



D8.13 Operational version of the CLIMA VRE and user guide of the Virtual Research Environment dedicated to climate indicators



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<ul style="list-style-type: none"> • Author(s) (Partner-OU): 	<ul style="list-style-type: none"> • Marcello G. Magaldi, Daniele Lagomarsino-Oneto, Roberta Sciascia (CNR-ISMAR Lerici), Andrea Lira-Loarca, Giovanni Besio (Università di Genova), Lorenzo P. Corgnati and Carlo Mantovani (CNR-ISMAR Lerici)
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1. INTRODUCTION

Virtual Research Environments (VREs) are online collaborative platforms designed to integrate software tools, data, and computational resources into a unified workspace. VREs support their users – mainly researchers, but not only – in finding solutions and addressing scientific and/or management questions (Assante et al., 2023). VREs are intrinsically transdisciplinary as they may span various disciplines like environmental research, social sciences, healthcare and bioinformatics, enabling users to conduct innovative and data-driven research in an efficient and collaborative manner. Being inspired by the Open Science and Findable, Accessible, Interoperable and Reusable (FAIR, Wilkinson et al., 2016) principles, their primary goal is to overcome several challenges in many current research fields, such as data fragmentation, resource limitations, and barriers to collaboration. Following these directions, VREs can be used not only for enhancing collaborations across disciplines but also for managing and analyzing large datasets and for ensuring reproducibility of analyses and obtained results.

The development of VREs started in the early 2000s with the emergence of e-infrastructures such as grid computing and collaborative research platforms. The original idea of providing mainly computational resources evolved over time to create integrated platforms that could gather and host services related to the different steps of scientific studies. A social web approach was used in the “myExperiment” platform (De Roure et al., 2009) to provide researchers with mechanisms to support the sharing of workflows within and across multiple communities. A simple and general structure of a typical VRE was already proposed by Keraminiyage et al. (2009) and contained to the two key elements of VREs (Figure 1). Researchers, who may be geographically separated, may interact thanks to: a) human-computer interfaces, like user-friendly Graphical User Interfaces (GUIs) for computer software; and b) VRE capabilities (“embedded functionalities”) to achieve success factors of collaborative research, like project management factors which include tools to clearly define responsibilities, to plan and use adequate resources, to establish project milestones and to perform an effective communication among users.

In 2013, the establishment of the Research Data Alliance (RDA, <https://www.rd-alliance.org>) laid the ground for the current VRE concept. Indeed, the RDA mission is to “build the social and technical bridges that enable open sharing and re-use of data” while its vision establishes that “researchers and innovators openly share and re-use data across technologies, disciplines, and countries to address the grand challenges of society”. In the last survey presented in February 2024, the RDA counts more than 14000 members, coming from more than 150 countries worldwide. Although the majority (around 70%) of the members belong to academia and research, several other types of organizations are represented in RDA as governmental and public bodies, press and media, funding agencies and large as well as small and medium enterprises (Figure 2). Such a variety of members underlines the collaborative potential of VREs.

The current level of maturity achieved by VREs is exemplified by the D4Science experience (Assante et al., 2019a; Candela et al., 2023), established as part of the European e-infrastructure initiative. Its goal is to support cross-disciplinary collaboration and open science by integrating tools and services into a cohesive environment. The D4Science structure (Figure 3) builds up on both the human-computer interfaces and the embedded functionalities of the early ideas but is more complex including external resource providers and both front and backend components (see also section 2 for more details).

Virtual Research Environments may represent one way research is conducted in the future, fostering innovation, collaboration, and efficiency. By leveraging platforms like D4Science, researchers can

overcome traditional barriers and engage in cutting-edge, inter- and transdisciplinary projects. As digital technologies continue to advance, VREs are expected to play an even greater role in shaping the future of scientific research.

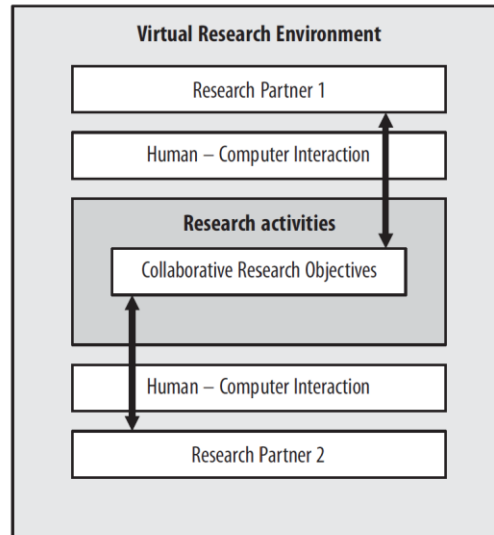


Figure 1: Structure of a typical VRE as put forth by Keraminiyage et al. (2009).

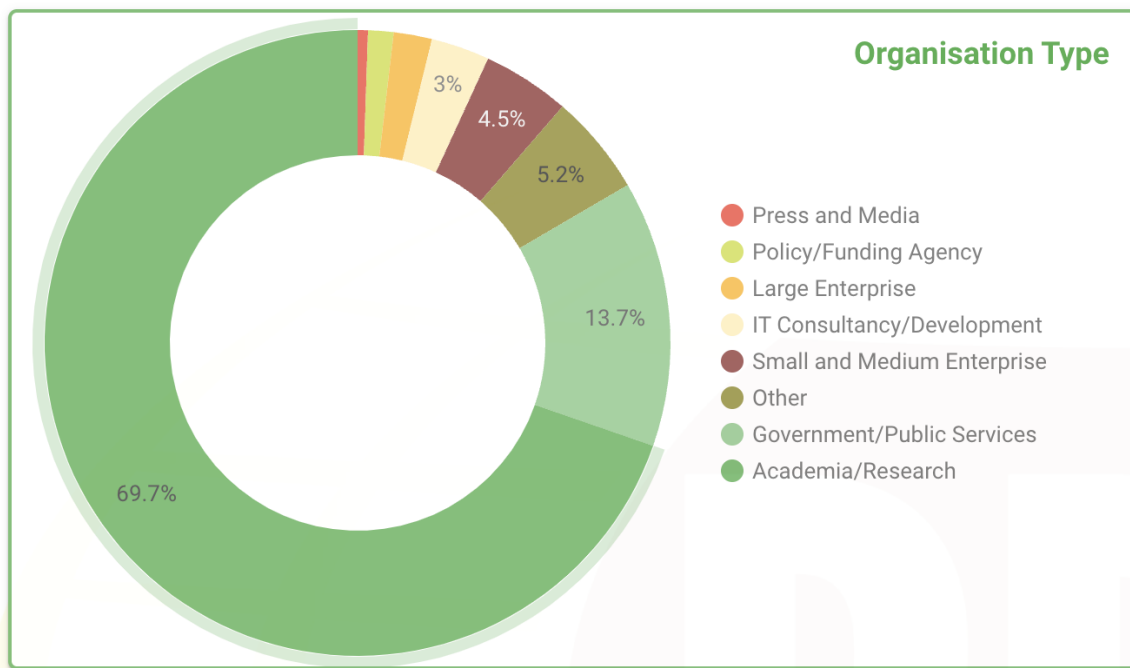


Figure 2: Distribution of members of the Research Data Alliance (RDA) by organization types introduced in February 2024 (source: <https://www.rd-alliance.org>).

Climate and climate change indicators

Climate change is one of the grand challenges of the 21st century, influencing every aspect of human and environmental systems. Its impacts – ranging from rising global temperatures and sea levels to extreme weather events – demand immediate and sustained actions. The last “State of the Climate in 2023” published by the American Meteorological Society points out that 2023 was the warmest year on record for North America, South America, and Africa. It was also the warmest year for Europe according to some datasets, while others put it in second place as for Asia (Blunden and Boyer, 2024). According to the International Renewable Energy Agency (IRENA), addressing climate change not only mitigates its impacts but also creates opportunities for innovation, job creation, and technological advancements. Transitioning to a low-carbon economy, for instance, fosters the development of renewable energy technologies and energy-efficient systems, contributing to sustainable economic growth (IRENA 2023; IRENA et al., 2024).

Climate change is also considered among the United Nations’ Sustainable Development Goals (SDGs, <https://www.un.org/sustainabledevelopment>) as they provide a universal framework for achieving a sustainable and equitable future. “Climate action” (SDG 13) is explicitly focused on combating climate change and its impacts, but addressing climate change is also at the basis for the success of other goals like:

- “No Poverty” (SDG 1): climate change exacerbates poverty by increasing vulnerability to natural disasters and disrupting livelihoods, especially in developing countries;
- “Zero Hunger” (SDG 2): rising temperatures and unpredictable weather patterns threaten food security by reducing agricultural productivity;
- “Clean Water and Sanitation” (SDG 6): climate change affects freshwater availability through altered precipitation patterns and glacier melt;
- “Life Below Water” (SDG 14) and “Life on Land” (SDG 15): ecosystems face unprecedented stresses due to climate-induced changes, threatening biodiversity.

Climate change is also the cornerstone of the current scientific strategies of many European Research Infrastructures (RIs) which play a fundamental role in both advancing climate science and informing policy decisions. The Integrated Carbon Observation System (ICOS, <https://www.icos-ri.eu>), for example, monitors greenhouse gas concentrations and fluxes across Europe, providing critical data for understanding carbon cycles and verifying emissions reductions. Its standardized observations support the development of effective climate policies. The LifeWatch research infrastructure (<https://www.lifewatch.eu>) focuses on biodiversity and ecosystem research, leveraging advanced technologies to study the impacts of climate change on species distribution and ecosystem services. The European Long-Term Ecosystem Research (eLTER, <https://elter-ri.eu>) addresses ecosystem responses to environmental changes, including climate dynamics. By integrating long-term datasets, eLTER improves predictions of ecosystem resilience and guides sustainable land-use practices. The DANUBIUS research infrastructure (<https://www.danubius-ri.de>) investigates river-sea systems, which are highly sensitive to climate change. Its research focuses on understanding sediment transport, water quality, and habitat changes, informing sustainable management of these critical interfaces. The Joint panEuropean Research Infrastructure for Coastal Observatories (JERICO, <https://www.jerico-ri.eu>) is specialized in coastal and marine observations, providing insights into ocean-atmosphere interactions and the impacts of climate variability on marine ecosystems. JERICO scientific strategy is based upon the three following Key Scientific Challenges (KSCs), all directly related to climate change:

- KSC#1: assessing and predicting the changes of coastal marine systems under the combined influence of global and local drivers;
- KSC#2: assessing the impact of rare/extreme events;
- KSC#3: unravelling the effects of climate and anthropogenic changes.

As underlined in Deliverable 8.3, climate indicators are essential for tracking changes in the Earth's climate system and evaluating the effectiveness of mitigation and adaptation measures. For example, indicators such as global surface temperature, sea level rise, and greenhouse gas concentrations are identified in the State of the Global Climate Series of the World Meteorological Organization (WMO) and offer scientific and quantifiable evidence of climate trends (e.g. WMO, 2023). Indicators help communicate the urgency of climate action to a broader audience, fostering societal engagement and behavioral change (OECD 1993; EEA 2017, 2023). They are also used for policy analysis and guidance as decision-makers are encouraged to look at them to design targeted interventions, monitor progress towards international commitments – like the Paris Agreement (<https://unfccc.int/process-and-meetings/the-paris-agreement>) – and allocate resources effectively. By integrating robust climate indicators into research and policymaking, societies can better anticipate risks, adapt to changes, and build resilience.

Following these directions, Activity 8.7 of the ITINERIS project is focused on developing the so-called “CLIMA VRE” which is a Virtual Research Environment to gather climatic variables from the different RIs of the project with the aim of identifying and developing climate indicators. The CLIMA VRE also considers extra-RI datasets coming from other initiatives funded by the European Union, like both the Copernicus Climate Change and the Copernicus Marine Services.

Scope and structure of the deliverable

This deliverable D8.13, together with the other two deliverables D8.12 and D8.14, represents the ITINERIS Intermediate Objective IO8.8 and aims to provide the user guide of the CLIMA VRE in its first operative, though not final, version. It must be also seen as another step for the full operative version of the CLIMA VRE which represents a specific objective (OBJ7) of the WP8 “Virtual Research Environments and Cross-disciplinary Activities” of the ITINERIS project.

The discussion within this deliverable is limited to the D4Science e-infrastructure (see section 2) since it is the one used by the CLIMA VRE and by the majority of the other VREs developed or under development in the WP8 of the ITINERIS project. There are several examples of other e-infrastructures like:

- the “VRE-Hub” developed at the European Organization for Nuclear Research (CERN, <https://vre-hub.github.io>) mainly in the fields of high-energy physics and astrophysics;
- the “BIH-VRE” offered by the Berlin Institute of Health at Charité (BIH, <https://www.bihealth.org>) for treating medical and health data;
- the “LifeWatch VREs” by the same research infrastructure to support ecological and biodiversity research and which include the ones developed by the Italian national node (<https://www.lifewatchitaly.eu/laboratori-virtuali>) on alien and invasive species and phytoplankton;
- the more specific “Swarm VRE” developed by the European Space Agency (ESA, <https://earth.esa.int/eogateway/tools/swarm-vre>) to analyse data from ESA's Swarm satellite mission dedicated to the measures of the Earth's geomagnetic field;
- the “EGI Federation” coordinated by the EGI Foundation (<https://www.egi.eu>) which is an international e-infrastructure set up to provide advanced computing and data analytics

services for research and innovation and includes national and intergovernmental computing and data centres spread across Europe and worldwide;

- the “EUDAT Collaborative Data infrastructure” (<https://eudat.eu>) supported by both the European Union General Directorates of Technology Research and Innovation (DG RTD) and of Communications Networks, Content and Technology (DG CONNECT). It offers heterogeneous research data management services and storage resources through its network of academic computing and data centres across 15 European nations, whereby data is stored alongside some of Europe’s most powerful supercomputers.

The description of the above e-infrastructures is beyond the scope of this document. In this deliverable D8.13, the user guide of the CLIMA VRE is provided in Section 2. In the first part of Section 2, the focus is on the D4Science infrastructure and on the specific gateway created on purpose for the ITINERIS project. The second part of the same section deals with the specific dashboard for the CLIMA VRE. A demonstration of the VRE operativity is provided in Section 3 with the interactive application for the Italian Sea Surface Temperature Demonstrator (ISSTD). Conclusions are drawn in Section 4 together with next steps and indications for the CLIMA VRE’s further development.

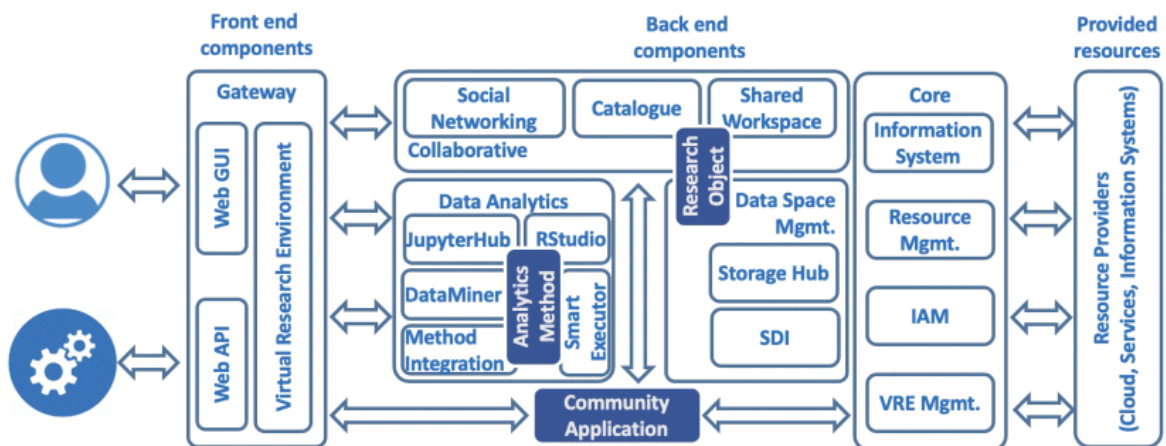


Figure 3: The D4Science service-oriented architecture shown in Candela et al. (2023). API: application programming interface; IAM: identity and access management; Mgmt.: management; SDI: spatial data infrastructure.

2. USER GUIDE OF THE ITINERIS CLIMA VRE

The CLIMA VRE is one of the virtual research environments developed within the ITINERIS project thanks to D4Science. It inherits important embedded functionalities as it uses a D4Science gateway specifically created for the project. These functionalities are described in the following paragraphs together with the general D4Science architecture.

The D4Science e-infrastructure

D4Science is an e-infrastructure designed to support data-intensive science by integrating resources, tools, and services across a wide variety of domains. To date, D4Science users are more than 24000 coming from more than 50 countries worldwide and using more than 170 different VREs. Its architecture (Figure 3) ensures scalability, flexibility, and interoperability, enabling collaboration among diverse communities (Assante et al., 2023; Candela et al., 2023). D4Science relies on the “gCube system” (Assante et al., 2019b, <https://www.gcube-system.org>) which is specifically designed to support the development and operation of VREs. The gCube system organizes and manages the infrastructure's various components, offering connections with the provided resources and both front-end and back-end functionalities. Users can interact directly with the e-infrastructure thanks to the front-end component while the logic of the system is implemented by the back-end component. The component dealing with the provided resources is the D4Science part providing both front-end and back-end components with resources, like computing, storage, data and software (Assante et al., 2023). The gCube system has the following main core functionalities (Assante et al., 2019b):

- the Information System: it acts as the registry of the entire infrastructure. It gives global and partial views of the resources and their operational state through query answering or notifications;
- the Resource Management: it is responsible for resource discovery, allocation, and monitoring. This ensures optimal utilization of computational and storage resources across the infrastructure;
- the Identity and Access Management system: it is the critical functionality for ensuring secure, controlled, and efficient access to the D4Science array of resources and services. This system is designed to address authentication, authorization, and auditing needs while maintaining flexibility and scalability to support diverse user groups and applications. It supports multiple authentication methods including:
 - the username and password method: it is the most common method for individual user accounts;
 - the OAuth2 Authorization Framework (Hardt, 2012): it provides secure and token-based access, often used for integrations with external applications;
 - the Federated Identity Providers: it allows users to authenticate using third-party systems, such as institutional logins or social identity providers (e.g. like Google or LinkedIn), through protocols like the Security Assertion Markup Language (SAML, OASIS 2005) or OpenID Connect (OpenID, 2014);
- the VRE management: it ensures the correct and optimal support for the specifications of each VRE in terms of both data and services. It consists of the following three phases:
 - a design phase: where authorised users can specify their needs for data and services for their virtual environment request;
 - a deployment phase: where D4Science administrators can approve a VRE request with relative specifications. Once approved, the deployment starts and the authorized users casting the VRE request act as VRE managers. VRE managers are enacted to monitor the automatic deployment of the real components needed to satisfy the specification request;

- an operation phase where authorised users are provided with facilities for managing the user of the VRE and changing the VRE services if needed.

Besides the custom-tailored requests by the users, in the D4Science architecture, each VRE is furnished with the following basic functionalities supporting collaboration and cooperation among its users (Assante et al., 2019a):

- a shared workspace: to store, organize and work on any document, tool or dataset useful for a specific research;
- a social networking area: to have discussions and inform the community on any topic (including working versions and releases of documents, tools or datasets);
- a data analytics platform: to execute data processing tasks either provided by the same VRE users or borrowed from other VREs or external sources;
- a catalogue-based publishing platform: to disseminate and make public any document, tool or dataset.

Each of the above functionalities germane to the operativity of the CLIMA VRE is briefly described in the next paragraphs.

The ITINERIS gateway and the social networking area

In the D4Science e-infrastructure, a gateway, often referred to as a Science Gateway, acts as a single entry point to similar VREs serving a particular research community, providing applications and services relevant to their scientific field. This customization ensures that users belonging to a community have a similar access to the tools necessary for data analysis, visualization, and other research activities. Following this direction, the D4Science ITINERIS VRE Gateway (<https://itineris.d4science.org>) was specifically designed for the ITINERIS project. Using the D4Science Identity and Access Management system, users can login with one of the methods listed above to enter the so-called ITINERIS Gateway dashboard (Figure 4). On the top left corner, on the side of the ITINERIS logo, the dashboard includes direct links to the shared workspace service (see below for details) and the message service which are denoted with two icons, an open folder and a closed letter envelope, respectively. On the top right corner, the user can set options for both her/his D4Science account and VRE profile (as the avatar and the password) as well as how to receive notifications for specific services like for the workspace, the social network area and the catalogue.

On the right side of the dashboard, under the “My Virtual Research Environments” tab, there are the links with the ITINERIS VREs users have already access to (namely the CLIMA, Critical Zone and Essential Variables VREs in the example of Figure 4). By clicking on the “Add more” button and by providing a mandatory motivation, users can request access to the other VREs available in the ITINERIS gateway (namely the AERO, ANAEE, Carbon, Downstream and Isotope VREs in the example of Figure 4, corresponding on the remaining Activities of the WP8 of the project). Users will be able to access the VRE once they are granted permission by one of the specific VRE managers. On the left side of the dashboard, under the “user home” tab, there is a direct link to the special shared folders for each VRE (see below for more details), considering also VREs belonging to other D4Science gateways (like the FisheriesAtlas VRE folder in the example of Figure 4).

In the middle of the dashboard, under the “News Feed” tab, there is a direct link with the social networking area of the D4Science gateway where VRE members can exchange ideas, inform and discuss with the other members about any topic using the usual social network rules, including the creation of new posts, tags (“@” to directly tag one member, “#” to refer to specific themes or keywords), interactions (thumb ups, direct reply and comment to a specific post), etc...

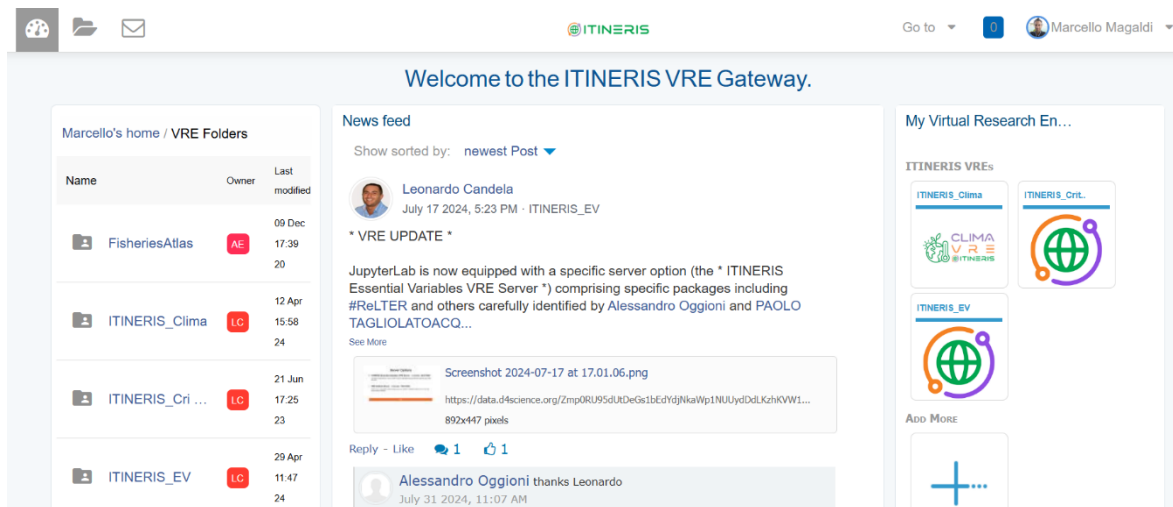


Figure 4: A screenshot of the D4Science ITINERIS Gateway dashboard.

The shared workspace

Figure 5 shows a screenshot of the D4Science shared workspace (Assante et al., 2019a). The service looks like a typical file manager showing file system structure with files organized in folders. A simple right click of the mouse activates the drop-down menu visible in Figure 5 which allows users to upload and download files, create private folders, publish data in the catalogue and share folders and data with other users. Each user has her/his own workspace named after her/him (for example “Leonardo’s workspace” as visible in the top left corner of Figure 5). In the user workspace, a special folder named “VRE folders” is recognizable by a white star (just below the “Leonardo’s workspace” in Figure 5). Documents, tools or datasets placed in this special folder are automatically shared with the other members of the VRE. Each other folder created under the workspace remains private (like for example the “CNR OpenScience TF private spaces” folder in Figure 5) until the user decides to share it with the usual permission rules:

- “Write Any”: all users can modify the content of the created folder;
- “Read Only”: only the user that created the folder can modify its content, all other users are only allowed to read;
- “Write Own”: users can only modify the content they created under the folder.

The workspace is also provided with a version control system to keep track of any file version uploaded to the workspace. Once selected a file, users can see all other versions by right-clicking on it and by clicking on “Versions”.

The CLIMA VRE dashboard

A user can enter the CLIMA VRE environment after having requested and obtained access to it. It is then welcomed by the so-called CLIMA VRE dashboard (Figure 6). On the top left corner, always on the side of the ITINERIS logo, the dashboard includes direct links to go back to the gateway dashboard, to the gateway shared workspace, catalogue and message services. The user can also search for specific keywords in the “News Feed” and start interacting with the social networking area of the gateway.

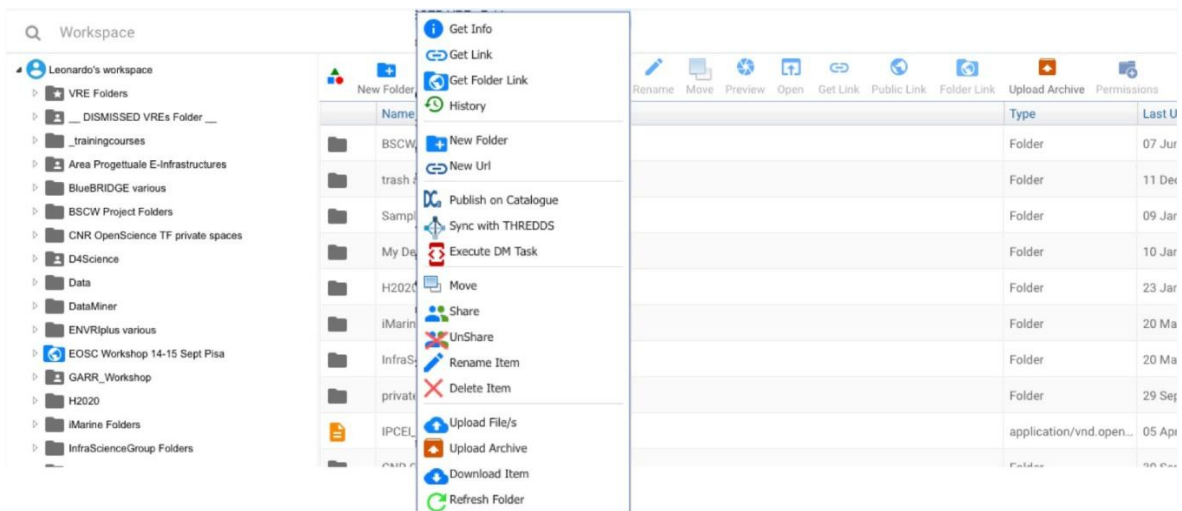


Figure 5: A screenshot of the D4Science shared workspace service shown in Assante et al. (2019).

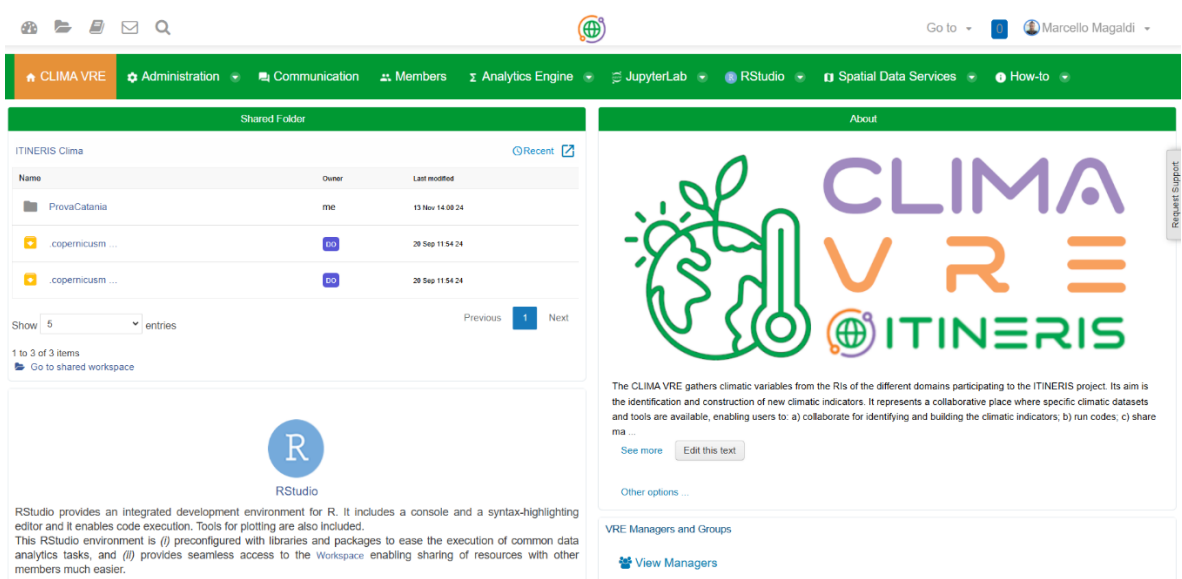


Figure 6: A screenshot of the CLIMA VRE dashboard.

On the right side of the CLIMA VRE dashboard, under the “About” tab lies a description of the CLIMA VRE together with its temporary logo. Just below it, there is a direct link to the profiles of the CLIMA VRE managers. On the left side, under the “Shared Folder” tab lies a link with the workspace service directly targeting the shared VRE folder named “ITINERIS Clima”. Just below it there is a link and a description of the RStudio service (see below for details).

The horizontal bar of the navigation menu is the most important part of the CLIMA VRE dashboard as it provides links to the specific functionalities of the virtual research environment which are described next.

The “Administration” section

The Administration section provides functionalities to VRE managers to manage users and groups, and to ensure a smooth operation of the VRE. It includes the following key features:

- “Manage Users and Groups”: it allows administrators to oversee the user base and group configurations. This includes assigning users to groups, defining roles and permissions, and modifying group structures to suit the needs of the VRE;
- “See Invites”: it provides a view of all pending invitations sent to potential VRE members. VRE managers can track the status of these invites, resend them if needed, or revoke them;
- “Create New User”: it enables VRE managers to manually create new user accounts, bypassing the invitation process. This functionality is particularly useful for adding members who may not have initiated their own registration;
- “Add Existing Users”: it facilitates adding users who are already registered within the D4Science infrastructure to the specific VRE. This ensures a quicker integration of existing community members;
- “Accounting Dashboard”: it offers an overview of resource usage and allocation within the VRE. Administrators can monitor computational resources, storage consumption, and other relevant metrics to ensure optimal utilization and identify potential bottlenecks. Figure 7 shows, as an example, the number of accesses to the JupyterLab service since the CLIMA VRE creation. The clear peak in October 2024 is due to the development of the demonstrator.

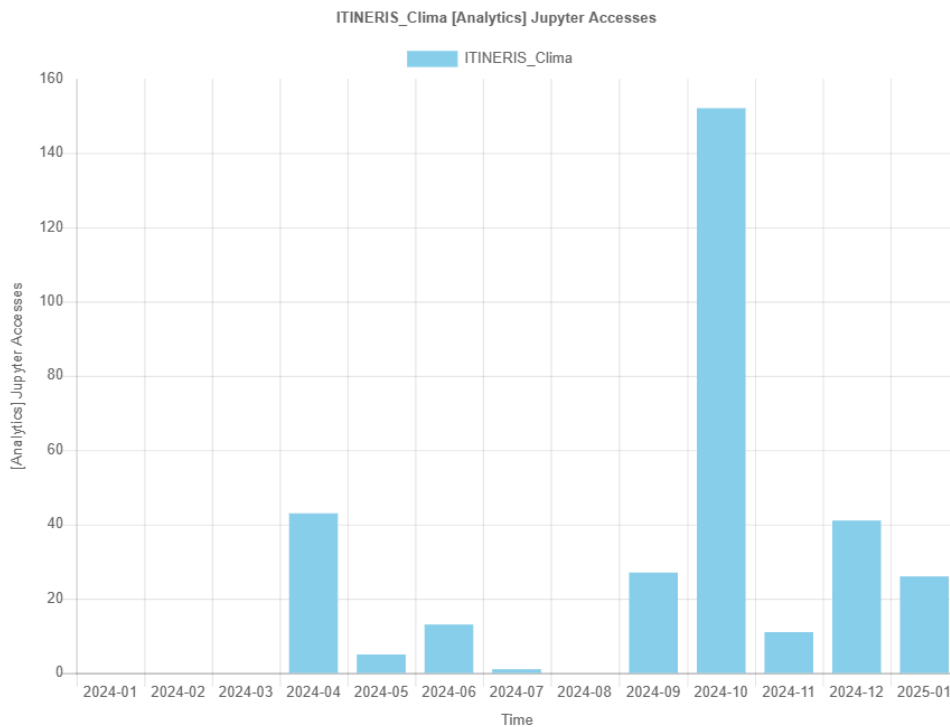


Figure 7: A screenshot of the CLIMA VRE accounting dashboard showing the accesses over time to the JupyterLab service.

The “Communication” section

The Communication Section represents the social networking area, called also “News Feed”, of the specific VRE. It is designed to foster collaboration and share information among VRE members and is the hub for exchanging messages, sharing updates, and maintaining active engagement within the VRE community. As also already described above, under this section, users can directly:

- share updates about new resources and media;
- send and receive private messages to/from other users through an Individual Messaging system;
- request technical support from the VRE managers or advice from other peers;
- have a look and decide to participate in threaded VRE discussions in the forum or discussion boards.

The “Members” section

This section allows users to view all other members of the VRE. It simply includes a member directory with a list of all registered members of the VRE, along with their roles and profiles. At the moment, 23 members are registered to the CLIMA VRE.

The “Analytics Engine” section

The Analytics Engine section provides advanced tools for data analysis. It is particularly useful for performing data mining operations, i.e. for analyzing large databases in order to generate new information. At the moment, this section is experimental for the CLIMA VRE, it does not include the DataMiner manager Web Interface (Coro et al., 2017) but only the more recent Cloud Computing Platform (CCP) service together with the relative CPP Method Importer tool (<https://ccp.cloud.d4science.org/docs>). The CPP represents the evolution of the Data Miner and allows users to execute predefined methods and monitor their execution. The Method Importer is the tool to define new methods, as well as manage and edit existing ones. The methods are gathered in categories according to their functionalities and have their own characteristics like:

- the name and version number: to indicate updates or improvements;
- the name of the author(s): the person(s) responsible for creating or maintaining the methods;
- the description: a brief explanation of the method’s purpose or functionality;
- the tags: relevant keyword that are pertinent for the methods.

By using the CPP service, users can select the methods to be executed in the “Methods List” section, execute them by filling the “Method Execution” form, and monitor their execution in the “Execution Monitor” section, which tracks scheduled, pending, and finished data processing jobs.

The “JupyterLab” section

This section gives access to the JupyterLab service by starting dedicated virtual servers. In the CLIMA VRE, users can either start a default VRE server which uses 4 cores for a total RAM of 16 GB or a larger and dedicated CLIMA VRE server which uses 16 cores with 64GB of RAM (Figure 8). Both server options are equipped with preinstalled modules and packages.

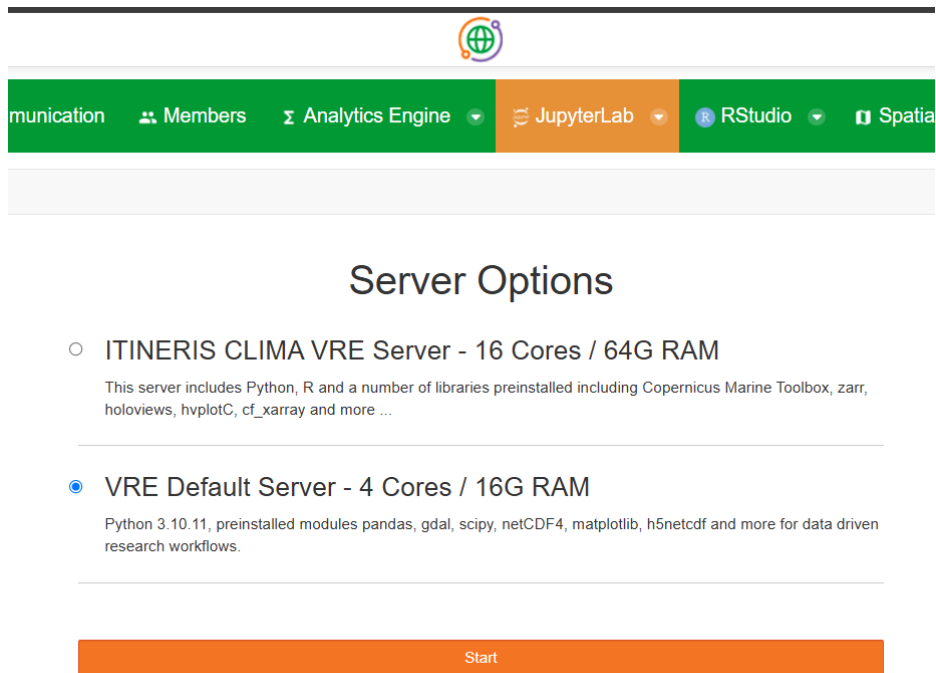


Figure 8: A screenshot of the JupyterLab section showing the two server options available for the CLIMA VRE.

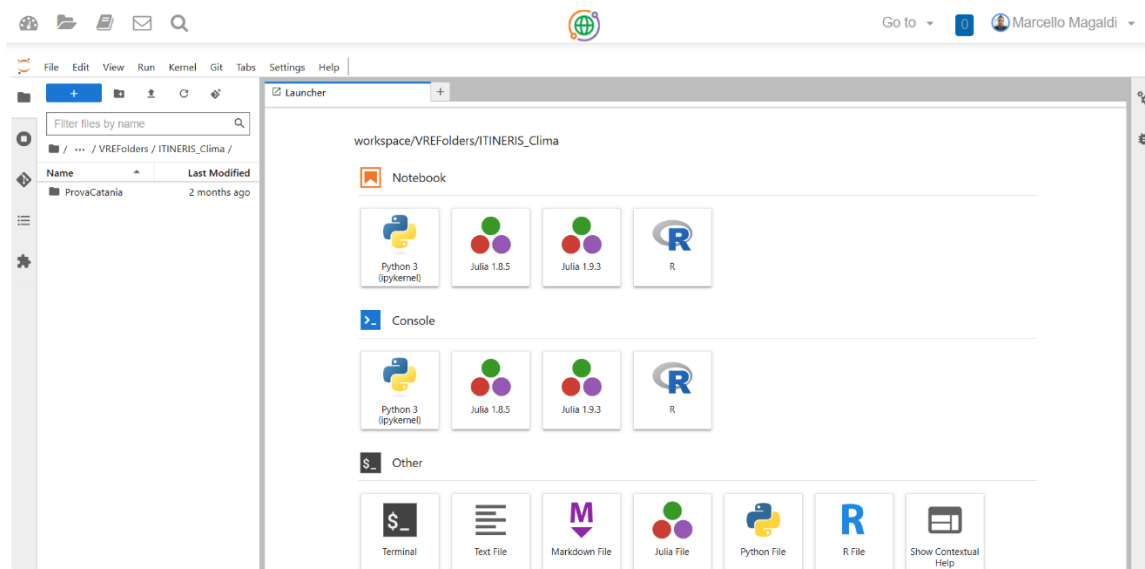


Figure 9: A screenshot of the JupyterLab Launcher showing the different software usable within the CLIMA VRE.

Speed test for the 16-core VM on a demanding dataset

Andrea Lira-Loarca and Marcello G. Magaldi

October, 2024, version 1.1

Import needed toolboxes

```
In [1]: import xarray as xr
import hvplot.xarray
from dask.diagnostics import ProgressBar
```

Install Google Cloud Storage File System (GCSFS) package - not needed when proper environment is setup

```
In [2]: pip install gcsfs
```

Figure 10: A screenshot of the initial part of the Speed test notebook of the CLIMA VRE.

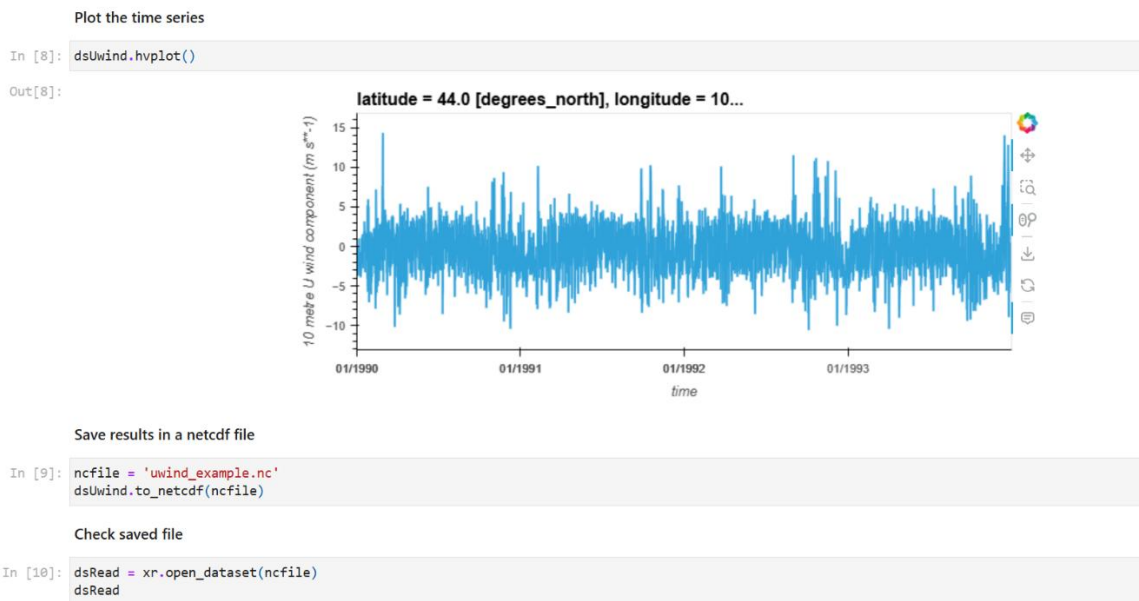


Figure 11: A screenshot of the final part of the Speed test notebook of the CLIMA VRE showing the 4-year time series for the closest point (44°N, 10°E) to Lerici (44°04'34.54"N, 9°54'39.96"E). The time series can be interactively explored thanks to the widgets on the right side of the plot.

JupyterLab (<https://jupyterlab.readthedocs.io>) is a flexible, web-based Integrated Development Environment (IDE) for interactive computing. It is the evolution of the Jupyter project (<https://jupyter.org>) and provides a powerful platform for data analysis, scientific computing, and machine learning, empowering researchers, developers, and data analysts to work efficiently with code, data, and visualizations. JupyterLab relies heavily on the use of the so-called “notebooks” which are interactive documents that combine in a single file live pieces of codes or scripts, equations, visualizations, and comments in the form of normal text expressed through the Markdown language (<https://daringfireball.net/projects/markdown>). JupyterLab supports over 100

programming languages (through the specific and so-called “kernels” in the Jupyter ecosystem, <https://github.com/jupyter/jupyter/wiki/Jupyter-kernels>) including Python, Java, R, Julia, Matlab, Octave, Fortran, C, Perl, Ruby, SQL and many more. Besides notebooks, JupyterLab provides a highly customizable, multi-document interface that enables users to work also with: a) text editors: to edit code, scripts, or plain-text files with syntax highlighting and rich language support; b) terminals: to access the underlying system shell for executing commands; c) file viewers: to open and interact with various file types, such as images, Markdown, Python, Julia and R files (Figure 9).

The JupyterLab is, at the moment, the main service offered by the CLIMA VRE (see also Figure 7) and also the service under which the Italian Sea Surface Temperature Demonstrator (see Section 3) has been developing.

As an example application, a “Speed test” notebook using Python is available in the CLIMA VRE (Figures 10 and 11). The script contained in the notebook gets accessed to the large (~90TB) cloud-optimized ERA5 data available on Google Cloud Storage (GCS, <https://cloud.google.com/storage/docs/public-datasets/era5>) to extract and save a full 4-year time series (from 1990 to 1993) for the zonal 10-m wind component for the town of Lerici. Using the dedicated CLIMA VRE server with 16 cores, the information are extracted and the final file (~400KB) is saved after less than 10 minutes in the Network Common Data Format (NetCDF, <https://www.unidata.ucar.edu/software/netcdf>). The script uses specific Python packages like “hvPlot” (see Section 3 for details) to control the obtained plot and interactively explore the large dataset with widgets (Figure 11).

The “RStudio” section

This section gives access to the RStudio service by starting, as in the case of the JupyterLab, a dedicated virtual server. In the CLIMA VRE, at the moment, users can only start a standard VRE v4 RStudio server which uses 4 cores for a total RAM of 8 GB (Figure 12). The standard server is equipped with community libraries preinstalled for the R software.

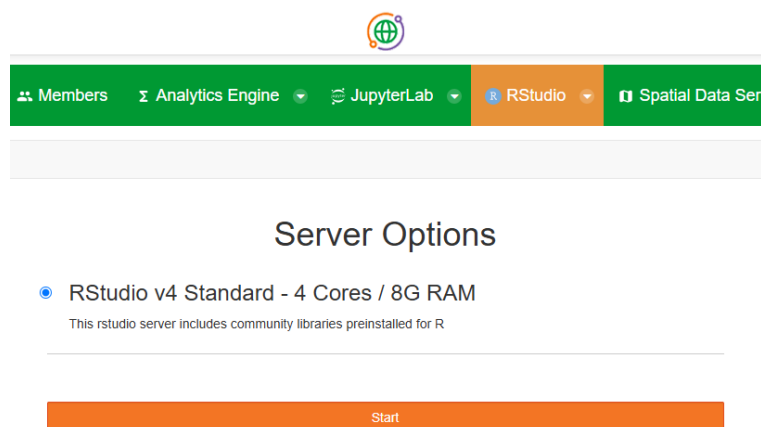


Figure 12: A screenshot of the RStudio section showing the server option available for the CLIMA VRE.

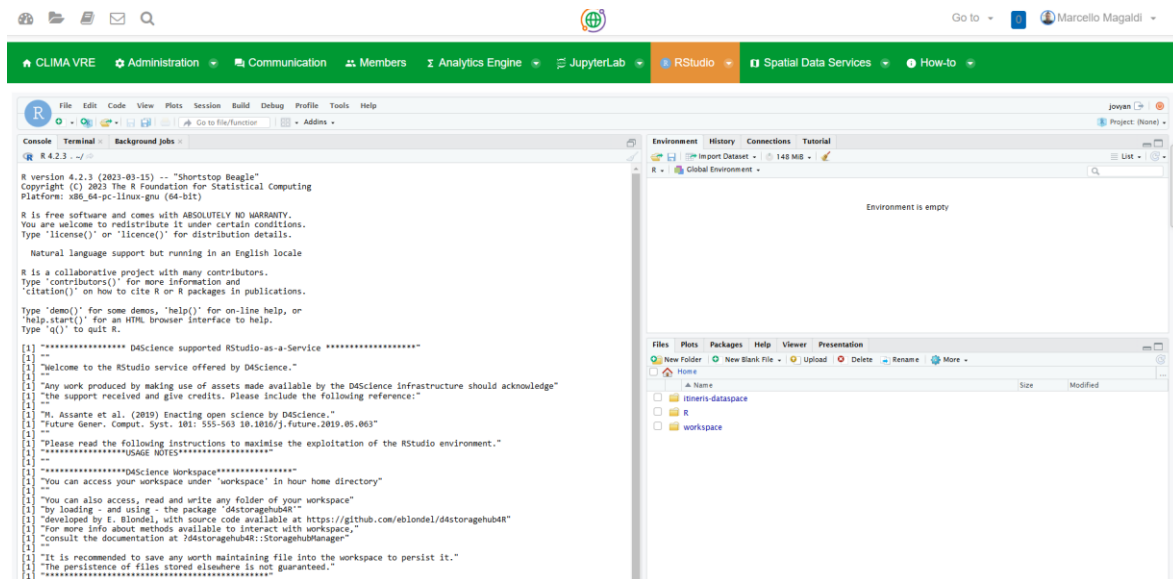


Figure 13: A screenshot of the RStudio environment available for the CLIMA VRE.

RStudio (<https://posit.co/products/open-source/RStudio>) is another example of Integrated Development Environment (IDE) specifically designed for R, a powerful language for statistical computing and graphics. It provides a comprehensive and user-friendly interface for data analysis, statistical modeling, and data visualization. RStudio is designed to simplify the workflow of writing, debugging, and executing R code. The interface is divided into multiple parts (Figure 13), each serving a distinct purpose. The source editor is where users can write and edit their scripts, with features like syntax highlighting, code completion, and error diagnostics to improve the coding experience. The console provides a space for running commands interactively, allowing users to see immediate results from their code. Additionally, RStudio offers panes for managing files, inspecting datasets, viewing plots, and accessing help documentation.

Like JupyterLab, RStudio incorporates tools for creating dynamic documents that combine code, output, and narrative text. This functionality is powered by “R Markdown”, which allows users to generate reports, presentations, and even interactive applications that dynamically update based on the underlying data and code. RStudio supports interactive plotting through packages like the Shiny app (<https://shiny.posit.co>), enabling users to build dynamic, web-based visualizations that enhance the communication of complex data insights. It also offers native support for Python alongside R, allowing users to incorporate Python scripts and libraries into their R projects, bridging the gap between two of the most widely used programming languages in data science.

The “Spatial Data Services” section

This section includes the spatial data services provided with the CLIMA VRE thanks to the D4Science e-infrastructure, namely GeoNetwork and GeoServer. These services are specifically tailored to address the needs of users working with geospatial information across various disciplines, adhering to international standards like those promoted by the Open Geospatial Consortium (OGC,

<https://www.ogc.org>) and ensuring compliance with the INSPIRE directive (Infrastructure for Spatial Information in Europe, <https://inspire.ec.europa.eu>).

GeoNetwork is a web-based cataloguing service that facilitates the discovery, access, and sharing of spatial datasets and services. It is particularly effective for managing metadata associated with geospatial data and ensuring that they are compliant with standards like ISO 19139, OGC, and INSPIRE metadata requirements. The platform provides a centralized repository for organizing metadata, making it easier for users to search for and retrieve spatial resources within the D4Science infrastructure. GeoNetwork also supports federated cataloguing, allowing metadata records from external sources to be harvested and integrated into the catalogue. GeoNetwork supports the creation of metadata records in INSPIRE-compliant formats and also includes tools for validating metadata against INSPIRE requirements, helping data providers ensure the quality and consistency of their records.

GeoServer is a server platform for publishing geospatial data and creating interactive visualizations. It enables users to store, manage, and serve spatial datasets in various formats, ensuring accessibility and interoperability. GeoServer is designed to work with GeoNetwork, allowing datasets documented in the metadata catalogue to be easily published. It supports a wide range of spatial data formats, including vector formats like Shapefiles and GeoJSON, as well as raster formats such as GeoTIFF and raster layers from NetCDF files. These formats are aligned with OGC standards, ensuring that data published through GeoServer can be consumed by a wide variety of client applications. Additionally, GeoServer supports PostGIS, enabling the integration of spatial data stored in relational databases. GeoServer also supports OGC-compliant web services, such as:

- Web Map Service (WMS): this service allows users to generate and retrieve dynamically geo-referenced map images. WMS is ideal for creating interactive maps that can be embedded in web applications, providing users with customizable visualization options for their spatial data;
- Web Feature Service (WFS): WFS enables the retrieval and manipulation of vector data in a standardized format. It allows users to query, download, and update geospatial features, making it a valuable tool for applications that require access to raw vector data;
- Web Coverage Service (WCS): This service provides access to raster data, allowing users to retrieve geospatial coverages for analysis and visualization;
- Web Map Tile Service (WMTS): WMTS delivers pre-rendered map tiles for efficient rendering and visualization, particularly in applications where performance and scalability are critical;
- Sensor Observation Service (SOS): GeoServer supports SOS, which is used to manage and retrieve sensor data and observations. This is especially useful for applications involving real-time environmental monitoring or Internet of Things (IoT) devices.

It must be pointed out that, like in the other ITINERIS VREs, the GeoServer service is not open to all CLIMA VRE members, and it is only accessible through a specific login.

3. THE ITALIAN SEA SURFACE TEMPERATURE DEMONSTRATOR (ISSTD)

As underlined in Deliverable 8.3, the sea surface temperature (SST) is considered as an essential climate variable not only for its fundamental role within the marine environment but also as it directly affects both the atmospheric circulation and the precipitation field. Leveraging mainly on satellite data, SST datasets are also among the most robust and reliable sources of information for the estimations of the global temperature field. The SST indicators are already available for the whole Europe and for the Baltic, Black, Mediterranean and North Sea areas in the Copernicus Climate Change Service (C3S). Following this direction, the same Deliverable 8.3 has suggested the preparation of a SST-based demonstration tool for the CLIMA VRE not only to prove its operativity but also to showcase the capabilities and potentialities of the virtual environment. Having in mind the specific target of a non-specialist audience, such a demonstration tool calculates, as key Italian climate indicators, the sea surface temperature anomalies for the four main Italian Seas, namely the Adriatic, Ionian, Ligurian and Tyrrhenian Seas.

The main idea of the Italian Sea surface temperature demonstrator (ISSTD) is to develop an interactive application that does not require any programming skills and thus is meant for users of any kind, including researchers and stakeholders. ISSTD offers the possibility to access the information from diverse datasets which may describe past, present and future climatic scenarios.

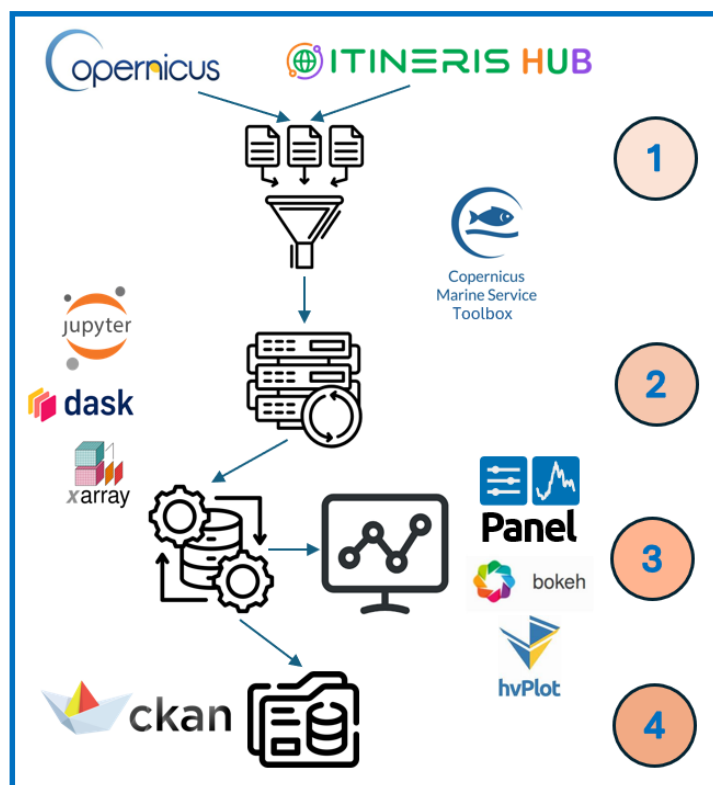


Figure 14: The different packages involved in the workflow of the Italian Sea surface temperature demonstrator (ISSTD). The four phases are: 1) harvesting; 2) harmonization; 3) data processing and visualization; 4) publication.

The ISSTD App back end component is based on the JupyterLab service, namely through the 16-core CLIMA VRE dedicated server. Its workflow involves different packages and is split in the following four different phases (Figure 14):

1. Data harvesting: predefined areas and SST datasets are interactively selected through the “Panel” package (see below). The current focus is on the different products available in the Copernicus Climate Change Service (C3S) and on their cloud-optimized versions for distributed access. The Copernicus Marine Toolbox is used for this purpose. The idea is to access similar datasets coming from the Italian Research Infrastructures (RIs) from the ITINERIS HUB in the future;
2. Data harmonization: format, variable names, spatio-temporal alignment happens mainly via the “dask” and “xarray” packages (see below);
3. Data processing and visualization: also for the processing, this phase mainly relies on the “dask” and “xarray” packages (see below) which are suited for distributed calculus and big data analysis. For the visualization, the ISSTD App uses the “Panel”, “bokeh” and “hvPlot” packages (see below);
4. Publication: this phase is still under development and aims at publishing the App results in the ITINERIS catalogue via the CKAN open-source data management system (<https://ckan.org>).

In the following paragraphs, the above toolbox and packages are briefly described to then show the App capabilities.

The COPERNICUS MARINE Toolbox

The Copernicus Marine Toolbox (<https://help.marine.copernicus.eu/en/collections/9080063-copernicus-marine-toolbox>) is a powerful software suite designed to facilitate access, analysis, and visualization of oceanographic data provided by the Copernicus Marine Service (CMEMS, <https://marine.copernicus.eu>). It includes reliable tools to process and utilize marine data for applications such as environmental monitoring, climate research, and marine resource management. The toolbox can provide access to a wide range of data products, including satellite observations, in-situ measurements, and model outputs, covering key variables such as sea surface temperature, salinity, currents, chlorophyll concentrations, and sea level anomalies.

The Copernicus Marine Toolbox supports formats such NetCDF, GRIB, and ASCII, and allows users to access datasets through APIs and data catalogue interfaces. The toolbox enables efficient downloading, filtering, and subsetting of large datasets, following specific customized spatial and temporal criteria. Built-in analytical functions allow users to compute derived variables, perform statistical analyses, and conduct spatial and temporal interpolations. As in the case of the ISSTD App, the Copernicus Marine Toolbox enables workflows that combine CMEMS data with external datasets or other software environments like Python, R, or MATLAB.

The DASK package

Dask (<https://www.dask.org>) is a flexible, open-source parallel computing library for Python designed to easily handle large-scale computations. It allows users to efficiently manage workflows that cannot fit into computer RAM or require significant computational resources. Dask achieves this by providing scalable, parallel, and distributed computation capabilities, making it an essential tool for data science, machine learning, and scientific computing workflows.

At its core, Dask is built around the concept of task scheduling, enabling users to break down complex computations into smaller, manageable tasks that can be executed in parallel. The library supports both single-machine and distributed environments, allowing users to scale from laptops, to powerful virtual machines like the one used for the ISSTD App, to large-scale clusters. Dask integrates smoothly with the broader Python ecosystem, making it a natural choice for Python users who rely on libraries like NumPy, pandas, and Xarray.

The XARRAY package

Xarray (<https://xarray.dev>) is an open-source Python library designed for working with multi-dimensional labeled datasets, offering robust tools for data analysis, manipulation, and visualization. Originally developed for processing climate and geoscientific data, Xarray has grown to be a versatile tool widely used in domains like oceanography, machine learning, and time series analysis. Its core strength lies in its ability to handle data with multiple dimensions – such as time, latitude, longitude, and depth – while preserving metadata.

Xarray introduces two main labeled data structures or classes of objects:

- DataArrays: multi-dimensional arrays with labeled axes (dimensions) and associated metadata;
- DataSets: collections of DataArrays with shared dimensions and metadata, similar to dictionaries of DataArrays.

These structures make it easy to query, index, and perform computations on datasets while keeping track of meaningful metadata such as variable names, units, and coordinates.

Xarray provides native support for reading and writing NetCDF files and integrates with OPeNDAP, enabling remote access to datasets hosted on servers. Building on its structures, it allows users to perform operations along specific dimensions of DataSet structures, such as summing, averaging, or applying custom functions. These operations are intuitive and take advantage of labeled dimensions, eliminating the need for manual axis management. Furthermore, users can perform complex indexing operations using dimension labels, such as selecting data by specific time ranges, slicing across spatial coordinates, or extracting subsets of data based on logical conditions.

Xarray integrates well with libraries like NumPy, pandas, matplotlib, and Dask. It enables users to leverage Dask for handling computations to larger datasets or distributed computing environments. By enabling chunking, users can analyze data that surpasses local memory constraints while maintaining the same intuitive API.

The BOKEH package

Bokeh (<https://bokeh.org>) is an open-source Python library for creating interactive, web-ready visualizations and dashboards. Designed to provide an elegant and efficient way to visualize data of varying complexity, Bokeh enables users to produce rich, interactive plots and layouts that are easily embedded in web applications. Its flexibility and performance make it an excellent choice for data scientists, analysts, and developers.

Bokeh excels in producing visualizations that move from simple plots to complex, multi-layered dashboards with interactive components such as sliders, widgets, and real-time streaming data. Its design philosophy emphasizes interactivity, high performance, and ease of integration into modern

web frameworks. It supports a wide range of interactive features, such as zooming, panning, tooltips, and selection tools. These capabilities allow users to explore data dynamically, making it easier to identify patterns, trends, and outliers. Bokeh provides a comprehensive set of plotting tools for creating bar charts, scatter plots, line graphs, heatmaps, and more. Bokeh also supports advanced visualizations, such as geospatial plots and network graphs. As many packages above, it integrates with popular Python libraries like pandas, NumPy, and Jupyter Notebook, allowing users to generate interactive visualizations directly from their existing workflows. It also supports exporting visualizations to static formats such as PNG and SVG.

The HVPLOT package

HvPlot (<https://hvplot.holoviz.org>) is an open-source Python library designed to simplify the creation of interactive visualizations for data analysis workflows. Even if it is built on top of other packages and of Bokeh, it is different from this latter as they serve different purposes. Bokeh is a low-level library and requires users to explicitly define plot elements, layouts and their interactivity. In contrast, hvPlot is a high-level library designed to make plotting simpler and more intuitive. HvPlot is then used to quickly visualize data with minimal effort and its integration with data libraries like pandas and Xarray allows users to generate plots directly from DataFrames or DataArrays, whereas Bokeh requires more setup to achieve similar results. On one hand hvPlot is particularly efficient when working with multi-dimensional data, providing built-in support for Xarray and Dask objects. On the other hand, if Bokeh can handle multi-dimensional data, it typically requires more effort and additional libraries for similar functionality.

By leveraging the underlying capabilities of Bokeh, hvPlot emphasizes interactivity, allowing users to zoom, pan, hover, and explore data dynamically and supports a diverse set of visualization types, including line plots, bar charts, scatter plots, histograms, box plots, and heatmaps.

The PANEL package

Panel (<https://panel.holoviz.org>) is an open-source Python library designed to create versatile, interactive applications for data visualization and analysis. Panel provides a high-level interface for building web-ready applications using Python, allowing data scientists, analysts, and developers to create sophisticated tools for exploring and presenting data. Panel supports a wide range of use cases, from simple widgets for data exploration to complex, multi-view dashboards and production-grade web applications. It is highly compatible with popular Python plotting libraries such as hvPlot, Bokeh, and matplotlib, enabling the integration of rich visualizations into interactive layouts. It provides a comprehensive suite of widgets, such as sliders, dropdowns, checkboxes, and text inputs, which can be linked to plots, functions, or other widgets. This makes it easy to create dynamic, interactive applications that respond to user inputs in real time. It also offers powerful layout management, allowing users to arrange visual and interactive components in grids, tabs, splitters, and other flexible structures. This ensures that applications are visually organized and easy to navigate.

Panel works well with Dask, enabling users to visualize and interact with large, distributed datasets. This capability is ideal for big data workflows and scalable computing.

The interactive APP

The Italian Sea surface temperature demonstrator uses the above libraries to subset and preprocess data. Specifically, to speed up computations and reduce resources consumption of the APP, data are preliminary processed to perform computational steps that are common in the analysis. These steps include:

- accessing data from cloud storage and repositories;
- masking and extracting data for each of the four Italian Seas;
- computing domain averaged time series of sea surface temperatures.

Each dataset is usually available as gridded SST fields and accessed through specific packages and APIs like those of the Copernicus Marine Toolbox for the CMEMS products. Masks for each of the four Italian Seas are defined as lists of geographic coordinates representing the vertices of the closed polygons including the sea points of interests (Table 1 and Figure 15).

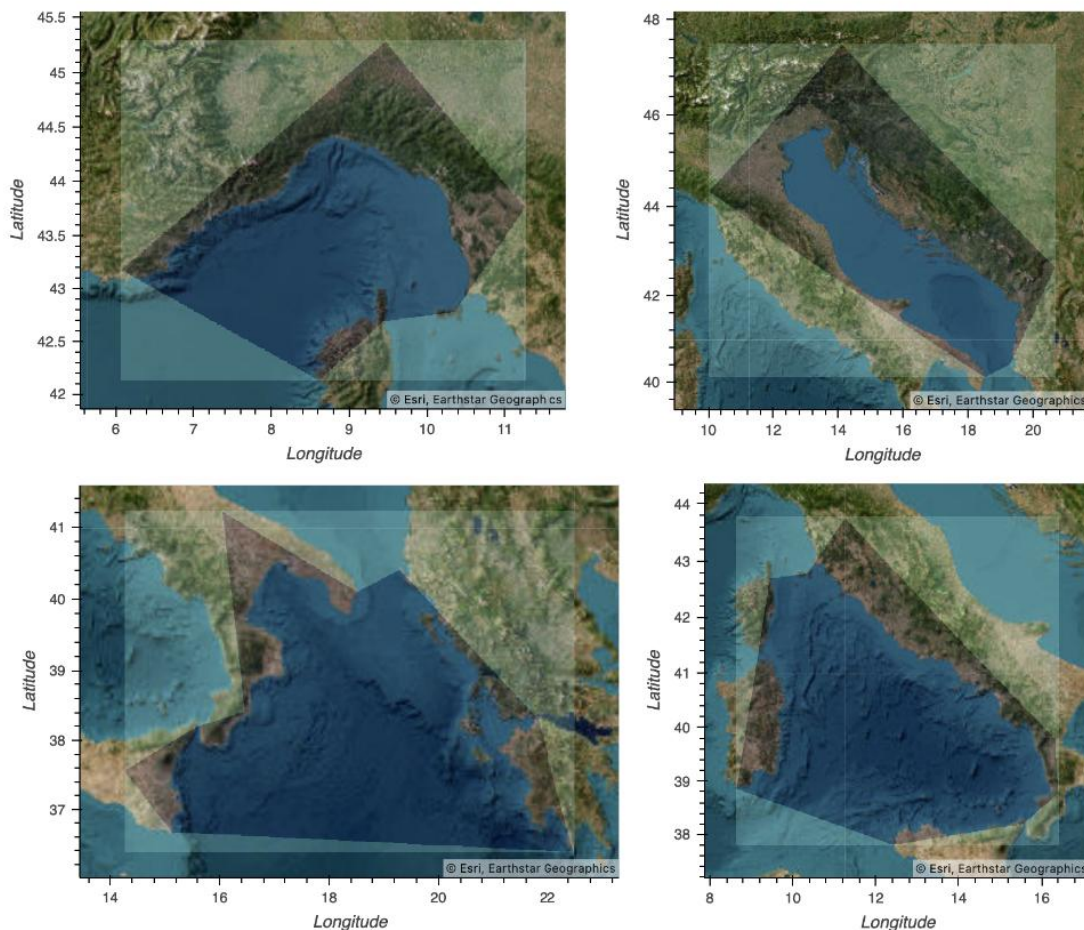


Figure 15: Polygons defining the four Italian sea masks: Ligurian (top-left panel); Adriatic (top-right panel); Ionian (bottom-left panel) and Tyrrhenian Sea (bottom-right panel). Each shaded rectangular area is a regional subset of the original gridded product. Dark regions are closed polygons which include the sea points considered in the calculations and analysis for each Sea.

Table 1 – Locations and geographic coordinates (latitudes, longitudes) defining the closed polygons used for the masking process for the four Italian Seas considered in the APP.

Adriatic Sea

- Capo Linguetta: 40.418, 19.300;
- Kosovo: 42.649, 20.674;
- Austria: 47.485, 14.117;
- Lunigiana: 44.343, 10.029;
- Punta Palascia: 40.108, 18.520.

Ionian Sea

- Capo Passero: 36.677, 15.131;
- Capo Matapan: 36.387, 22.483;
- Patraso: 38.296, 21.847;
- Capo Linguetta: 40.418, 19.300;
- Punta Palascia: 40.108, 18.520;
- Canosa di Puglia: 41.215, 16.067;
- Riace: 38.418, 16.470;
- Messina: 38.199, 15.573;
- Enna: 37.569, 14.273.

Ligurian Sea

- Tolone: 43.182, 6.070;
- Pianura Padana: 45.284, 9.473;
- Firenze: 43.765, 11.267;
- Elba centro: 42.782, 10.358;
- Bastia: 42.699, 9.450;
- Cargese: 42.137, 8.620.

Tyrrhenian Sea

- Messina: 38.202, 15.557;
- Calabria 1: 38.781, 16.414;
- Calabria 2: 39.795, 16.336;
- Firenze: 43.765, 11.267;
- Elba centro: 42.782, 10.358;
- Bastia: 42.699, 9.450;
- Capo Teulada: 38.865, 8.644;
- Capo Boeo: 37.802, 12.425.

After the mask definition, using Dask and Xarray functionalities, area-weighted averages of SST values are calculated for each Sea at every time step to produce a time series. Similarly, SST yearly averages at every grid point are computed and stored as gridded DataSet structures, with the same geographic resolution of the original product.



Figure 16: Starting panel of the ISSTD APP with a drop-down menu for the dataset selection and the “Load Data” button for its confirmation.

As initial step, the ISSTD interactively asks users to select the dataset for the following analysis. This choice can be confirmed by pressing the “Load Data” blue button in the initial panel of the APP (Figure 16). After confirmation, the application loads all preprocessed files for the selected data source and shows a new panel with new controls and plots (Figure 17).

On the top-left area of the APP, users can interact with the following controls (from top to bottom):

- *Dataset selection*: this is a drop-down menu that allows users to select the dataset for the analysis;
- *Sea switch*: this is a radio button that allows users to change the currently selected Sea among the four Italian options using and apply the mask definitions as explained above;
- *Year slider*: this slider object allows users to select a specific year within the time range covered by the chosen dataset;
- *Reference period slider*: this two-value slider object allows users to set the reference interval of years used to calculate the SST climatology (see also below for more details);
- *Download area*: this is another radio button that, once pressed, it allows users to download the analysed time series as CSV files.

The top-right area of the APP displays a map with the geographic distribution of the SST averages for the specific Sea and year selected thanks to the above controls (the Tyrrhenian Sea and the 1998 year for the example shown in Figure 17).

A comparison among the SST averages for the selected year in the four Italian Seas is presented in the middle left area of the APP while yearly trends for the selected years are compared to the selected period of reference (red thick line) in the middle right area. In the lower part of this area lies an additional control (*Year to plot slider*) which is a two-value slider allowing users to select the specific years (from 2010 to 2016 in the example of Figure 17) to be shown in the above plot for comparison with the reference period (from 1981 to 1995 in the example of Figure 17).

The final and bottom area of the APP shows the SST anomalies in time for the selected Sea and calculated from the selected period of reference. Relative warmer and colder intervals are highlighted with red and blue colors, respectively.

All plots are interactively and automatically updated every time any parameter is changed through one of the controls described above. Furthermore, displayed data in each plot can be explored using the widgets and tools on the right (for example zooming, panning, saving images) which mainly rely on the hvPlot and Bokeh functionalities.

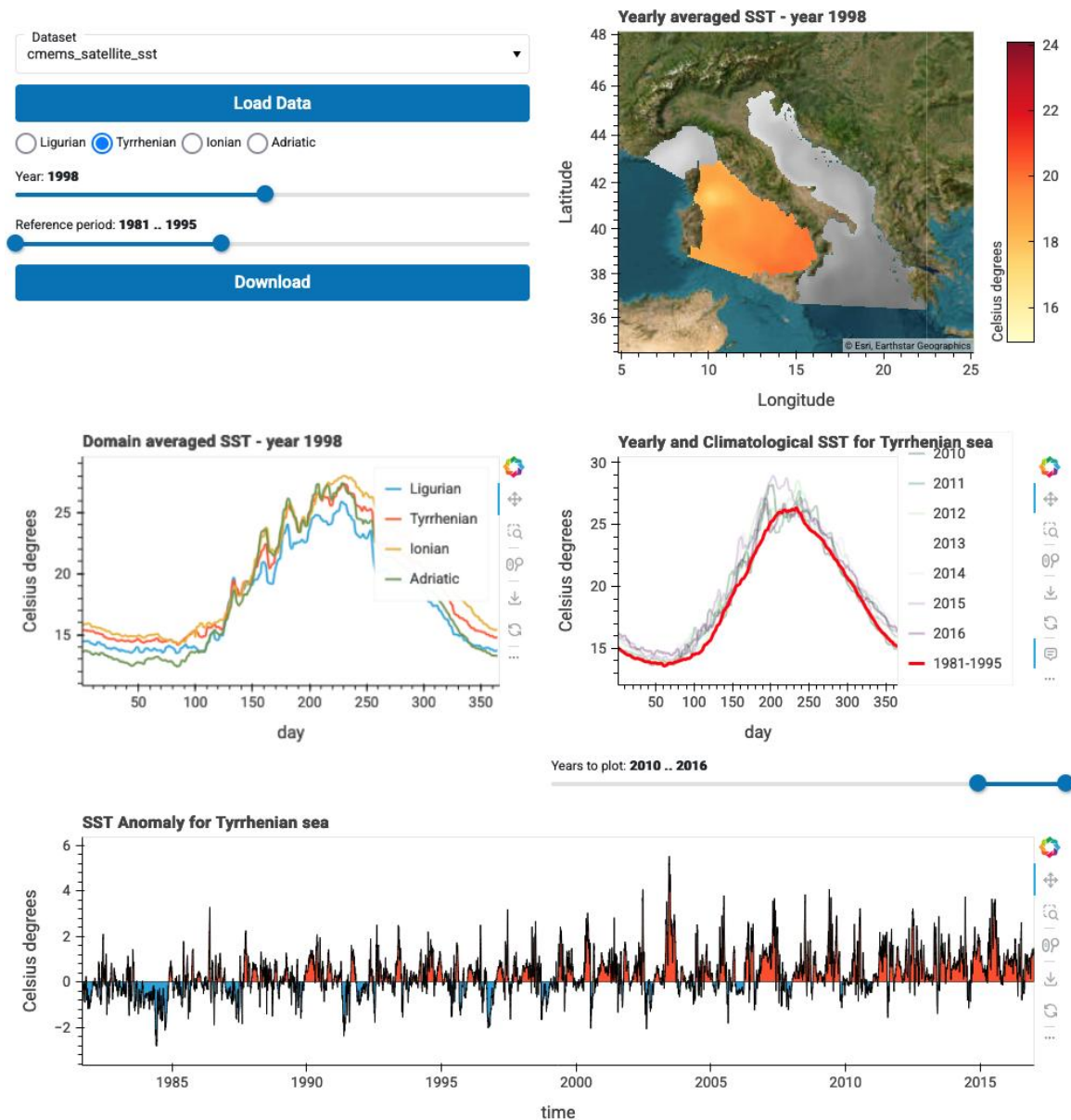


Figure 17: A comprehensive view of the ISSTD APP panel showing all controls and plots as they appear after selecting the data product source and pressing the initial “Load Data” blue button (top-left panel). The APP displays the SST yearly geographic distribution (top-right panel) and allows users to compare the different SST yearly averages in the four Italian Seas (middle left panel). Yearly trends for the selected years are also compared to the selected period of reference (red thick line, middle right panel). The time series of SST anomalies from the selected period of reference is calculated and displayed (bottom panel). The information spans many decades in time providing robust indications on the climatic trends. Figures are automatically updated when users interact with controls (sliders and buttons, see text for more details) while displayed data in each plot of the middle and bottom panels can be explored using the widgets and tools on the right.

The APP calculations use the following definitions:

- SST Climatology: if $T_{d,y}$ denotes SST daily values (d is an integer number from 1 to 366 indicating the day of the year and y is an integer in the range of years in the selected reference period R), the SST climatology is denoted with \bar{T}_d and defined by averaging value data for the same day of the year across the years in the selected reference period:

$$\bar{T}_d = \sum_{y=\min(R)}^{\max(R)} T_{d,y}.$$

Note that the selected reference period R is controlled through the *Reference period slider* in the APP and that the value for $d = 366$ is averaged over less points as it considers only leap years;

- SST Anomaly: denoted with $\delta T_{d,y}$, the SST Anomaly is defined as the deviation from the SST climatological signal:

$$\delta T_{d,y} = T_{d,y} - \bar{T}_d,$$

with positive and negative values indicating respectively warmer and colder days compared to the reference period.

4. CONCLUSIONS AND NEXT STEPS FOR THE CLIMA VRE

Two are the main objectives achieved thanks to this Deliverable 8.13:

- a) the user guide of the CLIMA VRE is provided (see Section 2) with specific focuses on the i) description of the functionalities of both the D4Science ITINERIS and CLIMA VRE dashboards and ii) architecture of CLIMA VRE and overview of open-source packages involved;
- b) a demonstration of the CLIMA VRE operativity is proved with the development and use of the Italian Sea Surface Temperature Demonstrator (ISSTD) App (see Section 3).

Suggestions and next steps for the CLIMA VRE development are envisioned following the directions described below:

- Improvements on the ISSTD App, namely in terms of:
 - Considering even more datasets as source of SST data, especially those that will be available under the ITINERIS HUB and also projections under different scenarios to have an idea of the projected SST anomalies;
 - Enlarging the harmonization phase to combine different datasets, especially important for more robust indications coming from the alignment of several projection products;
 - Computing optimization thanks to the setup of a dedicated environment, the continuous evolution and improvement of the VRE resources (including cloud

- computing options) and specific rechunking methods to ease the loading and the preprocessing of data of demanding datasets;
- Finalizing the publication phase of the APP obtained results with the use of both the Spatial Data Services and the CKAN data management system.
- Development of climate indicators related to one or more Italian Seas: following the example by Cyr and Galbraith (2021), use both a variable combination and data-driven approach to propose one or more climate indices. Following this direction, the main idea is to leverage on some of the facilities belonging to different marine RIs – like the EMSO and JERICO moorings in the Western Mediterranean basin – to develop a Ligurian Sea Climate Index.

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