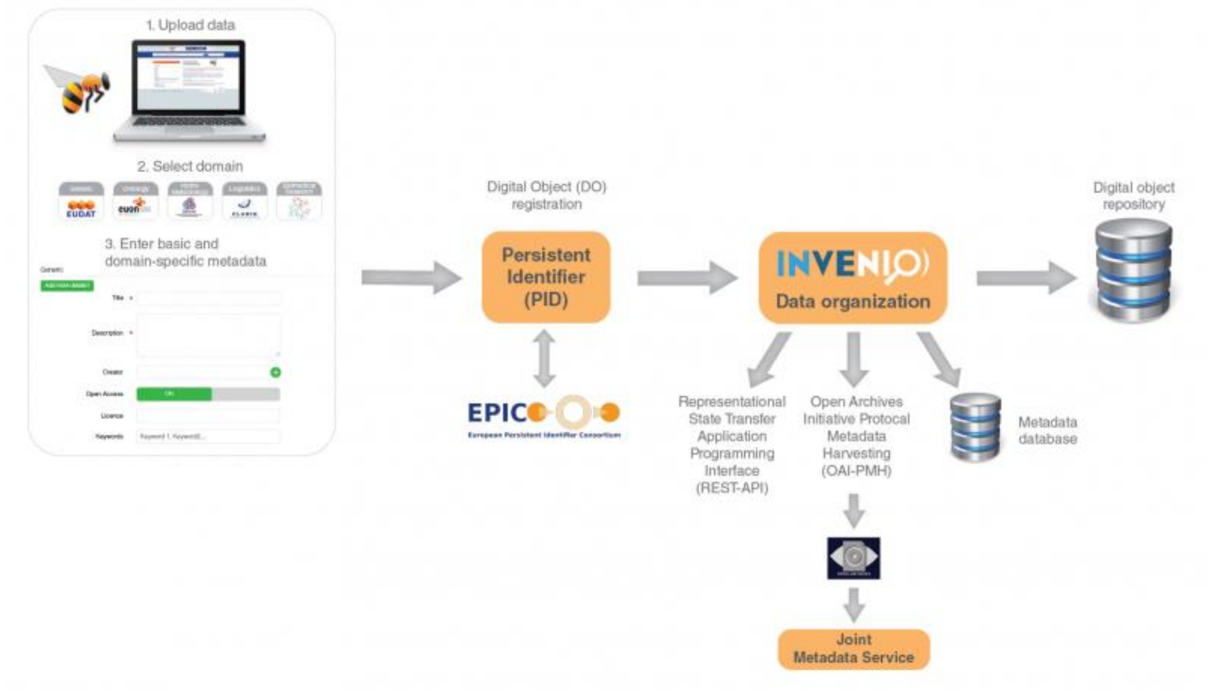
1. Upload data
2. Select domain
3. Enter basic and domain-specific metadata
Digital Object (DO) registration
Persistent Identifier (PID)
EPIC
European Persistent Identifier Consortium
INVENIO
Data organization
Digital object repository
Representational State Transfer Application Programming Interface (REST-API)
Open Archives Initiative Protocol Metadata Harvesting (OAI-PMH)
Metadata database
Joint Metadata Service

Figure 6: B2SHARE Architecture

B2NOTE

B2Note allows easily creating, searching and managing annotations. An annotation is a keyword or commentary attached to a data object (data collection, file) that explains or classifies it. B2NOTE is a standalone service for annotating data content hosted within the EUDAT CDI.

There exist three types of annotations in B2Note

- The semantic tag, a keyword from an ontology (a semantic tag coming from identified ontology repositories - currently only Bioportal
- The free-text keyword, to be created and used when a specific semantic term is not found
- The comment, a more comprehensive annotation

B2NOTE Features;

- Creation RDF triples
- Harvests information from ontology repositories
- Supports semi-automatic annotation using text mining
- Supports manual data annotation
- Easy to use user interface
- Integrated in B2Share: access files with B2Share, then annotate them with B2Note.
- Annotations are created and stored in a machine-readable format using the W3C Web Annotation model
- Annotations are searchable (in opposite to hand-written annotations).

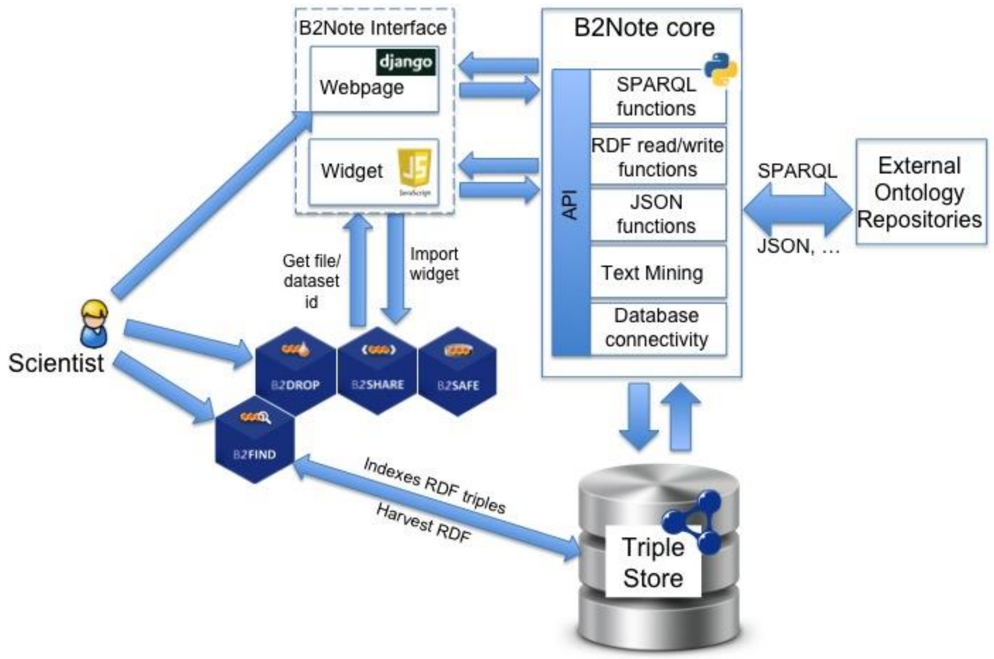

Figure 7: B2NOTE Components & Architecture

B2DROP

B2DROP is a secure and trusted data exchange service for researchers and scientists to keep their research data synchronized and up-to-date and to exchange with other researchers.

The service is simple to use and open to all researchers, scientists, communities alike to synchronise and exchange data with one or multiple users. B2DROP will be fully integrated with the B2 suite of services to allow user-friendly data sharing.

An ideal solution to:

- store and exchange data with colleagues and team members,
- synchronise multiple versions of data,
- ensure automatic desktop synchronisation of large files.

B2DROP Features

- Cloud Storage Federation, collaboration with GEANT in OpenCloudMesh
- B2DROP as a workspace area to computing facilities
- Integration with EUDAT CDI (e.g. B2SHARE)

Users can:

- Define with whom to exchange data, for how long and how
- Are offered up to 20GB of storage space for research data
- Access and manage permissions to files from any device and any location.

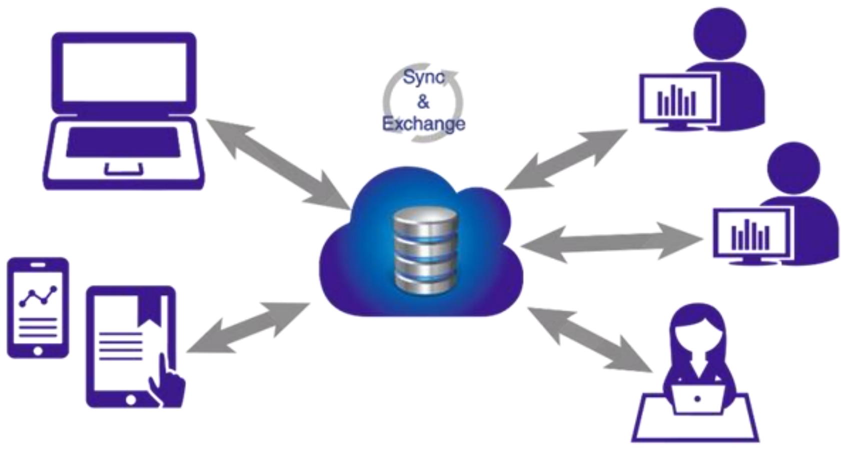

Figure 8: B2DROP

B2HOST

The EUDAT Collaborative Data Infrastructure offers a Service Hosting Framework called B2HOST that allows communities to deploy and operate their own applications and data-oriented services on machines next to the data storage location. Reasons for such services next to the data can be:

- Volume of the data is too large to be transferred efficiently on demand to third party data processing and analysis facilities
- Licensing restrictions that prevent even the smallest volume of data from being copied to a third party which provides the compute facilities.

In both cases, the use of B2HOST allows for the data to remain local, with a (community-specific) service interfacing between the data and external clients.

Resource providers within EUDAT offer service hosting capabilities in tandem with their storage service. These provide access to resources such as bare-metal or virtualized machines with basic execution system platforms (operating systems with a selection of software, tools and libraries). The only allowable use of these resources is for EUDAT communities to deploy and operate data-oriented services hosted at specific data centres. Community service managers can request the appropriate resources through B2HOST. Community service managers can also offer resources and join B2HOST.