D4.6 Blue Cloud VRE Operation Report (Release 2)

Work Package	WP4, Developing and operating the Blue Cloud VRE, its services and Virtual Labs
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0.5	06/10/2022	Trust-IT	Review and suggestions
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1.0	20/10/2022	CNR	Review and suggestions analysed and managed

Table of Contents

Table of Figures

Table of Tables

Executive summary

The Blue-Cloud project developed a cyber platform bringing together and providing access to multidisciplinary data from observations and models, analytical tools, and computing facilities essential to support research to better understand and manage the many aspects of ocean sustainability. The Blue-Cloud platform architecture consists of two major families of components: (a) the *Blue Cloud Data Discovery and Access* service to serve federated discovery and access to 'blue data' infrastructures, and (b) the *Blue Cloud Virtual Research Environment (VRE)* to provide a Blue Cloud VRE as a federation of computing platforms and analytical services.

This Deliverable D4.6 "Blue Cloud VRE Operation (Release 2)" is the revised and updated version of the D4.1 "Blue Cloud VRE Operation (Release 1)" [10]. It reports on the Blue-Cloud Virtual Research Environment (VRE) by complementing the architecture and infrastructure described in [9], where the constituents have been discussed. Specifically, 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.

9 Blue-Cloud VLabs were created and operated in the first period, while an additional 5 Blue-Cloud VLabs were created and operated in the second reporting period, from M17 (February 2021) to M35 (September 2022), bringing the total on 14 operational VLabs. Two VLabs of the second reporting period are specifically conceived to support the developments of the Blue-Cloud Demonstrators: *(i)* **The Plankton Genomics VLab** has been developed in the context of the Demonstrator #2, and *(ii)* **The Marine Environmental Indicators Dev VLab** has been developed in the context of the Demonstrator #3 - Marine Environmental Indicators. In order to support the Blue-Cloud Hackathon[1] event held in February 2022 the *(iii)* **Blue-Cloud Hackathon VLab** has been developed. Finally, in the framework of the Blue-Cloud synergies programme two additional VLabs were developed as pilots to support the work of *(iv)* the **JERICO-CORE** multi-platform research infrastructure dedicated to a holistic appraisal of coastal marine system changes, and *(v)* the **JONAS initiative**, addressing the issue of underwater noise in the Atlantic Seas.

These working environments are serving more than 1,300 users in total spread across more than 20 countries. Up to mid of September 2022, a total of more than 25,700 working sessions have been executed, with an average of 1,286 working sessions per month since the start of the Blue-Cloud project in October 2019. A total of more than 2,230 analytics sessions have been executed by the users of the VLabs, with an average of 55 working sessions per month.

From M17 (February 2021) to M35 (September 2022), a total of 212 tickets have been created and managed in the Blue-Cloud Project Issue Trackers (85% have been closed). Moreover, 34 tickets related to Blue-Cloud have been created in the D4Science overall context (88% have been closed).

[1] Blue-Cloud Hackathon: https://blue-cloud.org/events/blue-cloud-hackathon

1. Introduction

The Blue Cloud Architecture [8][9] consists of two major families of components:

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

The Blue-Cloud Virtual Research Environment components range from services to promote collaboration among its users to services supporting the execution of analytics tasks embedded in a distributed computing infrastructure and services enabling the co-creation of entire Virtual Laboratories [4]. This part of the overall Blue Cloud platform is built on the D4Science infrastructure and the gCube open-source technology [1][2] and deployed in the Blue Cloud gateway (accessible at https://blue-cloud.d4science.org) to make the services and Virtual Laboratories available.

The Blue Cloud platform development is driven by the needs and requirements underlying the development of selected demonstrators [6]. An up-to-date picture of the development of the demonstrators is described in [7]. In reality, this is the result of a co-creation approach in VLab development [4]. The co-creation process, when exploited to promote the development of VLabs, suggests following a participatory process where the activities of software developers and service providers are intertwined with the activities of the VLab designated community that bring specific value to the VLab. In fact, VLabs consists of two complementary parts: a) the *community-agnostic part*, i.e., services offering basic or advanced functionality exposing a common behaviour when instantiated in diverse contexts; b) the *community-specific part*, i.e., services offering a peculiar functionality or data, sometimes implemented by combining into specific workflows the community-agnostic part with context-specific services or data. The collaborative and participatory development of these two parts makes possible for (a) community-agnostic software developers and service providers to incrementally develop solutions matching the needs of diverse communities by promptly testing them in real usage scenarios; (b) VLab designated community members to actively contribute to the incremental development of the VLab by bringing in their peculiarity and diversity.

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 from M17 (February 2021) to M35 (September 2022).

The deliverable maintains the structure of the previous release (D4.1, Release 1) and it is organised as follows. Section 0 describes the policies and procedures governing the planning and deployment of Virtual Laboratories. Section 3 reports several indicators on the operation of the VRE and VLabs, their users and uses. Section 4 describes the Virtual Laboratories that have been deployed and operated during the period and reports on their usage statistics. For each Virtual Laboratory, the deliverable describes the goal and the main facilities offered to their users. Section 5 concludes the report by describing some concluding remarks.

2. Blue-Cloud VRE and VLabs Planning and Procedures

The Blue-Cloud VRE is built on the D4Science infrastructure and the gCube open-source technology [2019a, 2019b]. From the end-user point of view, the Blue Cloud services and Virtual Laboratories are accessible through the Blue Cloud gateway (https://blue-cloud.d4science.org).

The development of the Blue-Cloud VRE counts on the availability of new versions of the enabling technology that are made available by https://code-repo.d4science.org/gCubeCI/gCubeReleases. These versions are produced by taking into account the requirements (with the relative priority) formulated by the Blue-Cloud community via the specification of the demonstrators [2020c, 2020d] that might correspond to new facilities to be developed or request for enhancements of existing facilities as well as requests for resolving malfunctions.

The technology supporting the development of the Blue-Cloud VRE for the second reporting period (M17 to M35) was included in the following 14 gCube open-source software releases that have been deployed into the D4Science production infrastructure powering the VRE: 5.0 (Feb. 2021), 5.1 (Mar. 2021), 5.2 (May. 2021), 5.3 (June. 2021), 5.4 (Aug. 2021), 5.5 (Oct. 2021), 5.6 (Nov 2021), 5.7 (Jan. 2022), 5.8 (Mar. 2022), 5.9 (Mar. 2022), 5.10 (Apr. 2022), 5.11 (May. 2022), 5.13 (Jul. 2022), and 5.13.1 (Sep. 2022).

All the requests are modelled and managed by an issue tracker operated by D4Science and available at https://support.d4science.org, created and configured for users to create tickets for tasks, requests for support, incidents, VLabs creation, etc. An additional Blue-Cloud issue tracker has been created in the second reporting period as a Blue-Cloud public Support Service[2] open not only to the project members but also to the Blue-Cloud community at large, i.e., Hackathon participants, partners in synergy projects, students and any practitioner interested in the Blue-Cloud technology.

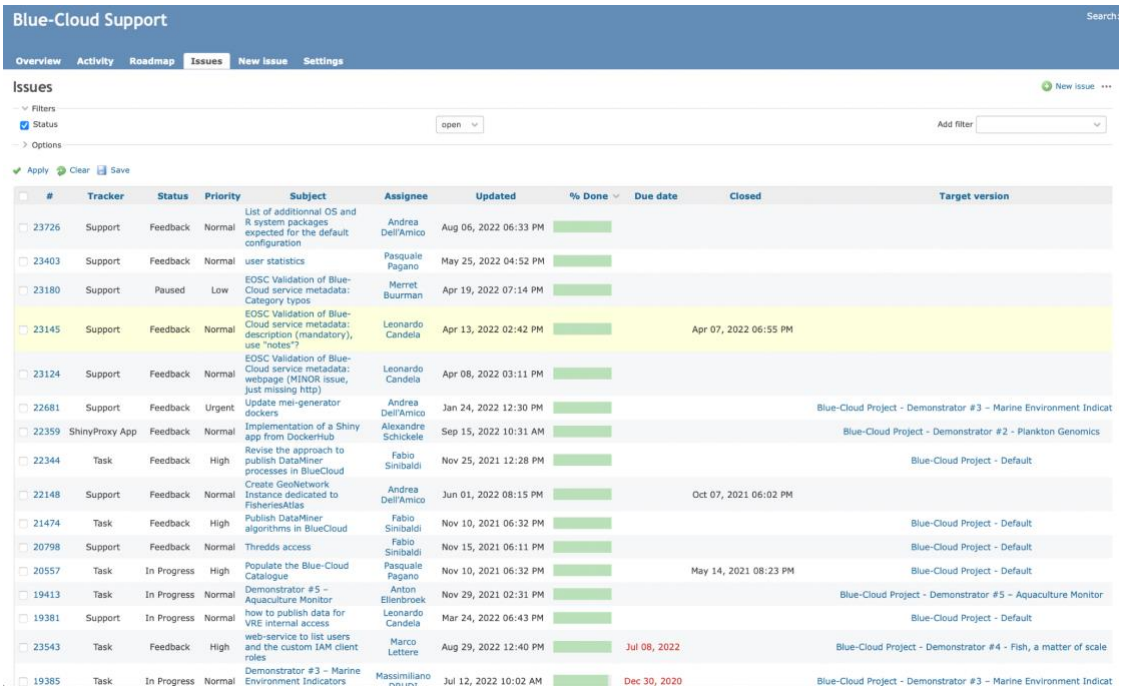

Figure 1. A screenshot of the Blue-Cloud Support issue tracker

[2] https://support.d4science.org/projects/blue-cloud-support

2.1. Procedures

Deployment and operation of VLabs is a collaborative effort involving the WP4 team called to deploy and configure the technology and to create VLabs expected by the work package working to jointly develop and onboard their technology, i.e., WP3.

The procedure leading to VRE and VLabs deployment is a consolidated one; it is the procedure inherited from the D4Science infrastructure and described in the D4Science Wiki:

https://wiki.d4science.org/index.php?title=Virtual_Research_Environments_Deployment_and_Operation

For the needs of Blue-Cloud, it was decided to support this activity by the project activity tracker. A specific VRE tracker has been created with the goal of capturing the entire process from specification to operation. The specification of the VRE/VLab is produced by the VRE/VLab designer/requester. This specification must contain:

- VLab name and abstract;
- Membership policy, i.e., whether the VLab is open or restricted, who is allowed to invite members; VRE expected datasets;
- VLab expected functionalities;
- VLab due date;

The following statuses are supported:

- ***Planned***: the WP4 team is fine with the specification, i.e., the specification contains enough details to proceed with the creation, and acknowledges that the creation of the VLab is feasible by the due date initially requested (or liaise with the designer/requester to find a mutually suitable date);
- ***Available***: the VLab is up and running and ready to be validated by the user designer/requester;
- ***Released***: the VLab has been validated, and the target community can start using it;
- ***Removed***: the VLab has been disposed as for the request of its manager;
- ***Rejected***: the requested VLab cannot be created as the requirements outlined for it cannot be satisfied.

3. Blue-Cloud VRE and VLabs Creation, Deployment, and Operation

This section briefly describes the facilities used by VLab creators for the actual deployment of VLabs, reports the complete list of deployed and operated VLabs, and offers a characterisation of each available VLab.

The act of definition and deployment of a new VLab is supported by a wizard (cf. Figure 2) that enables authorised users to transform the opened requests according to the procedure described in Chapter 2 into an actual specification and then, automatically, into a working VLab made available by the Blue-Cloud gateway. Through the wizard, the user is requested to specify: (i) the descriptive information characterising the expected VLab (i.e., name, description, duration), and (ii) the functionalities and datasets to be made available in the specific VLab by selecting among the available ones. The resulting list of functionalities is derived from the feasible functionalities created thanks to the software version and services hosted by the underlying infrastructure.

During the second reporting period the VRE Definition wizard was enhanced with the capability of setting up the JupyterHub cluster. Specifically at definition time it is possible to select the server option(s), in terms of libraries, memory and number of CPUs needed, for the newly created VLab as shown in Figure 2.

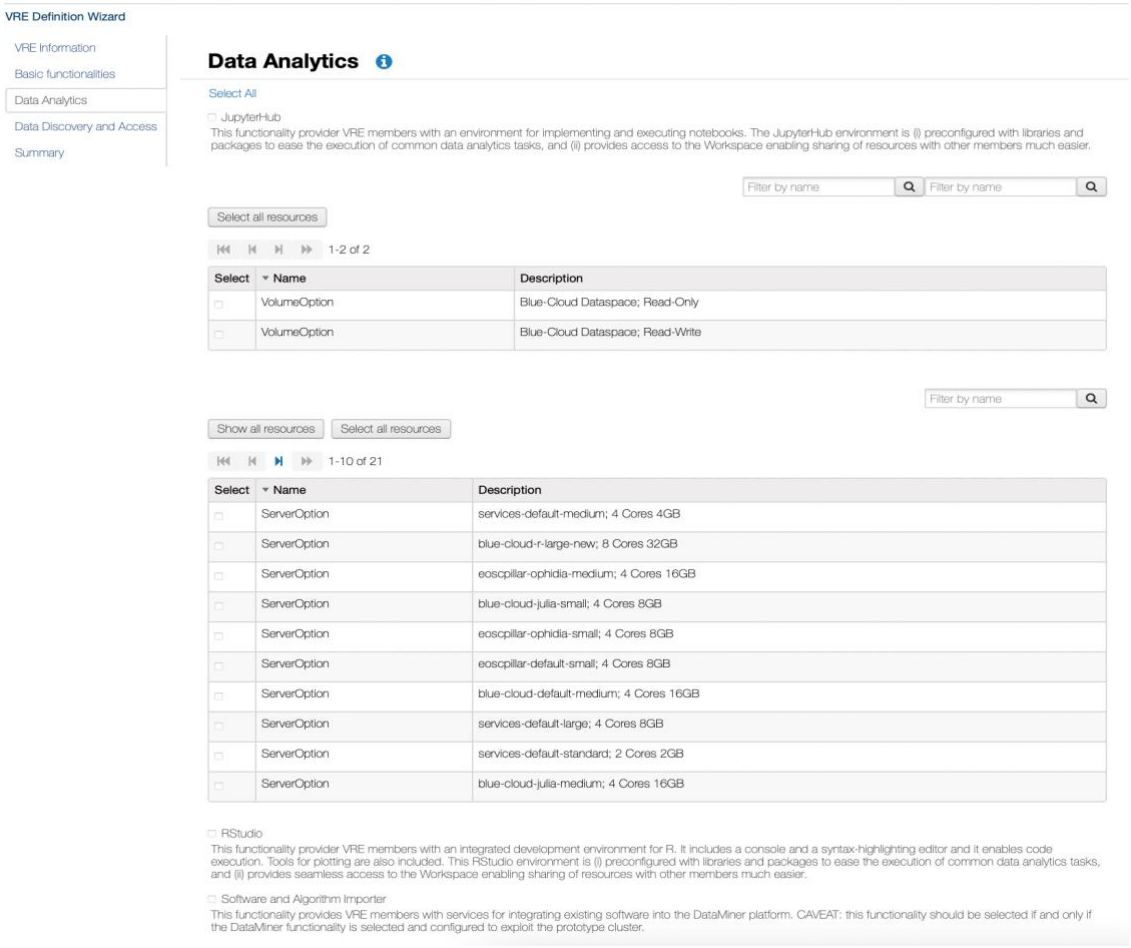

Figure 2. VLab Creation Wizard Screenshots for JupyterHub Server Options selection

So far, a total of ***14 VLabs*** were created and/or operated to serve the needs arising in the context of the Blue-Cloud project. Specifically, a total of 9 VLabs during the first period until M17, and 5 VLabs during the second period until M35.

The following VLabs were specifically conceived to support the developments of the Blue-Cloud Demonstrators and were existing prior to M17:

1. The **Aquaculture Atlas Generation VLab** is developed in the context of the Demonstrator #5 - Aquaculture monitor (cf. Sec. 4.1.2);
2. The **Fisheries Atlas VLab** is developed in the context of the Demonstrator #4 - Fish, a matter of scales (cf. Sec. 4.1.3);
3. The **GRSF_Pre VLab** is developed in the context of the Demonstrator #4 - Fish, a matter of scales (cf. Sec. 4.1.4);
4. The **Marine Environmental Indicators VLab** is developed in the context of the Demonstrator #3 - Marine Environmental Indicators (cf. Sec. 4.1.6);
5. The **Zoo and Phytoplankton EOV VLab** is developed in the context of the Demonstrator #1 - Zoo- and Phytoplankton EOV products (cf. Sec. 4.1.7).

Additionally for the same purpose, the following VLabs have been created during the second reporting period until M35:

6. The **Plankton Genomics VLab** has been developed in the context of the Demonstrator #2 - (cf. Sec. 4.1.8);
7. The **Marine Environmental Indicators Dev VLab** has been developed in the context of the Demonstrator #3 - Marine Environmental Indicators (cf. Sec. 4.1.6) and specifically needed by Demonstrator #3 developers in order to prepare and test new updates before the deployment to the "official" VLab (cf. Sec. 4.1.9) of this demonstrator #3.

The following VLabs were conceived to support project activities and/or to provide their users with development and demonstrative environments and were existing prior to M17:

8. The **Alien and Invasive Species VLab** was a demonstration oriented VLab showcasing how a web-based, comprehensive, collaborative working environment supporting decision-makers and scientists in predicting the spread of an invasive species (possibly alien) in a new environment can be developed (cf. Sec. 4.1.1);
9. The **HealthyOcean VLab** was developed to support the liaison between the REV Ocean team[3] and the Blue-Cloud team regarding several initiatives including the Ocean Data Platform (cf. Sec. 4.1.5).

Another two were developed to support the Blue-Cloud community with cross-thematic services:

10. The **Blue-Cloud Lab VLab** was developed to provide the Blue-Cloud community with a working environment to experiment with Blue-Cloud facilities (cf. Sec. 4.3.1);
11. The **Blue-Cloud Project VLab** was devised to support Blue-Cloud project activities and discussions (cf. Sec. 4.3.2);

The following additional series of VLabs was created during the second reporting period until M35 as a result of the synergies established between Blue-Cloud and other projects, Research

[3] REV Ocean website https://www.revocean.org/

Infrastructure, and initiatives related to the field:

12. The **JERICO CORE VLab** has been developed as a pilot supporting the collaboration between Blue-Cloud VRE and the JERICO Coastal Oceans Resource Environment (JERICO CORE). - (cf. Sec. 4.2.2);
13. The **JONAS VLab** has been developed as a pilot supporting the JONAS Project - Joint Framework for Ocean Noise in the Atlantic Seas initiative - (cf. Sec. 4.2.3).

Finally, to support the Blue-Cloud Hackathon event that was held in February 2022 the following VLab was developed:

14. The **Blue-Cloud Hackathon VLab** (cf. Sec. 4.2.1).

3.1. VRE and VLabs Operation

The operation of the VRE and the VLabs requires the management of requests for support, issues, and malfunctions. A total of 212 tickets have been created and managed in the Blue-Cloud Project Issue Trackers (160 in the project consortium one, 55 in the support one). Table 1 reports the specific (85% have been closed). Moreover, 34 tickets related to Blue-Cloud have been created in the D4Science overall context (88% have been closed).

Ticket type	*Total number*	*Open / in progress*	*Closed*
Incident	9	0	9
Support	136	18	118
Task	58	7	51
VLab	5	0	5
Other	4	1	3

Table 1. Tickets created in the 2 Blue-Cloud Issue Trackers

Table 2 reports the complete list of VLabs created and/or operated during the 2 reporting periods: 9 VLabs from October 2019 to January 2021 in shaded background, 5 VLabs from February 2021 to September 2022) in regular background.

VLab name	**Start date**	**Membership**	**#Users[4]**
Alien and Invasive Species	Oct. '19	Open	253
Aquaculture Atlas Generation	Oct. '19	Restricted	131
Blue-Cloud Lab	Oct. '19	Open	210
Blue-Cloud Project	Oct. '19	Private	130

[4] Number of members of the VLab in September 2022.

VLab name	Start date	Membership	#Users[4]
Fisheries Atlas	Dec. '20	Restricted	30
GRSF_Pre	Jun. '20	Restricted	15
HealthyOcean Lab	Nov. '19	Restricted	7
Marine Environmental Indicators	Apr. '20	Restricted	175
Zoo and Phytoplankton EOV	Jul. '20	Restricted	134
Plankton Genomics	Feb. '21	Restricted	52
Blue-Cloud Hackathon	Nov. '21	Open	164
JERICO-CORE	Dec. '21	Private	7
Marine Environmental Indicators DEV	July. '22	Private	7
JONAS	Aug. '22	Private	6

Table 2. List of Blue-Cloud VLabs

In Figure 3, the number of VLabs operated per month from February 2021 to September 2022 is reported. As indicated earlier, prior to February 2021 a total of 9 VLabs were already existing as documented in D4.1 Blue-Cloud VRE Operation (Release 1) [10]. During the reporting period five (5) additional VLabs have been created.

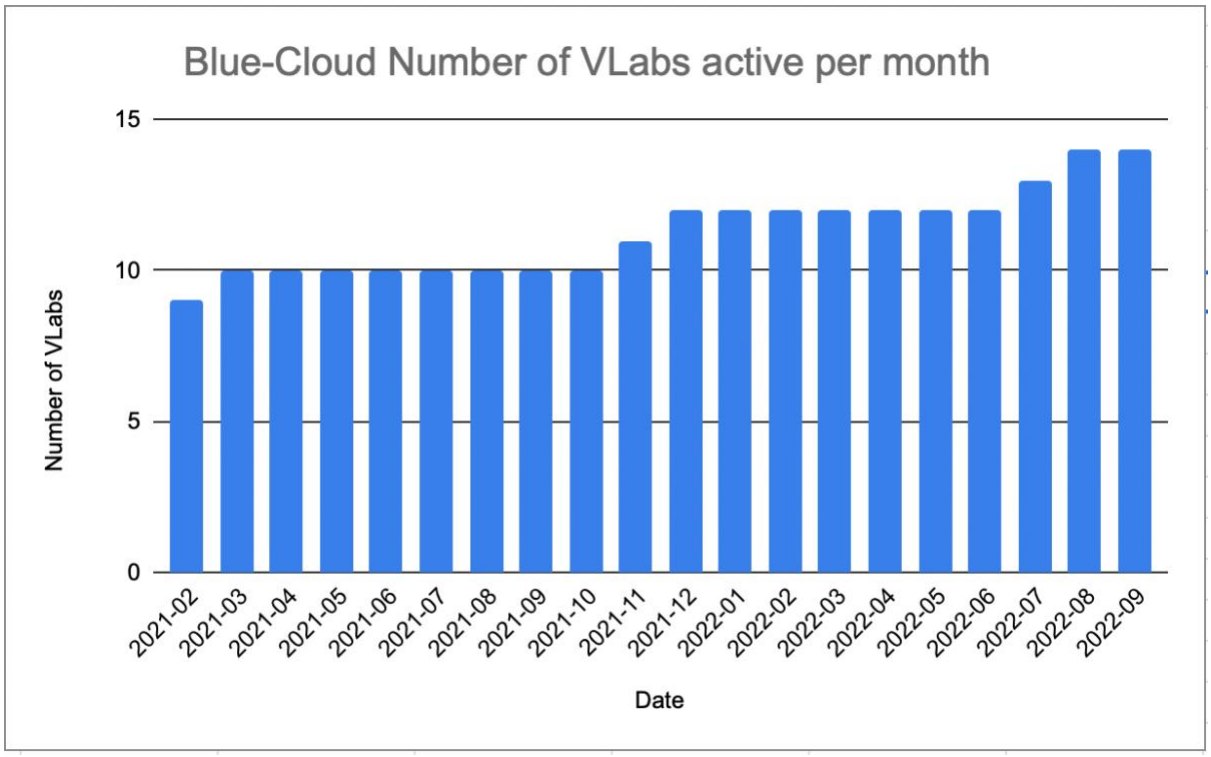

Figure 3. Number of VLabs operated per month (Feb. '21 -Sep. '22)

3.2. VRE and VLabs User Base

In Figure 4, the overall number of users benefitting from the facilities offered by the existing VLabs is reported, i.e., in September ’22, the 14 existing VLabs are serving more than 1,300 users. It is notable that during the beginning of 2022 a large number of registrations occurred; this is a consequence of the large participation to the Blue-Cloud Hackathon event that occurred between the end of January and February 2022.

Detailed figures per VLab are reported in the VLab dedicated sections of this document.

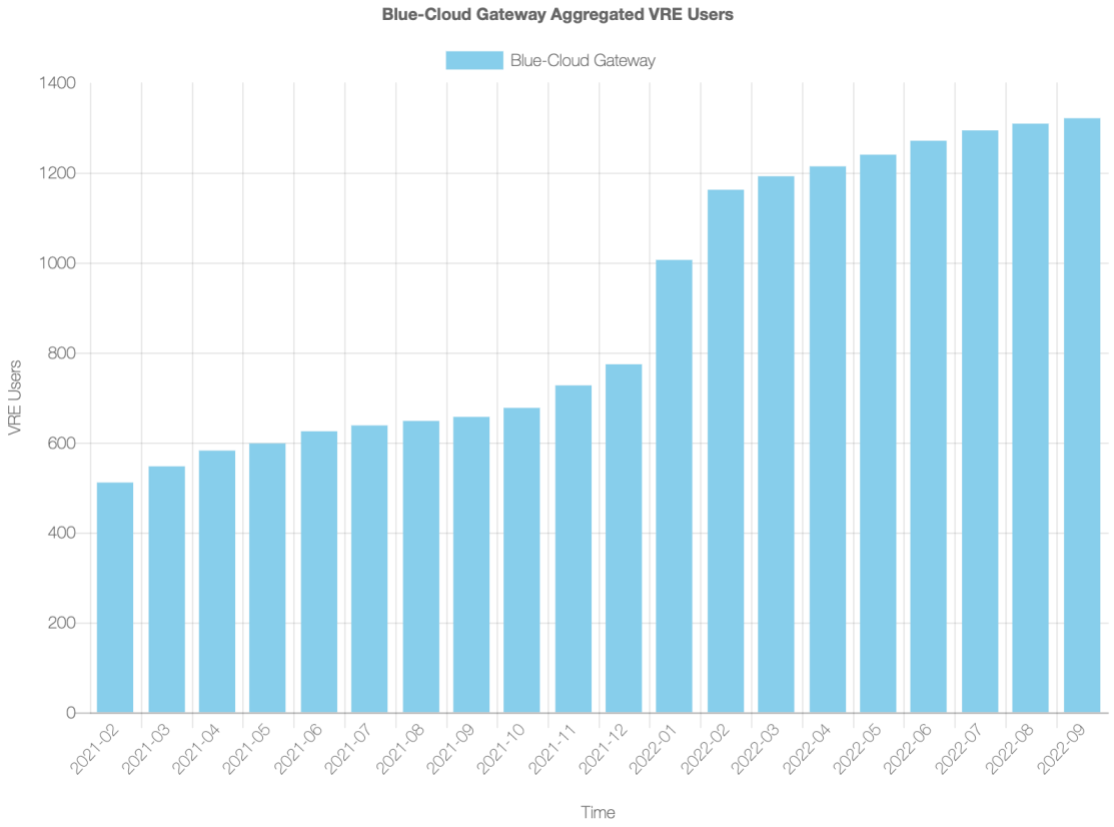

Figure 4. Number of users served by Blue-Cloud VLabs

Figure 5 reports the overall geographical distribution of the sessions registered in the second reporting period by highlighting the standard deviation of the average session duration: darker countries have session duration greater than the average session duration. Countries and Cities accessing the Blue-Cloud VRE are far more than the ones registered in the first reporting period.

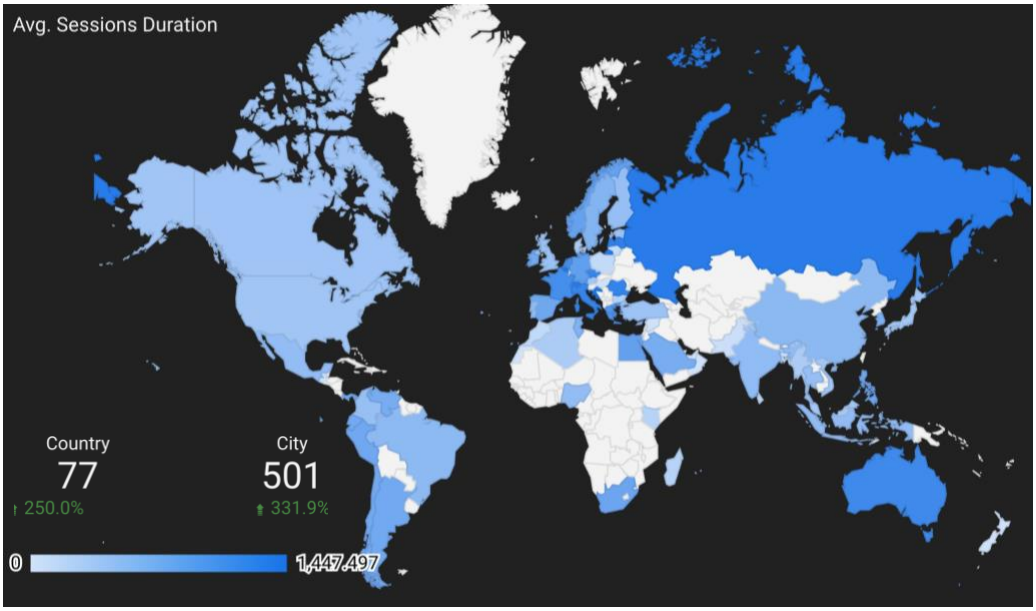

Figure 5. Geographical distribution of the sessions in the second reporting period

By analysing the email addresses of the users (which is what they are using to log in), it can be observed that: 36.4% of the users come from 100 Universities; 13.8% of the users belong to 38 International Organizations; 35.6% of the users belong to 98 National Organizations; 14.2% of the users exploited a commercial email provider (e.g., Gmail).

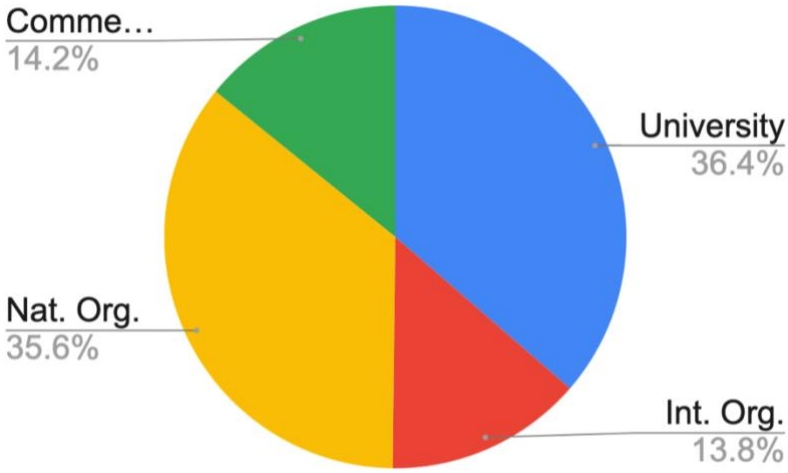

Figure 6. Users Provenance

The Universities are (alphabetic order):

Aalborg University	Arab Academy for Science, Technology and Maritime Transport	Burapha University	Chongqing University	College of Westchester

EPFL	Erlm: Un Établissement, 5 Écoles - Regional La Marsa	ETH Zurich	Facultad de Ciencias	Faculty of Sciences of the University of Lisbon
Free University of Bozen-Bolzano	Ghent University	Halu Oleo University	Hebrew University of Jerusalem	Imperial College London
Institut Barcelona D'Estudis Internationales (IBEI)	Institut Polytechnique de Paris	International Islamic University	Istanbul Technical University	Jacobs University
King Abdullah University of Science and Technology	KIT – The Research University in the Helmholtz Association	La Rochelle Université	Mt. San Antonio College	Nanjing University of Science
Natural Language Processing Lab. National Tsing	Hua University - Taiwan	Pacific Ridge School	Politécnico do Porto	San José State University
Sapienza Università di Roma	Sorbonne université	Southeast University, China	Technische Universität Berlin	Texas A&M University
The University Of The South Sewanee	Trakya University	Trinity College Dublin	Tsinghua University	Tuscia University (Università degli Studi della Tuscia)
UBO - Université de Bretagne Occidentale	Umeå University	Universidad Católica de Valencia	Universidad Complutense Madrid	Universidad de Granada
Universidad de Guadalajara	Universidad de los Andes	Universidad de Málaga	Universidad Simón Bolívar	Universidad Técnica Particular de Loja
Universidade de Aveiro	Universidade Tecnica do Atlantico	Università Ca' Foscari	Università degli Studi di Milano – Bicocca	Università degli studi di Parma
Università degli Studi di Roma "Tor Vergata"	Università degli studi di Trieste	Università del Salento	Università di Bologna	Università di Bologna
Università di Genova	Università di Pisa	Universitas Pendidikan Indonesia	Universitat Autònoma de Barcelona	Universität Bremen
Université Abdelmalek Essaadi	Université catholique de Louvain	Université de Liège	Université Ibn Zohr: UIZ	Université PSL (Paris Sciences & Lettres)
University College Cork	University College Dublin	University of Algarve	University of Amsterdam	University of Bergen
University of Cadiz	University of Cambridge	University of Évora	University of China Academic of Science	University of Gothenburg
University of Kentucky	University of Liège	University of Maryland	University of Minnesota	University of Montpellier
University of New Mexico	University of Osijek	University of Queensland	University of Sao Paulo	University of Technology Sydney
University of Uthrect	University of Veterinary Medicine, Vienna	University of Zurich	Vrije Universiteit Brussel	Wageningen University & Research.

The International and National Organizations include research centers, research infrastructures, and not profit organizations, as for example:

BSC	CYFRONET	CMCC	CNR	CNRS
CSC	DKRZ	EGI	EMBL	European Marine Observation and Data Network (EMODnet)
FAO (UN)	LifeWatch	GeoMar	GRNET	ICES
IFREMER	INRAE	INRIA	A Bussola.farm É Uma Empresa Agro 4.0 Da Amazônia	Agenzia regionale per la protezione dell'ambiente del Friuli Venezia Giulia
Alfred Wegener Institute	Athena RC	Basque Centre for Climate Change	Blue Lobster	Centro Tecnológico del Mar
Coastal Ocean Observing and Forecasting System (Spain)	CREAF public research centre	Cyprus Ministry of Agriculture, Rural Development and Environment	Flanders Marine Institute	Israel Oceanographic and Limnological Research
Latvian Institute of Aquatic Ecology	OceanData Platform	RedCLARA	Republic Hydrometeorological Service of Serbia	South African National Biodiversity Institute
St. Lawrence Global Observatory	Sustainable Fisheries	The Oceanic Platform of the Canary Islands.		

3.3. VRE and VLabs Usage Indicators

Figure 7 reports the overall number of working sessions initiated per month via the Blue-Cloud VRE. Up to September 2022, a total of more than 25.700 working sessions have been executed by the users, with an average of 1.286 working sessions per month. It is notable that during the beginning of 2022 a large number of sessions occurred, even in this case we believe it is a consequence of the large participation to the Blue-Cloud Hackathon event that occurred between the end of January and February 2022.

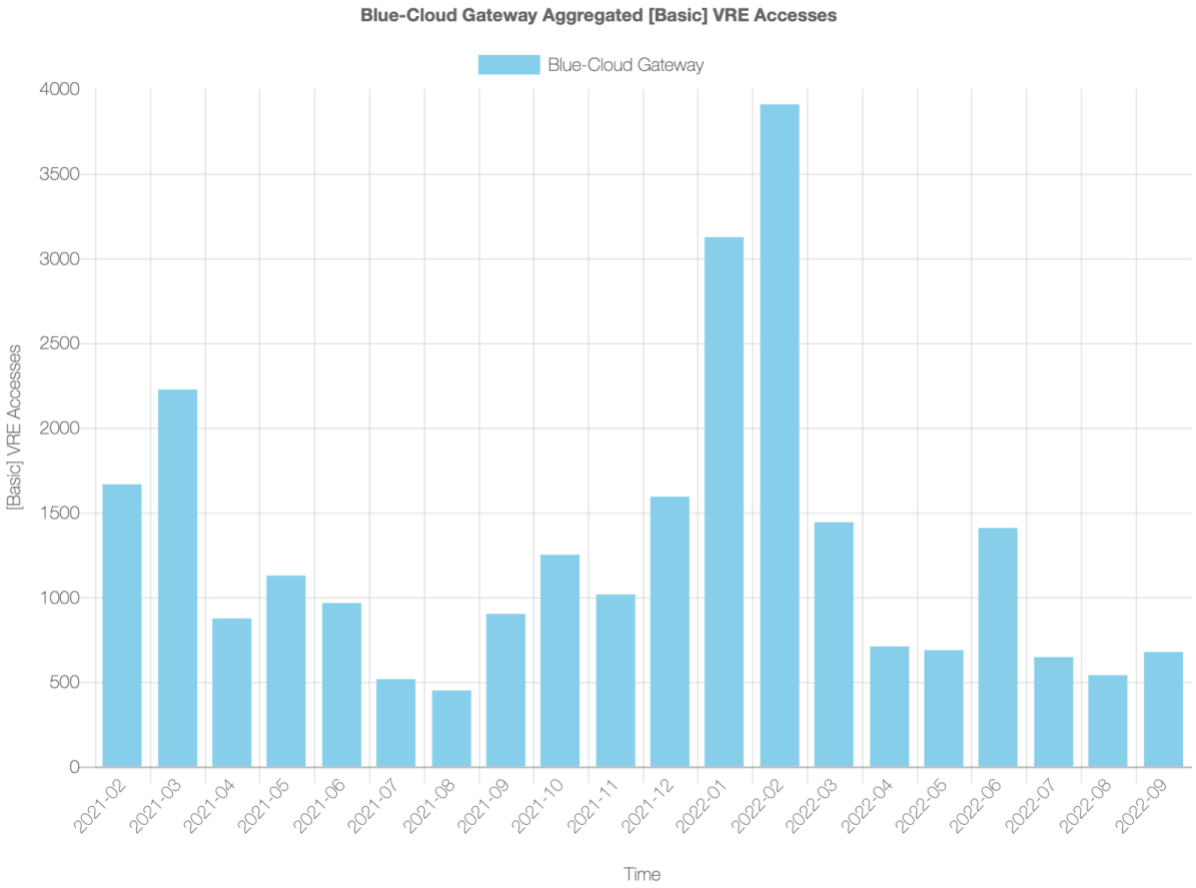

Figure 7. VLab Accesses per month

Figure 8 reports the overall number of working sessions initiated per month via the Blue-Cloud VRE among the 5 Blue-Cloud Demonstrators. The **Zoo and Phytoplankton EOV VLab** developed in the context of the Demonstrator #1 - Zoo- and Phytoplankton EOV products (cf. Sec. 4.1.7) and the **Marine Environmental Indicators VLab** got the best results in terms of access on average with respect to the other VLabs developed in the context of the other Demonstrators. Up to September 2022, a total of more than 15.000 working sessions have been executed by the users in the Demonstrator VLabs, with an average of 790 working sessions per month.

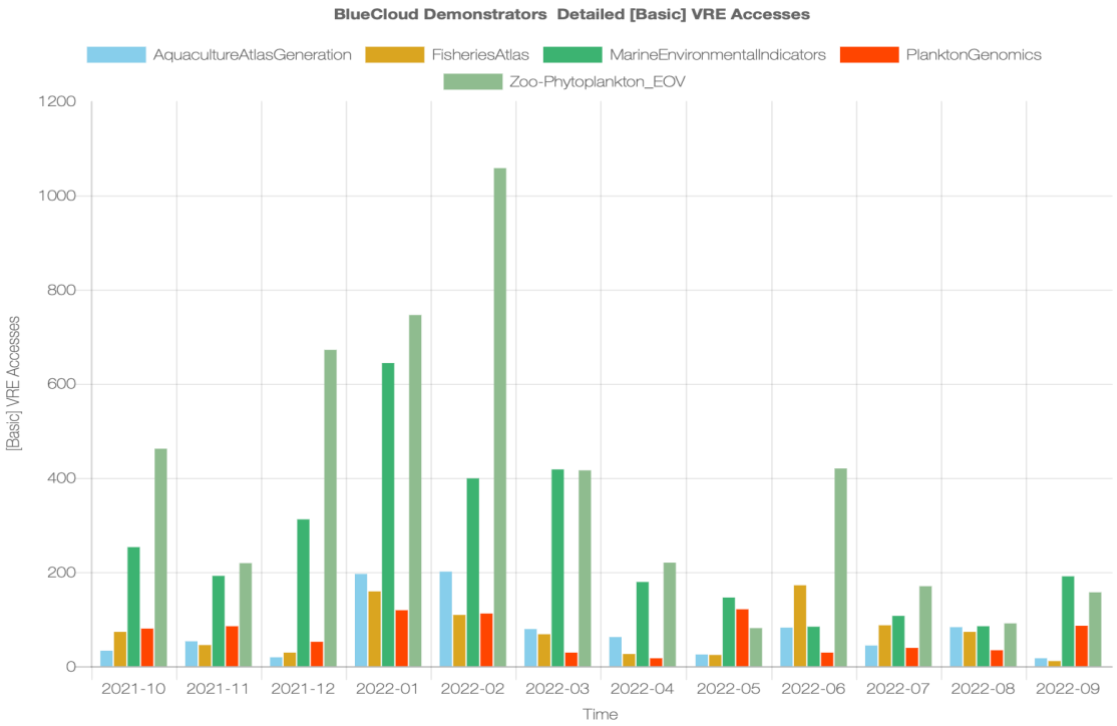

Figure 8. Demonstrators VLab Accesses per month

Figure 9 and Figure 10 report the overall number of working sessions initiated per month via the Blue-Cloud VRE among the 5 Blue-Cloud Demonstrators for the exploitation of the Analytics tools JupyterHub and RStudio. Up to September 2022, a total of more than 2.230 analytics sessions have been executed by the users in the Demonstrator VLabs, with an average of 55 working sessions per month. JupyterLab seems to be preferred by VLab users with a total of more than 1.300 accesses, while RStudio totalised 900 circa.

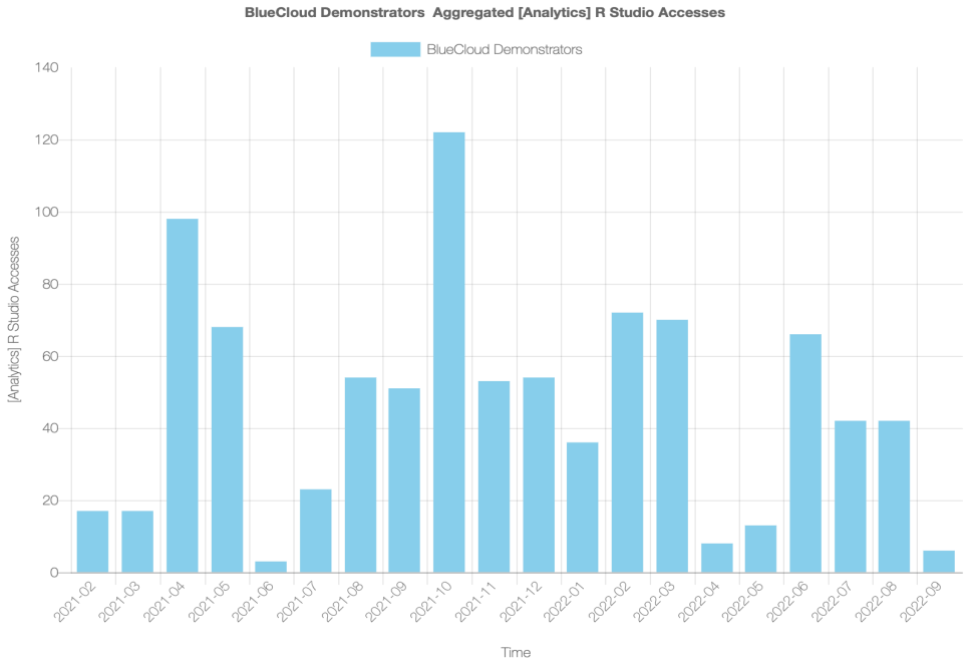

Figure 9. Demonstrator VLabs Accesses to RStudio per month

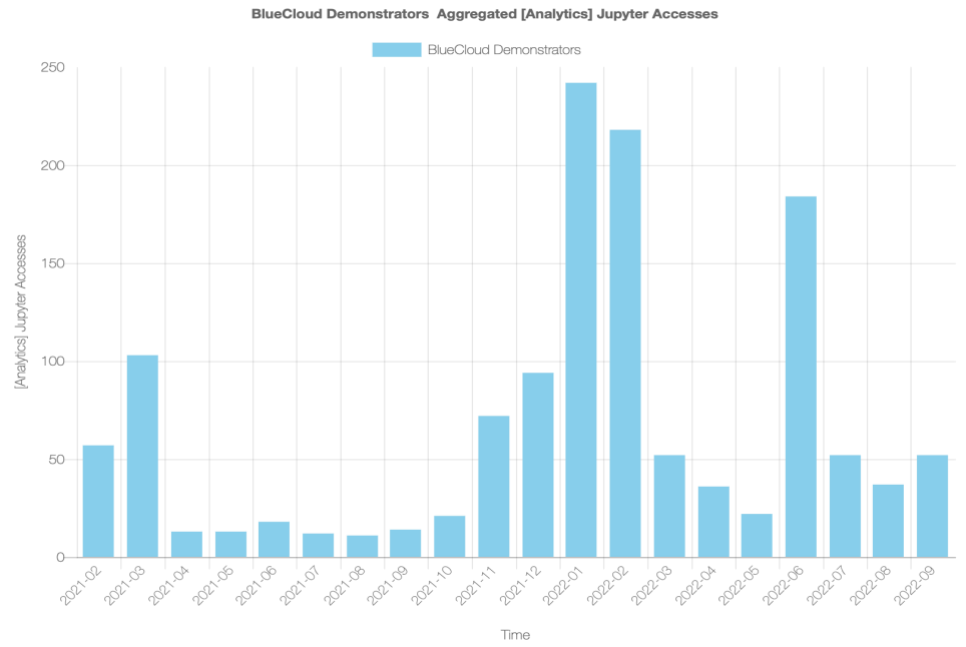

Figure 10. Demonstrator VLabs Accesses to JupyterHub per month

Figure 11 reports the overall number of jobs submitted per month via the Blue-Cloud VRE among the 5 Blue-Cloud Demonstrators. The high variance in the exploitation of the high throughput computing platform was well-managed by the Blue-Cloud VRE that automatically scaled up to manage peaks in the exploitation of the VLab services.

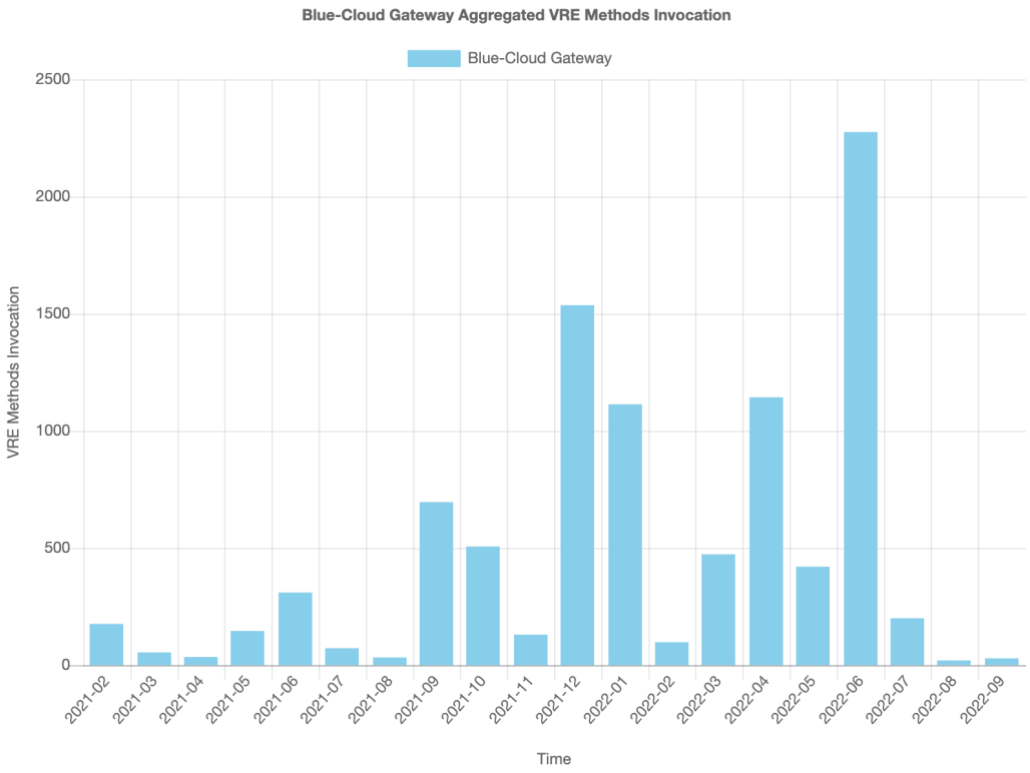

Figure 11. Demonstrator VLabs methods execution per month

4. Blue-Cloud VLabs

All the VLabs are equipped with:

- A ***shared workspace*** to enable every user to store and organise the information objects he/she is interested in working with. In addition to that, the user is allowed to collaborate with other users by sharing objects and messages;
- A ***user management facility*** to enable authorised users (i.e., VLab Managers) to manage other users using or wanting to access the VLab. VLab Managers can (i) authorise users for access to the VLab, (ii) assign or withdraw roles to users, (iii) remove users, and (iv) send communications to the current users;
- A ***social networking facility*** to enable users to use the common facilities typical of social networks – e.g., posting news, commenting on posted news – yet adapted to the settings of working environments like those characterising Blue-Cloud. Users can post news as well as applications;
- A ***notification facility*** to alert users on relevant activities as they happen. These notifications offer a sense of anticipation and create a productivity boost. Users receive an alert (through a priori selected channels, e.g., email, web portal, Twitter) notifying them when something of interest has happened in their VLab(s);
- A ***members facility*** to provide users with a list of VLab co-workers, i.e., the list of members partaking in the VRE and contributing to it;
- A ***messaging facility*** to provide users with a cloud-based common email environment. The distinguishing feature is represented by its integration with the rest, e.g., it is possible to send any information object residing in the workspace (regardless of how "big" and "complex" it may be) as an attachment without consuming bandwidth.

A brief description of each available VLab, including the ones created in the previous reporting period, is reported in the following sections.

4.1. VLabs supporting Blue-Cloud demonstrators

4.1.1. Alien and Invasive Species VLab

The Alien and Invasive Species VLab is a web-based, comprehensive, collaborative working environment supporting decision-makers and scientists in predicting the spread of an invasive species (possibly alien) in a new environment. The VLab hosts examples of suitable habitat maps produced for today and 2050 in new areas for more than 11,000 species. It also provides models and workflows to combine environmental data with species observations in their habitats to predict their future spread.

This VLab is available at https://blue-cloud.d4science.org/web/alienandinvasivespecies

This VLab stems from previous initiatives (BlueBRIDGE project[5]). From the Blue-Cloud point of view, it has been in operational status since October '19, i.e., when the Blue-Cloud gateway was released.

[5] https://www.bluebridge-vres.eu/

The uptake of this VLab from Blue-Cloud was due to the willingness to have a developed working environment to be used for demonstrative purposes for Demonstrator designers and implementers. It is currently serving 253 users distributed as in the following chart.

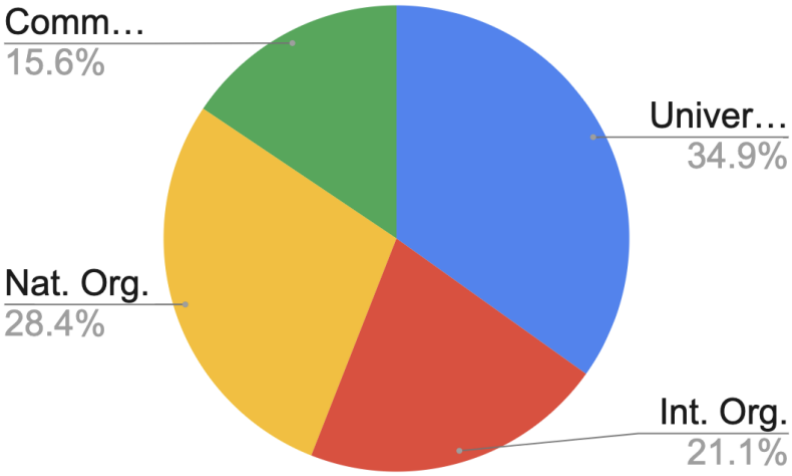

Figure 12. Alien and Invasive Species VLab Users Provenance

A screenshot of the VLab is available in Figure 13. It shows the home page and the menu items for accessing the VLab facilities.

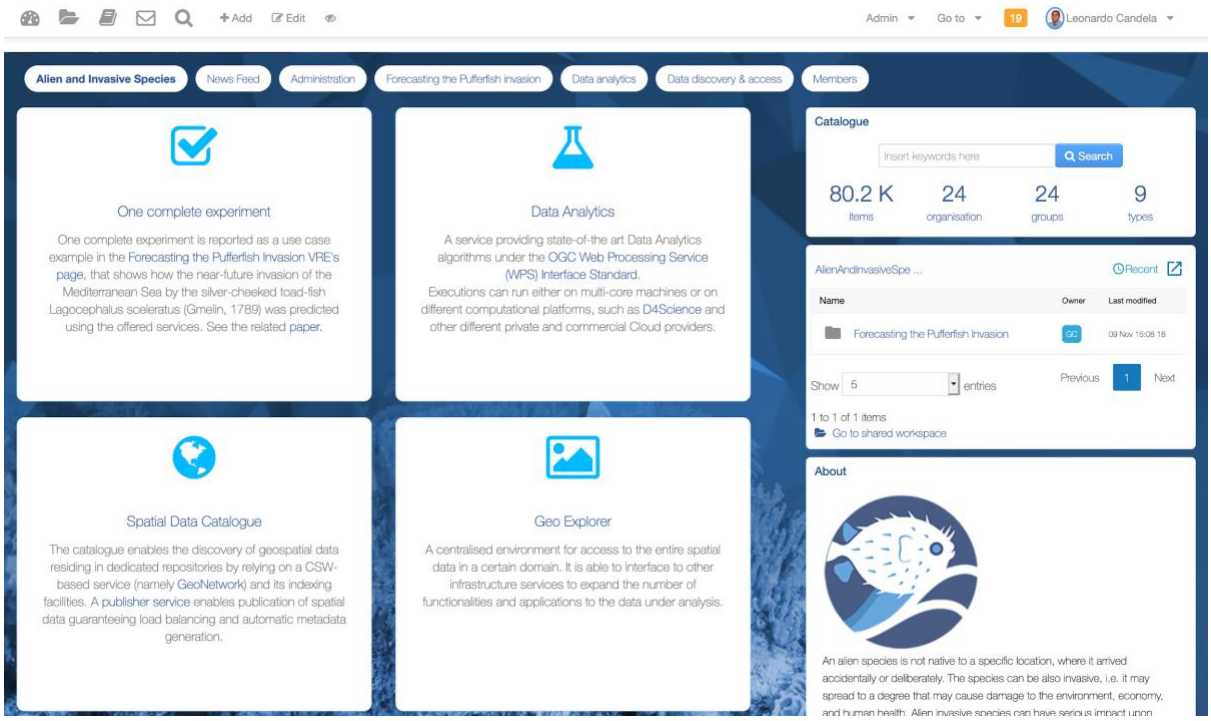

Figure 13. A screenshot of the Alien and Invasive Species VLab

In addition to the basic functionality, e.g., a workspace for sharing objects of interest and a user management facility for managing membership, this VLab is specifically equipped with the following functionalities:

- a ***data analytics facility*** enabling users to benefit from the offerings of the Data Miner

service [1][2] and interactively execute a large array of data analytics tasks on datasets. As of January '21 the facility offers ***66 ready to use method implementations*** ranging from Bayesian methods to maps comparison and data clustering;

- a ***geospatial data discovery facility*** enabling users to have access to species distribution maps;
- a ***species data discovery facility*** enabling users to have seamless access to species data (including occurrence points) across several data providers;
- a ***catalogue facility*** enabling users to have access to more than ***70k objects*** including datasets, research objects, training material, code lists, and series;

4.1.2. Aquaculture Atlas Generation VLab

The Aquaculture Atlas Generation VLab is developed in the context of the Demonstrator #5 - Aquaculture monitor [7].

This VLab is available at https://blue-cloud.d4science.org/web/aquacultureatlasgeneration

This VLab actually stems from the BlueBRIDGE project and it has been further developed thanks to the demonstrator implementation. From the Blue-Cloud point of view, it has been in operational status since October '19, i.e., when the Blue-Cloud gateway was released. It is currently serving 131 users distributed as in the following chart.

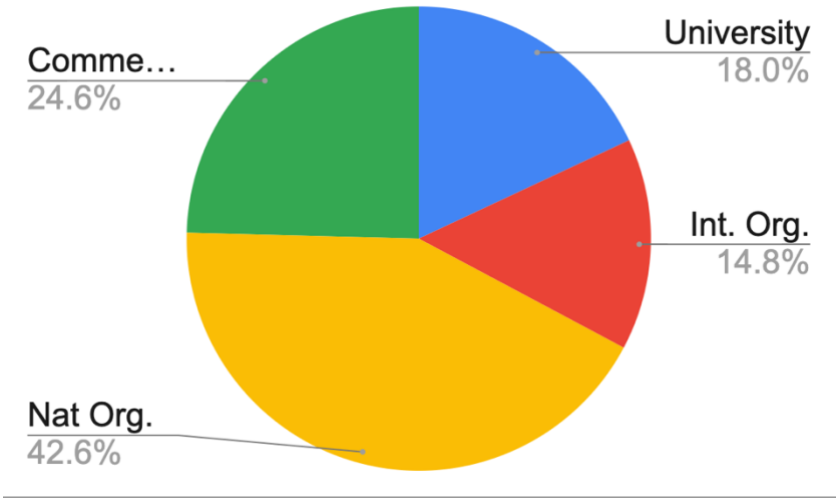

Figure 14. Aquaculture Atlas Generation VLab Users Provenance

A screenshot of the VLab is available in Figure 15. It shows the home page and the menu items for accessing the VLab facilities.

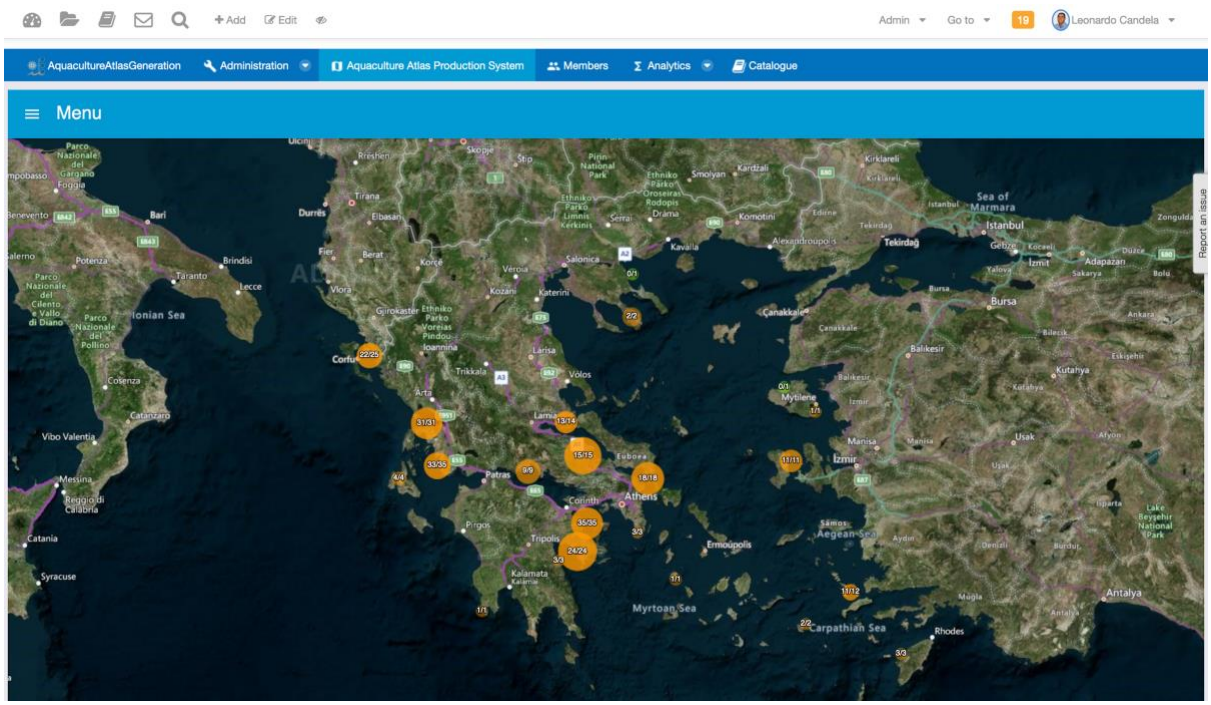

Figure 15. A screenshot of the Aquaculture Atlas Generation VLab

In addition to the basic functionality, e.g., a workspace for sharing objects of interest and a user management facility for managing membership, this VLab is specifically equipped with the following functionalities:

- the ***Aquaculture Atlas Production Systems*** map-viewer enabling users to identify and assess (for authorised users only) aquaculture farms. In particular, the tool visualizes the results of fish cage detection algorithms based on VHR optical images (ACUITY toolbox) and allows users to edit map features and to generate output as FAO NASO Maps;
- the ***data analytics*** facility enabling users to benefit from the offerings of the Data Miner service [1][2] and interactively execute a large array of data analytics tasks on datasets. It has been configured to serve ***4 specific algorithms***, i.e., those underlying the Aquaculture Atlas Production System facility (Geographic Proximity Tool, AAPS Public Publisher, AAPS Staging Publisher, AAPS NASO Publisher);
- the ***RStudio*** facility enabling users to use a fully-fledged RStudio® working environment directly from the VRE. This environment is integrated with the rest of VLab facilities, e.g., it is possible to use files from the workspace and to store new files within the workspace;
- the ***Catalogue*** facility enabling users to publish, search and browse datasets and other products of interest for the specific use case. This environment has been configured to give access to datasets stemming from the Greece and Indonesia cases.

4.1.3. Fisheries Atlas VLab

The Fisheries Atlas VLab is developed in the context of the Demonstrator #4 - Fish, a matter of scales [2020d]. This environment is conceived to provide its users with facilities supporting the development of an online overview of harmonized time-series of catch and effort. This VLab is available at https://blue-cloud.d4science.org/web/fisheriesatlas

This VLab has been in operational status since December 2020. It is currently serving 30 users distributed as in the following chart.

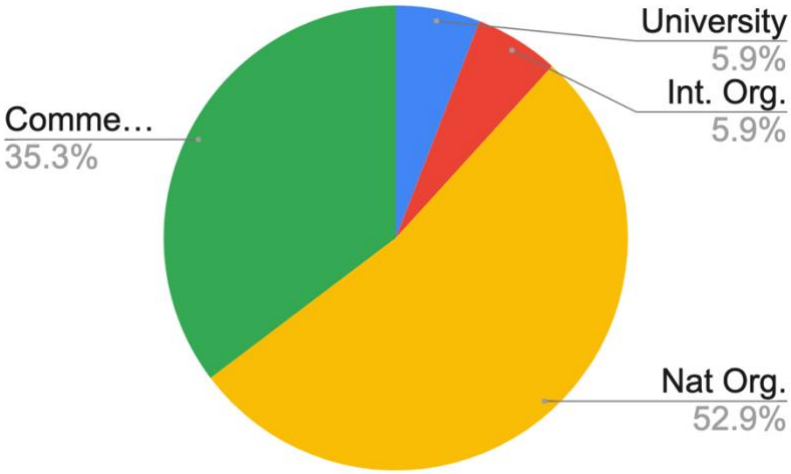

Figure 16. Fisheries Atlas VLab Users Provenance

A screenshot of the VLab is available in Figure 17. It shows one specific app of this VRE (the map viewer) and the menu items for accessing the VLab facilities.

Figure 17. A screenshot of the Fisheries Atlas VLab

In addition to the basic functionality, e.g., a workspace for sharing objects of interest and a user management facility for managing membership, this VLab is specifically equipped with the following functionalities:

- the ***RStudio*** facility enabling users to use a fully-fledged RStudio® working environment directly from the VRE. This environment is integrated with the rest of VLab facilities, e.g., it is

possible to use files from the workspace and to store new files within the workspace;

- a ***geospatial data catalogue*** facility enabling users to search and access ***more than 3500 datasets, services and maps*** of interest for the community;
- two ***repositories for geospatial datasets***, one based on GeoServer technology and another one based on THREDDS Data Server.
- a ***map viewer*** providing users with a seamless data discovery and visualization of information including FAO and IRD produced Tuna Atlas layers; FAO Productions and trade national statistics; Selected Regional Fisheries Organizations data; Selected EMODnet layers; Selected CMEMS products; Selected species distribution maps; Selected FAO and VLIZ layers;

4.1.4. GRSF_Pre VLab

The GRSF_Pre VLab is developed in the context of the Demonstrator #4 - Fish, a matter of scales [3][7]. GRSF stands for Global Record of Stocks and Fisheries. This environment is conceived to provide its users with a working environment to validate new content in the GRSF Knowledge Base [3] and therefore it is not a public service. the GRSF team uses this environment to validate data harvests from 3 global GRSF sources that are now published into the GRSF Admin[6] and GRSF VREs[7].

This VLab is available at https://blue-cloud.d4science.org/web/grsf_pre

This VLab has been in operational status since June 2020. It is currently serving 15 users. Those users assess and validate the procedure and tools for data management that are then exploited in the GRSF Admin VLab (42 users) accessible at https://i-marine.d4science.org/web/grsf_admin. The result of the data assessment and validation performed in the GRSF Admin VLab is then published in the public GRSF VLab accessible at https://i-marine.d4science.org/web/grsf (96 users) and distributed via the GRSF catalogue, https://i-marine.d4science.org/web/grsf/data-catalogue (3140 visits per month in average), and listed as component of the FAO knowledge base at https://www.fao.org/fishery/en/knowledgebase/175.

A screenshot of the VLab is available in Figure 18. It shows the catalogue facility displaying the available records.

[6] The GRSF Admin environment (https://i-marine.d4science.org/web/grsf_admin) provides authorized users with an environment and tools for building an integrated catalogue on stocks and fisheries information, i.e. for defining the authoritative version of the stocks and fisheries records made available by the GRSF official catalogue.

[7] The GRSF environment https://i-marine.d4science.org/web/grsf implements the "Global Record of Stocks and Fisheries" by providing users with an environment and tools for accessing stocks and fisheries information collated from three database sources: (i) Fisheries and Resources Monitoring System (FIRMS): http://firms.fao.org, (ii) RAM Legacy Stock Assessment Database: http://ramlegacy.org, and (iii) FishSource: http://www.fishsource.com

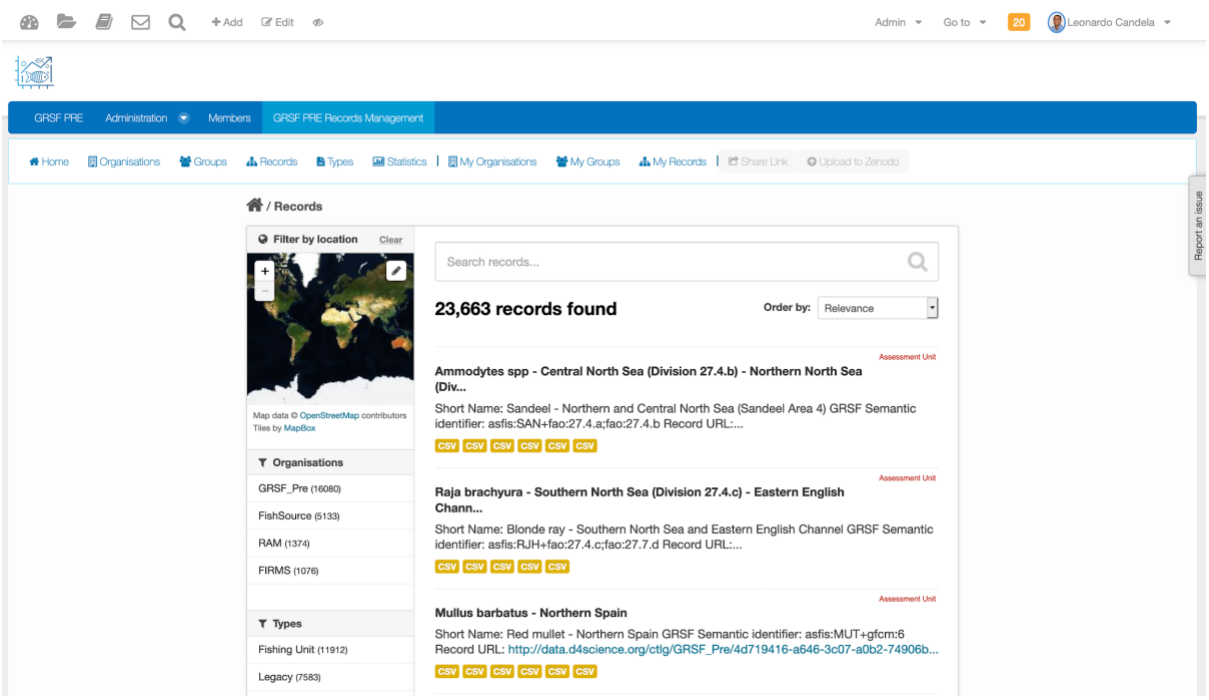

Figure 18. A screenshot of the GRSF_Pre VLab

In addition to the basic functionality, e.g., a workspace for sharing objects of interest and a user management facility for managing membership, this VLab is specifically equipped with the following functionalities:

- a ***catalogue facility*** enabling users to visualise the GRSF candidate records stemming from the integration facility and manage their approval. This catalogue has been populated with ***more than 23,500 records*** including Fishing Unit, Assessment Unit, and Marine Resource;

4.1.5. HealthyOcean VLab

The HealthyOcean VLab was developed to support the liaison between the REV Ocean team[8] and the Blue-Cloud team regarding several initiatives including the Ocean Data Platform. This VLab is available at https://blue-cloud.d4science.org/web/healthyocean-lab

This VLab has been in operational status since November 2019. It supported the collaboration among a small group of users (7 users) that had the possibility to exchange large data collections and ideas in a controlled and private environment.

A screenshot of the VLab is available in Figure 19. It shows the home page and the menu items for accessing the VLab facilities.

[8] REV Ocean website https://www.revocean.org/

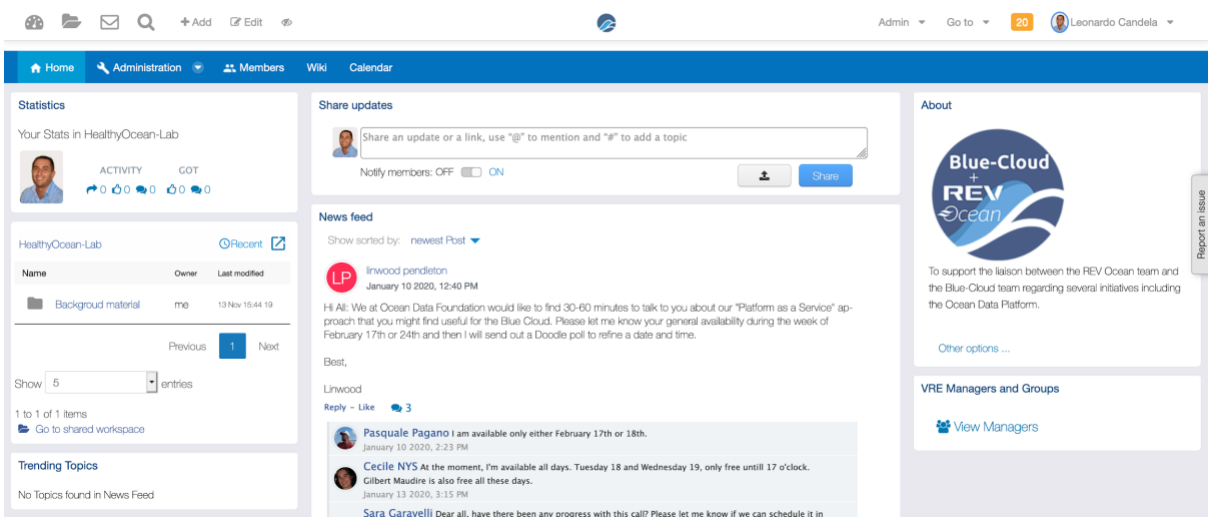

Figure 19. A screenshot of the HealthyOcean VLab

In addition to the basic functionality, e.g., a workspace for sharing objects of interest and a user management facility for managing membership, this VLab is not equipped with specific facilities since it was mainly conceived to support the cooperation between the two teams.

4.1.6. Marine Environmental Indicators VLab

The Marine Environmental Indicators VLab is developed in the context of the Demonstrator #3 - Marine Environmental Indicators [7]. It is conceived to provide its users with facilities to (i) identify environmental quality indicators in selected marine regions/areas; (ii) obtain new added-value data applying big data analysis and machine learning methods on the multi-source data sets, and (iii) to perform online and on the fly operations such as selecting portion of a dataset, to perform statistical analysis or display the data.

This VLab is available at https://blue-cloud.d4science.org/web/marineenvironmentalindicators

This VLab has been in operational status since April 2020. It is currently serving 175 users distributed as in the following chart.

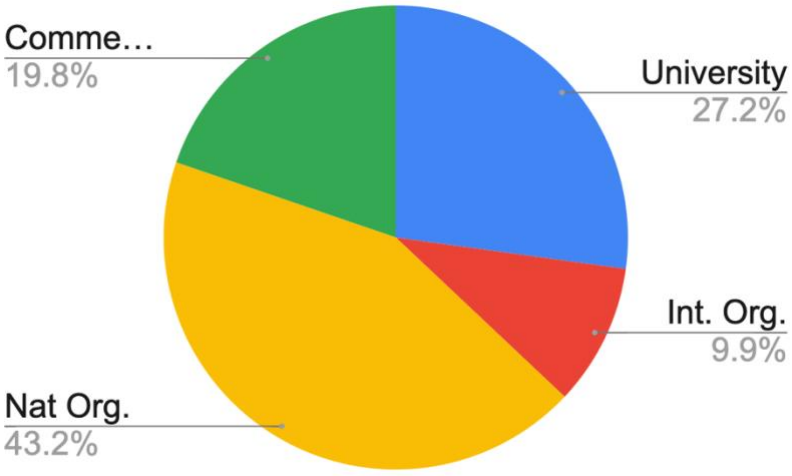

Figure 20. Marine Environmental Indicators VLab Users Provenance

A screenshot of the VLab is available in Figure 21. It shows the MEI Generator app specifically developed for this community and the menu items for accessing the VLab facilities.

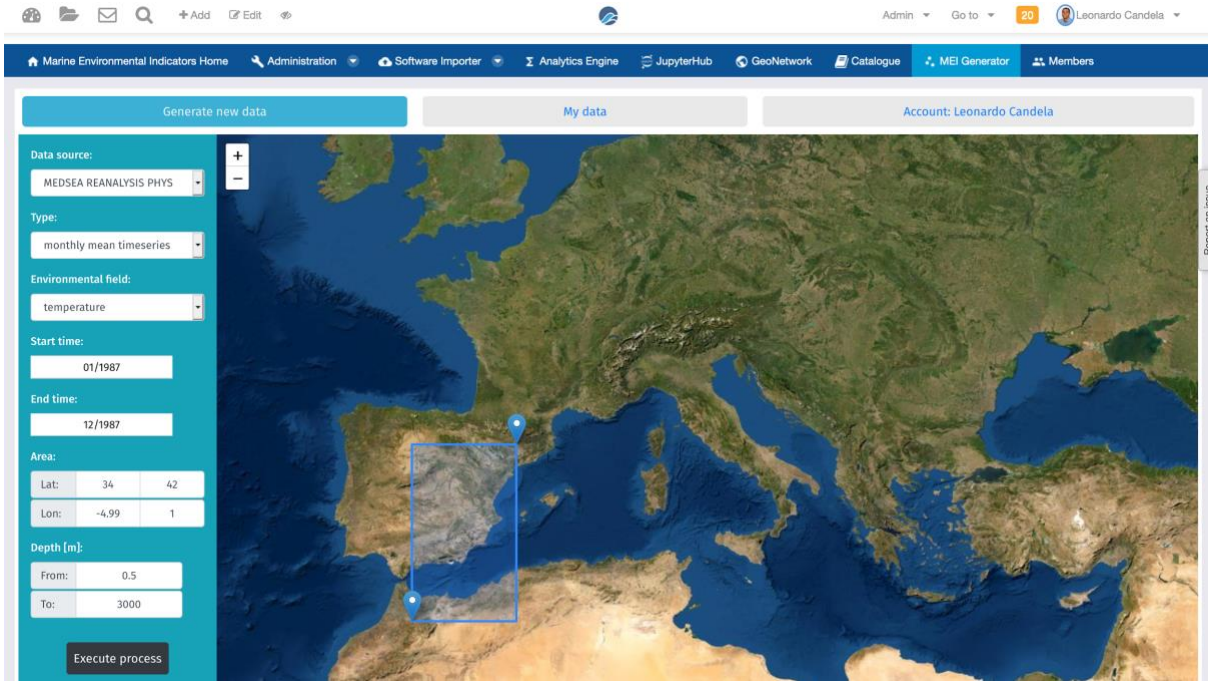

Figure 21. A screenshot of the Marine Environmental Indicators VLab

In addition to the basic functionality, e.g., a workspace for sharing objects of interest and a user management facility for managing membership, this VLab is specifically equipped with the following functionalities:

- a ***software importer facility*** enabling users to onboard existing software and algorithm implementations into the Data Miner platform [1][2];
- a ***data analytics facility*** enabling users to benefit from the offerings of the Data Miner service [1][2] and interactively execute a large array of data analytics tasks on datasets. As of January '21 the facility offers ***19 ready to use method implementations*** including preliminary versions of algorithms for computing the Storm Severity Index (dataset providing users insights on atmospheric wind/storm circumstances that impact the circulation of seas such as the Mediterranean Sea) and the seastat algorithm (i.e., the analytics process behind the MEI Generator app described below);
- the ***JupyterHub*** facility enabling users to develop and execute Jupyter notebooks. This environment is integrated with the rest of VLab facilities, e.g., it is possible to use files from the workspace and to store new files within the workspace. Two specific notebooks have been developed and shared: a ***Model Development notebook*** to design, optimize and train a model; and a ***Prediction notebook*** to use a trained model and classify the profiles of a dataset into the different classes.
- the ***geospatial data catalogue*** facility enabling users to search and access geospatial products of interest for the community. At the time of writing this deliverable the catalogue has not been populated yet with products of interest;
- the ***Catalogue*** facility enabling users to publish, search and browse datasets and other products of interest for the specific use case;
- the ***MEI Generator app*** facility, i.e., a specific web application aiming at providing its users with a user interface facilitating the steps of generating new data starting from the existing

ones and accessing and visualising the data previously calculated by the user.

One important feature of this VLab is that the environment was configured to serve two main classes of users: “VLab developers” and “VLab users”. The former class of users has full access to all the facilities discussed above. The latter class of users has access only to the JupyterHub and MEI Generator app.

4.1.7. Zoo and Phytoplankton EOV VLab

The Zoo and Phytoplankton EOV VLab is developed in the context of the Demonstrator #1 - Zoo- and Phytoplankton EOV products [7][11]. This environment is conceived to support a methodology to generate: (i) zooplankton products based on in situ observations of abundance of different zooplankton species in a region encompassing the North-East Atlantic; (ii) global ocean three-dimensional (3D) products of chlorophyll-a (Chla) concentration, that is a proxy for total phytoplankton biomass, based on Argo vertical profiles matched up with satellite imagery; (iii) a mechanistic model using near real-time data to quantify the relative contributions of the bottom-up and top-down drivers in phytoplankton dynamics.

This VLab is available at https://blue-cloud.d4science.org/web/zoo-phytoplankton_eov

This VLab has been in operational status since July 2020. It is currently serving 134 users distributed as in the following chart.

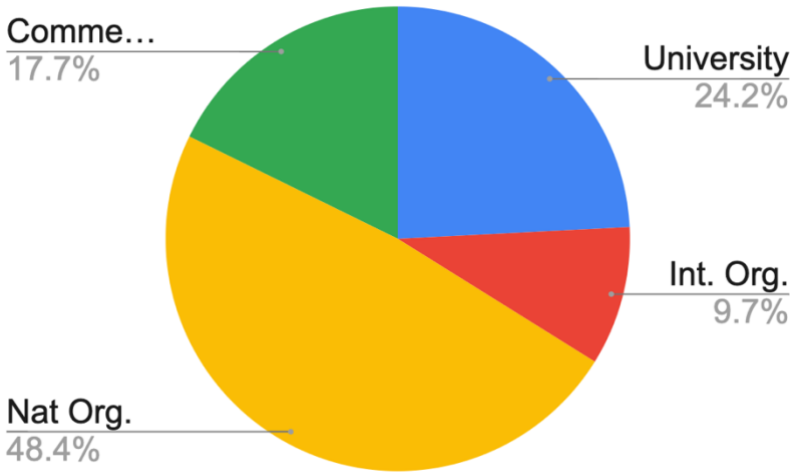

Figure 22. Zoo and Phytoplankton EOV VLab Users Provenance

A screenshot of the VLab is available in Figure 23. It shows the Data Miner GUI and the menu items for accessing the VLab facilities.

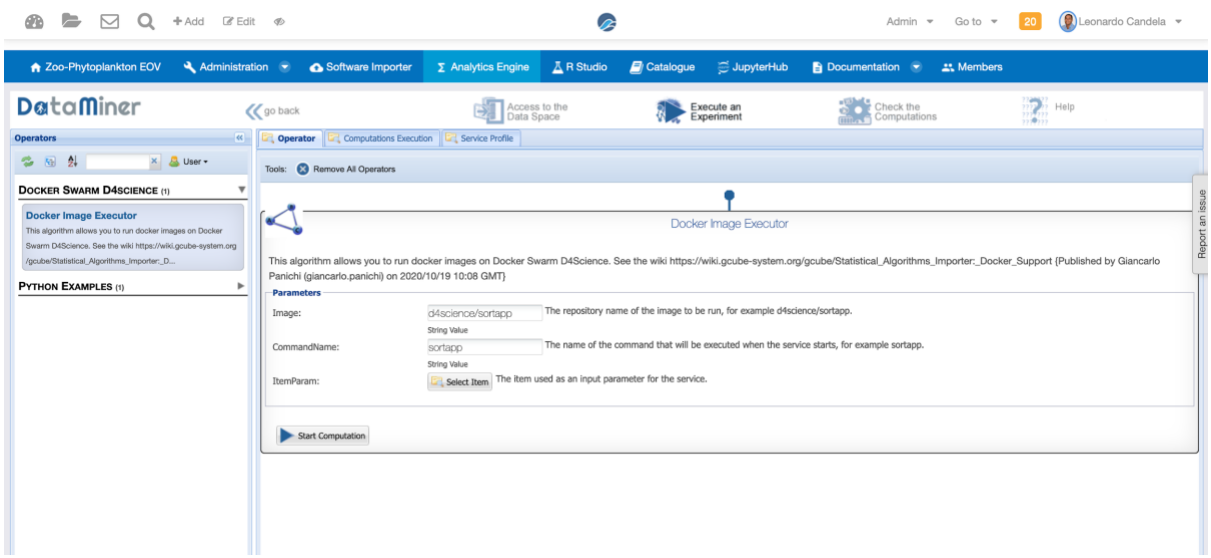

Figure 23. A screenshot of the Zoo and Phytoplankton EOV VLab

In addition to the basic functionality, e.g., a workspace for sharing objects of interest and a user management facility for managing membership, this VLab is specifically equipped with the following functionalities:

- a ***software importer facility*** enabling users to onboard existing software and algorithm implementations into the Data Miner platform [1][2];
- a ***data analytics facility*** enabling users to benefit from the offerings of the Data Miner service [1][2] and interactively execute a large array of data analytics tasks on datasets. As of January '21, the facility offers two ready-to-use method implementations. In particular, the ***Docker Image Executor*** algorithm that was specifically conceived to enable users to execute any algorithm packaged as a docker image. This algorithm is exploited to support the execution of the ***DIVAnd algorithm*** (Data-Interpolating Variational Analysis in n dimensions)[9];
- the ***RStudio*** facility enabling users to use a fully-fledged RStudio® working environment directly from the VRE. This environment is integrated with the rest of VLab facilities, e.g., it is possible to use files from the workspace and to store new files within the workspace;
- the ***Catalogue*** facility enabling users to publish, search and browse datasets and other products of interest for the specific use case;
- the ***JupyterHub*** facility enabling users to develop and execute Jupyter notebooks. This environment is integrated with the rest of VLab facilities, e.g., it is possible to use files from the workspace and to store new files within the workspace. Specific notebooks have been developed and shared: a notebook to create monthly fields of the vertical distribution of SOCA-Chl and a notebook to produce plots.

4.1.8. Plankton Genomics VLab

The Plankton Genomics VLab is developed in the context of the Demonstrator #2- Zoo- and Phytoplankton EOV products [12]. This environment focuses on plankton involving genomics analysis in its methodology. It showcases a deep assessment of plankton distributions, dynamics and fine-grained diversity to molecular resolution, focusing on two areas:

[9] https://github.com/gher-ulg/DIVAnd.jl

1. Species and functions discovery: discovery of as yet undescribed biodiversity from genetic and morphological signals from the characterisation of their geographical distributions, co-occurrences/exclusions and correlation with environmental contexts.
2. Biodiversity and ecology: exploration of genetic and morphological markers of plankton diversity and abundance, in particular the new ones discovered above, to predict their spatiotemporal distribution and serve as high-resolution EOVs for biological processes.

This VLab is available at https://blue-cloud.d4science.org/web/planktongenomics

This VLab has been in operational status since February 2021. It is currently serving 52 users distributed as in the following chart.

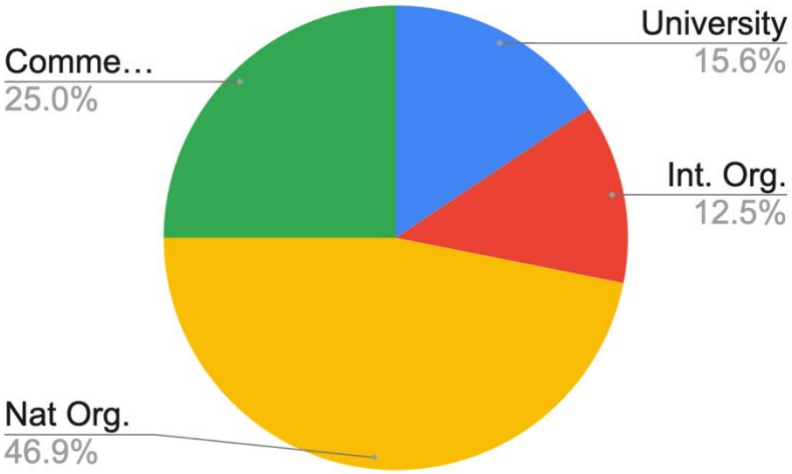

Figure 24. Plankton Genomics VLab Users Provenance

A screenshot of the VLab is available in Figure 25. It shows the Jupyter Notebook 1 developed in the JupyterHub VLab facility.

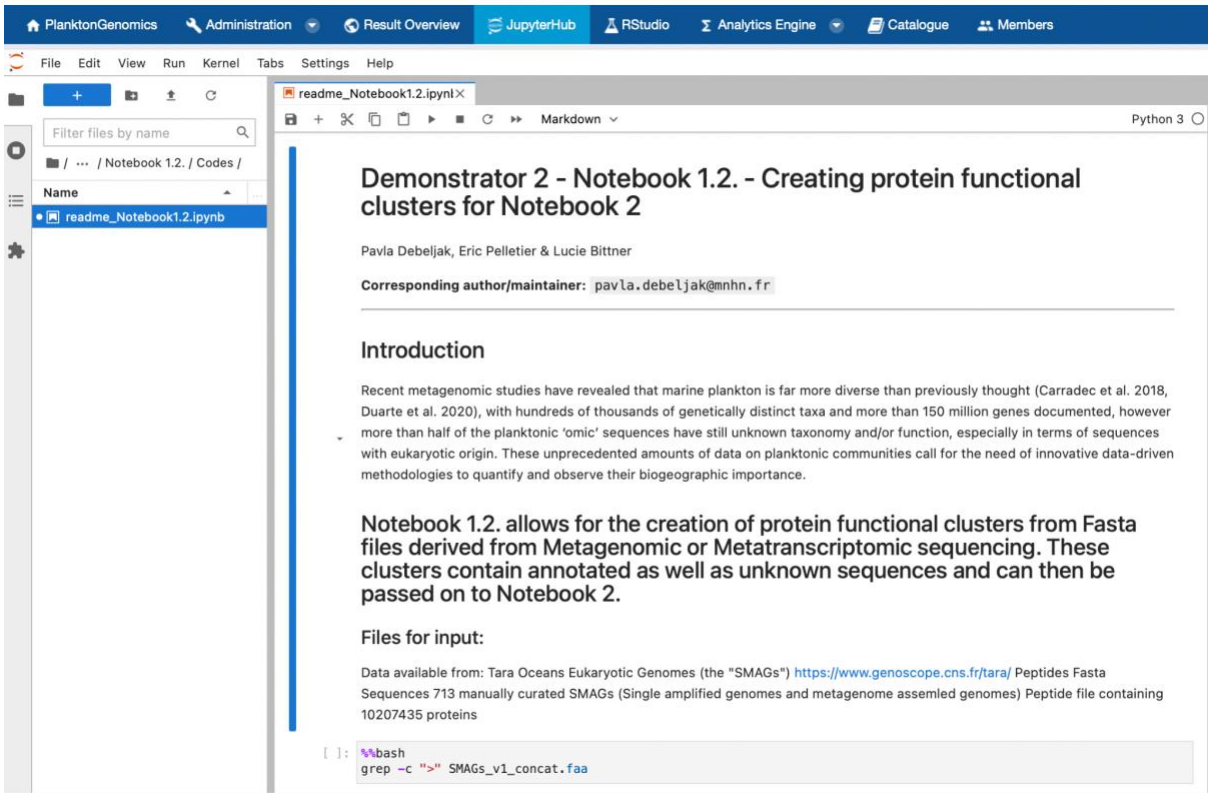

Figure 25. A screenshot of the Plankton Genomics VLab

4.1.9. Marine Environmental Indicators DEV VLab

The Marine Environmental Indicators DEV VLab is developed in the context of the Demonstrator #3 - Marine Environmental Indicators [2020d]. This is the development-oriented Virtual Lab supporting the Marine Environmental Indicators VLab. It is specifically needed by Demonstrator #3 developers in order to prepare and test new updates before the deployment to the "official" VLab (cf. Sec. 4.1.6) of this demonstrator #3.

This VLab has been in operational status since July 2022. It is currently serving 7 users.

4.2. Additional VLabs serving external user communities

4.2.1. Hackathon VLab

Over 7-9 February 2022, the Blue-Cloud Hackathon brought together nearly 150 participants from a diverse community of marine science practitioners, computer scientists and innovators to test Blue-Cloud's web-based ecosystem of Open Science services and resources to address selected Ocean challenges. The Blue-Cloud Hackathon has been an open invitation to marine scientists & researchers, data scientists, ICT experts, innovators, students, and anyone passionate about the Ocean to explore and test Blue-Cloud: A new, Open Science platform for the marine domain offering a wealth of data, analytical tools and computing power to support you in developing solutions for a

safe, healthy, productive, predictive and transparent Ocean.

Participants have been challenged to develop applications that contribute to improving knowledge of marine ecosystems; support the transition to a greener, blue economy; advance Ocean literacy; and/or enhance international collaboration towards achieving the Sustainable Development Goals (SDGs) of the United Nations Agenda 2030.

This VLab has been in operational status since November 2021. It is currently serving more than 160 users, however since the event was terminated in March 2022 it is no longer in use.

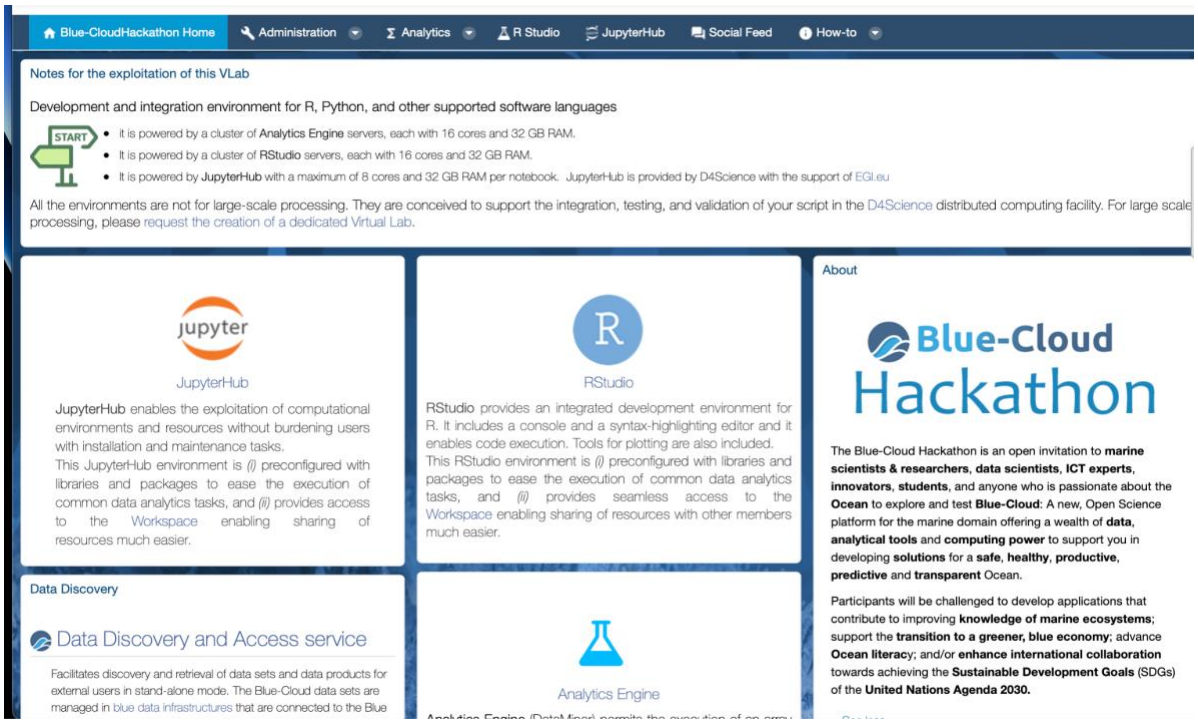

Figure 26. A screenshot of the Blue-Cloud Hackathon VLab

4.2.2. JERICO CORE VLab

The **JERICO CORE VLab** is developed as a pilot supporting the collaboration between Blue-Cloud VRE and the JERICO Coastal Oceans Resource Environment (JERICO CORE). The VLab offers to any JERICO user a working environment for JERICO CORE tools and data to further their research and application needs (Access is restricted to project users only).

This VLab has been in operational status since December 2021

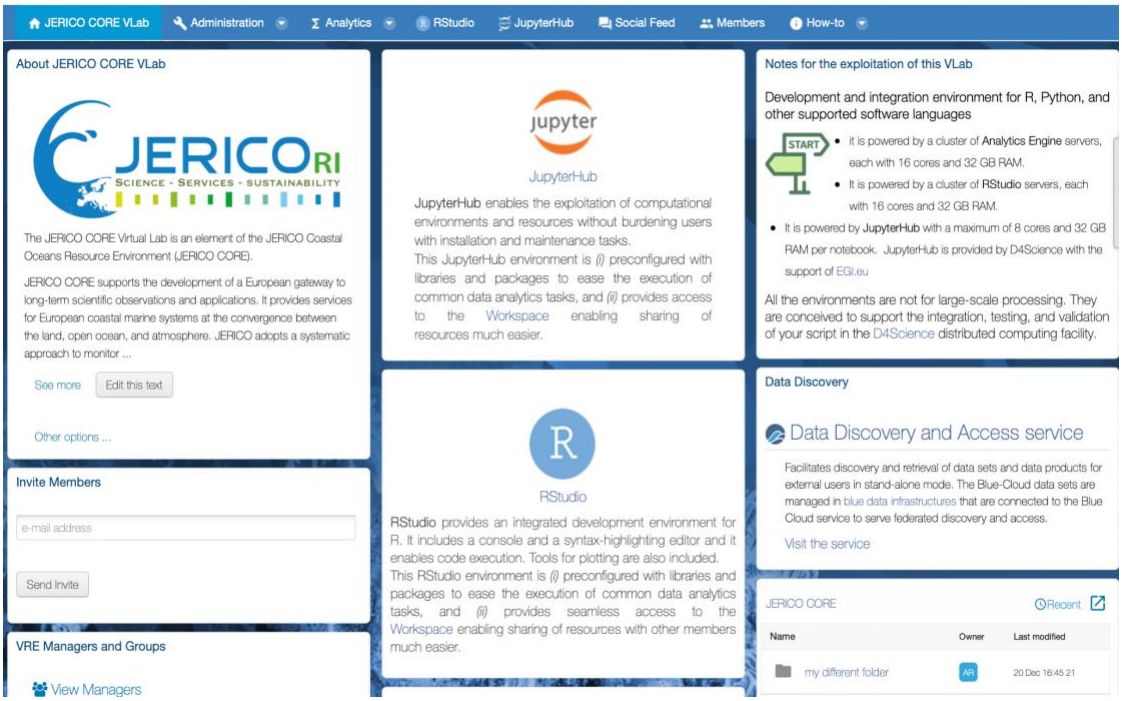

Figure 27. A screenshot of the JERICO-CORE VLab

4.2.3. JONAS VLab

The JONAS VLab is developed as a pilot supporting the JONAS Project - Joint Framework for Ocean Noise in the Atlantic Seas initiative. The VLab offers to any JONAS user a working environment for Blue-Cloud tools and data to further their research and application needs (Access is restricted to project users only). At the time of writing this VLab has just been created.

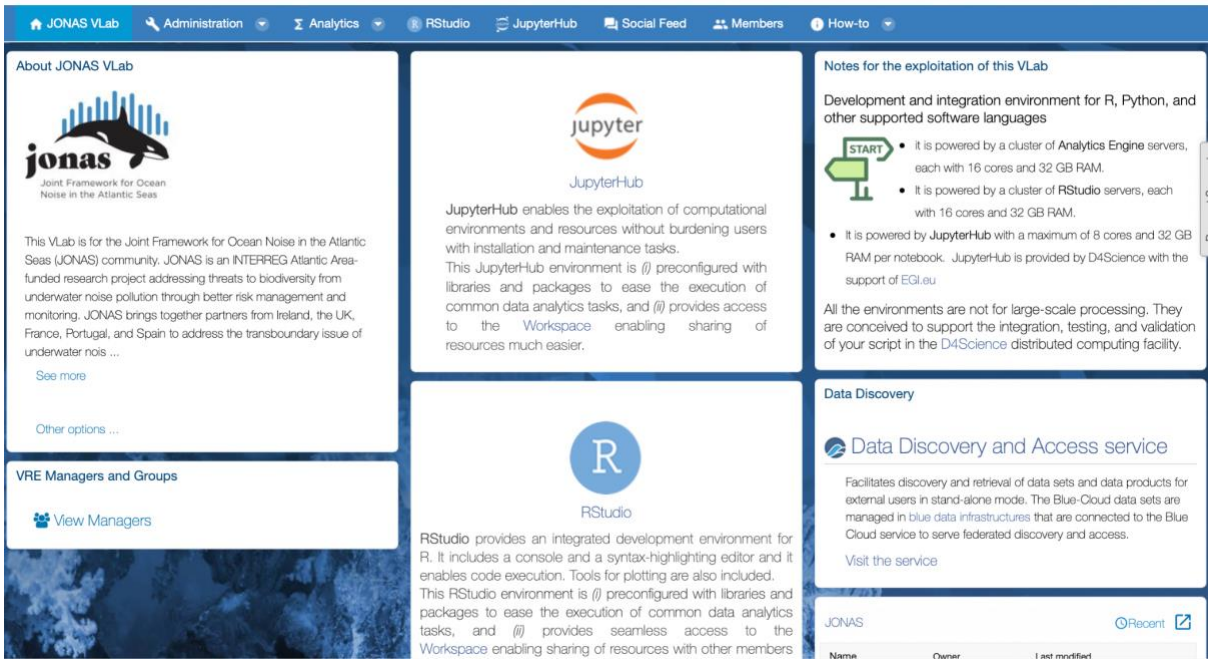

Figure 28. A screenshot of the JONAS VLab

Figure 22. A screenshot of the JONAS VLab

4.2.4. Training session on how to use and exploit the VLabs

In order to clarify aspects of usage of the VRE and the VLabs created, respond to questions from users from JERICO, Jonas and other projects that expressed interest in and investigate further functionalities needed, an online training session was organised on 7th of October 2022 aimed to present the potentialities and services included in the VRE following a use-case based approach. The training was led by Pasquale Pagano and Massimiliano Assante, managers of VRE and D4Science. Training materials are available on the JERICO Core and Jonas VLabs, on the Blue-Cloud Project VLab (see Section 4.3.2) as well as from the public Support Centre available online[10]

4.3. VLabs supporting project activities

4.3.1. Blue-Cloud Lab

The Blue-Cloud Lab VLab is developed to provide the Blue-Cloud community with a working environment to experiment with Blue-Cloud facilities. This VLab is available at https://blue-cloud.d4science.org/web/blue-cloudlab

This VLab has been in operational status since October '19, i.e., when the Blue-Cloud gateway was released. It is currently serving 210 users distributed as in the following chart.

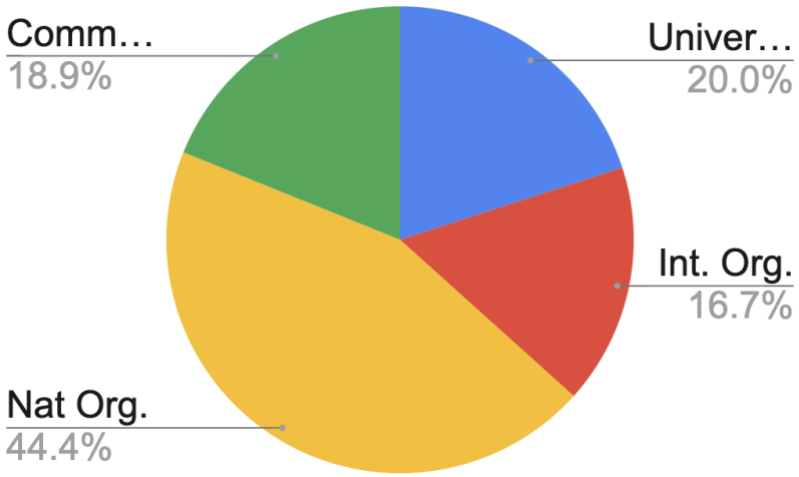

Figure 29. Blue-Cloud Lab VLab Users Provenance

A screenshot of the VLab is available in Figure 30. It shows the home page and the menu items for accessing the VLab facilities.

[10] https://blue-cloud.org/support-centre/support-material/

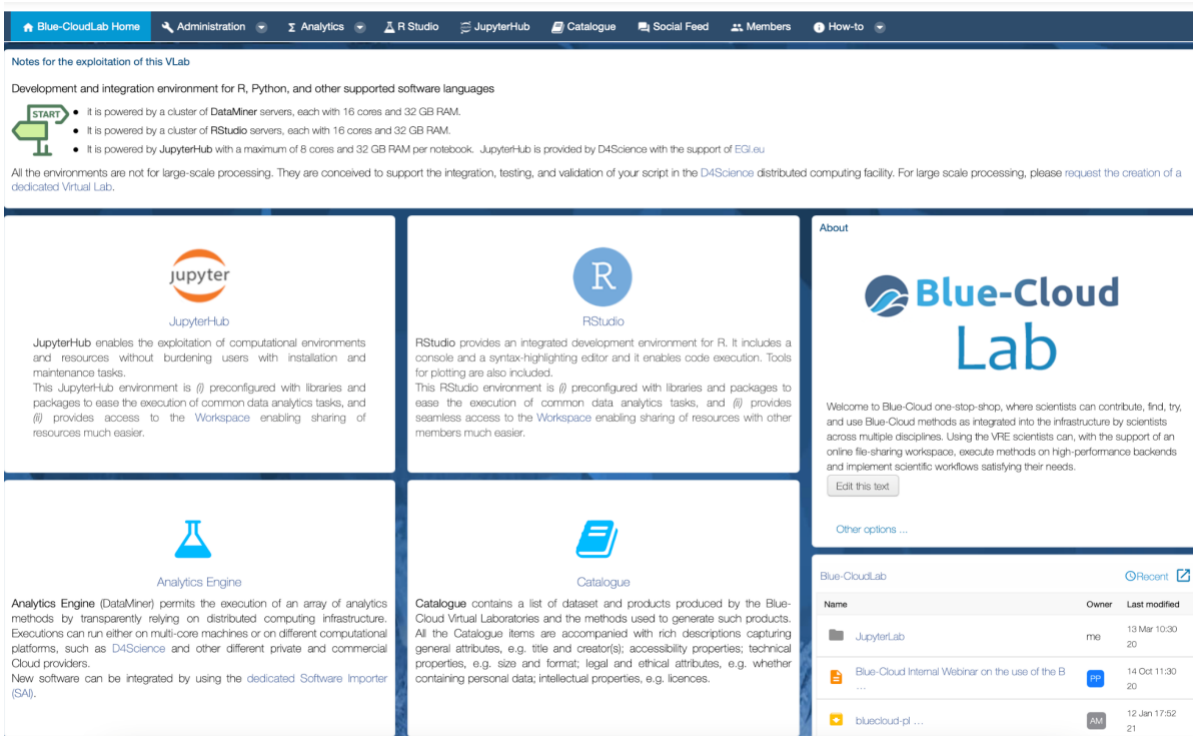

Figure 30. A screenshot of the Blue-Cloud Lab VLab at M35

In addition to the basic functionality, e.g., a workspace for sharing objects of interest and a user management facility for managing membership, this VLab is specifically equipped with the following functionalities:

- a ***data analytics facility*** enabling users to benefit from the offerings of the Data Miner service [1][2] and interactively execute a large array of data analytics tasks on datasets. As of January '21 the facility offers ***39 ready to use method implementations*** ranging from Bayesian methods to maps comparison and data clustering;
- the ***RStudio*** facility enabling users to use a fully-fledged RStudio® working environment directly from the VRE. This environment is integrated with the rest of VLab facilities, e.g., it is possible to use files from the workspace and to store new files within the workspace;
- the ***JupyterHub*** facility enabling users to develop and execute Jupyter notebooks. This environment is integrated with the rest of VLab facilities, e.g., it is possible to use files from the workspace and to store new files within the workspace;
- the ***Catalogue*** facility enabling users to publish, search and browse datasets and other products of interest for the specific use case.

4.3.2. Blue-Cloud Project VLab

The Blue-Cloud Project VLab was devised to support Blue-Cloud project activities and discussions. Only members of the Blue-Cloud consortium have access to it. The Blue-Cloud Project VRE is available at https://blue-cloud.d4science.org/web/blue-cloudproject

This VLab has been in operational status since October '19 and it is currently serving 130 users, namely the Blue-Cloud Consortium members. A screenshot of the VRE is provided in Figure 31. It shows the home page and the menu items for accessing the VLab facilities.

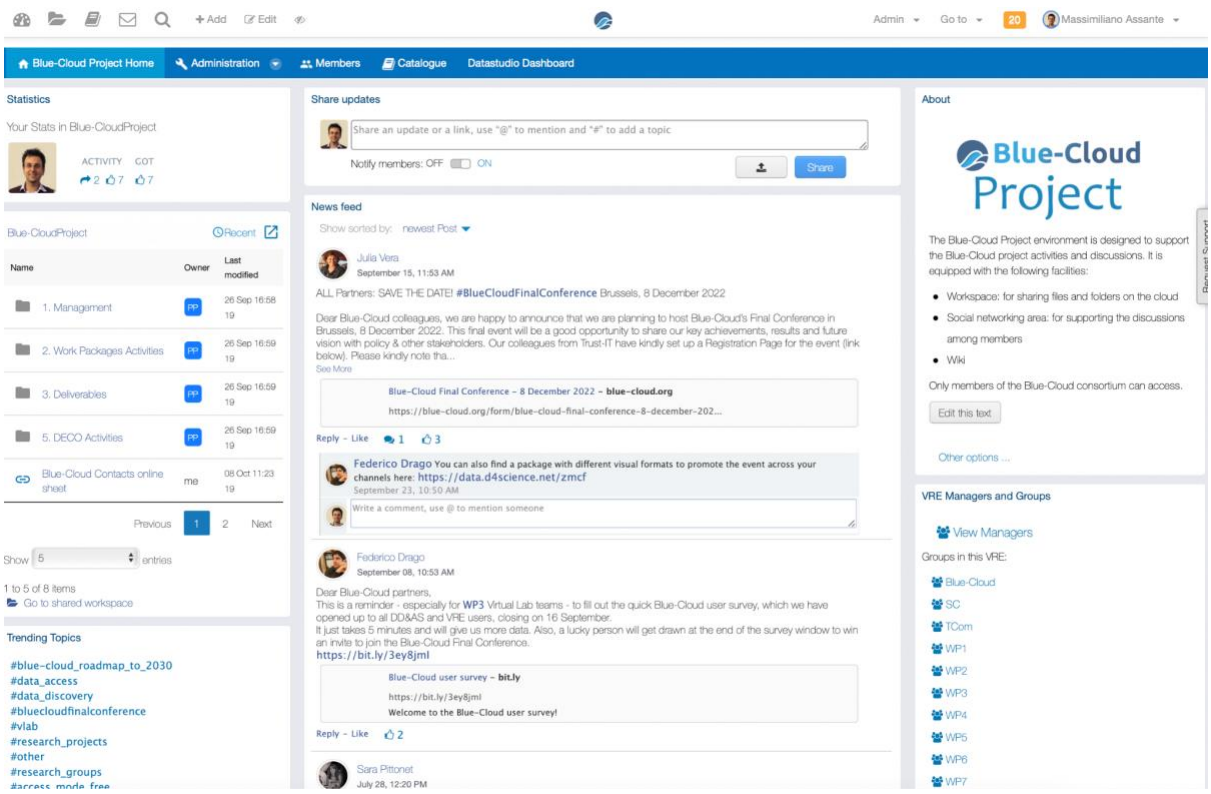

Figure 31. A screenshot of the blue-cloud Project VLab at M35

In addition to the basic functionality, as a social networking area for supporting the discussions among members and a user management facility for managing membership, this VLab is specifically equipped with a ***Catalogue*** facility enabling users to publish, search and browse products of interest for the specific community. In particular, this catalogue is planned to be populated with ***project deliverables*** and ***service descriptions*** characterising the service portfolio developed by the project.

5. Concluding Remarks

This deliverable presented the Blue Cloud Virtual Research Environment by complementing the architecture and infrastructure previously described in [5] where the constituents were discussed. In particular, this deliverable described how the constituents have been deployed, exploited, and operated to support the development of the Blue Cloud gateway, https://blue-cloud.d4science.org, its underlying infrastructure, and the VLabs.

In addition to the 9 Blue-Cloud VLabs created and operated in the first period, 5 Blue-Cloud VLabs were created and operated in the second reporting period. Seven (7) of available VLabs are conceived to support the developments of the Blue-Cloud Demonstrators, while the others are conceived to support project activities and/or to provide their users with development and demonstrative environments.

These working environments are serving more than 1,300 users in total spread across more than 77 countries and 236 institutions including universities, research infrastructures, and research institutes. Up to September 2022, a total of more than 25,700 working sessions have been executed by the users, with an average of 1,286 working sessions per month, since the start of the Blue-Cloud project in October 2019. A total of more than 2,230 analytics sessions have been executed by the users in the Demonstrator VLabs, with an average of 55 working sessions per month.

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