IS-ENES3 DELIVERABLE (D -N°5.1)

Compute service requirements and state of the art approaches

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Revision Table			
Version	**Date**	**Name**	**Comments**
0.1	22/05/19	Christian Pagé	Initial version template draft with structure proposal
0.2	13/01/20	Christian Pagé	Begin of C4I material writing. Ideas on content of every section.
1.0	10/02/20	Christian Pagé	Consolidation and adaptation of structure given partners contributions.
1.0R	13/02/20	Christian Pagé	Ready for Internal Review.
1.0F	26/02/20	Christian Pagé	Final version ready to submit after review and additions of ESMValTool contributions by Björn.

Abstract

In order to design and develop a Compute Service to support better data access to the European ESGF Research Infrastructure, it is mandatory to collect user requirements, gaps and challenges on computing aspects for analysis and processing. To this aim a virtual workshop has been organized to gather this information. This deliverable summarizes the outcome of this workshop. This provides needed information to design and plan the future ENES Compute Service that will be developed within the IS-ENES3 project.

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Dissemination level		
PU	Public	X
CO	Confidential, only for partners of the IS-ENES3 project	

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Executive Summary

Considering the large increase in data volume of climate data in recent years and continuing, the ENES Research Infrastructure (RI) can no longer solely focus on data storage and federated data access. The need of data processing as close as possible to the data storage is now a strong requirement of providers and users. Within the IS-ENES3 project, Compute Services will be designed and implemented for the IS-ENES RI.

In order to properly develop Compute Services, it is needed to assess requirements from future providers and users, as well as survey the current state-of-the-art technology among the providers of data processing services within the climate RI. To fulfill this objective, an IS-ENES3/ESGF Virtual Workshop on Compute and Analytics was organized on Dec 2nd, 2019, and the agenda can be seen here:
https://is.enes.org/events/workshops/is-enes3-esgf-virtual-workshop-on-compute-and-analytics
This activity was planned in the context of WP5 - Task 4. Overall, the workshop resulted in a very good summary of current approaches within different service providers, and discussions were quite active among the participants. It contributed to survey potential technologies and approaches that can be used to design the ENES Compute Service within the next few months.

Currently there is a clear trend visible toward consolidation and harmonizing the processing services provided by the ENES Climate Data Infrastructure (CDI) centers. The quality assurance of the diagnostic software and the reproducibility of the results of the analysis already offered by the ESMValTool are strong requirements of the community. With the pangeo software stack and associated current deployments at HPC centers (e.g. NCAR) as well as the cloud, the support for pangeo will also be a strong requirement for the ENES CDI centers. The need to support flexible, research project specific processing software environments has to be satisfied. This requires the centers to invest in new containerization and container orchestration approaches. A current challenge all ENES CDI compute service providers face is the provisioning of common “public” processing services to be used by the broader European (and international) climate science community, because of the missing cost models to cover the (often extensive) resource usage. The current VA (Virtual Access) and TNA (Trans-National Access) based schemes of H2020 projects are quite insufficient and cross-institutional agreements need probably to be negotiated, which are closely related to the issue of establishing a sustainable ENES CDI and an organisational legal form for this entity.

1. Compute Service: Current situation – Status Report

Currently, several climate data providers within the ESGF Climate Research Infrastructure are providing compute services for their users. Several approaches and solutions have been developed and implemented, according to the requirements of users and the providers resources and funding. Technologies are also evolving very rapidly, and the landscape of tools and approaches is very different from what it was only a few years ago.

During the IS-ENES3/ESGF Virtual Workshop on Compute and Analytics that took place on Dec 2nd, 2019, providers of data processing services presented their approach and implementation. In this section a review of the current state-of-the-art is presented, along with corresponding User Requirements and Challenges.

1.1 Situation Analysis - State of the Art

climate4impact Platform

The IS-ENES climate4impact (C4I) platform has been running since 2011. It provides easier access to climate simulations for end users, especially the climate change impact modelling community.

The objectives of the platform are complementary to the Copernicus C3S. The characteristics of the C4I Platform are as follows:

- *Targeted at climate science researchers as well as the climate change impact community, to explore climate data, download needed data, and perform on-demand analysis*
  - Make all ESGF climate model data and services (CMIPs, CORDEX) accessible
  - Enable users to explore all MIPs on ESGF or other datasets available using OpenDAP
- *Connect to ESGF web services*
  - Search, Catalog Support, Security
  - Several projects and experiments
- *Enable Visualization via ADAGUC Software*
  - Visualization system using Web Map Services
  - Web Coverage Services for data transformation
- *Provide Analysis Services using (Py)WPS to perform calculations*
  - icclim open-source software for on-demand climate indices calculation
  - Data sub-selection
  - Personal store for processing results
- *Run an operational service*
  - Deployed in the cloud
  - Is one of the official CMIP6 dissemination portals

- *Promote Users' engagement: climate research community, climate impact community as well as interdisciplinary research community*

The C4I Platforms provides several processing capabilities, ranging from time and spatial subsetting with a graphical User Interface (UI) using OGC WCS Standard, to simple statistics such as time average, to more complex calculations such as climate indices and indicators (provided by the icclim software). And even more complex tools such as statistical downscaling is provided through an interface to the University of Cantabria Downscaling Portal.

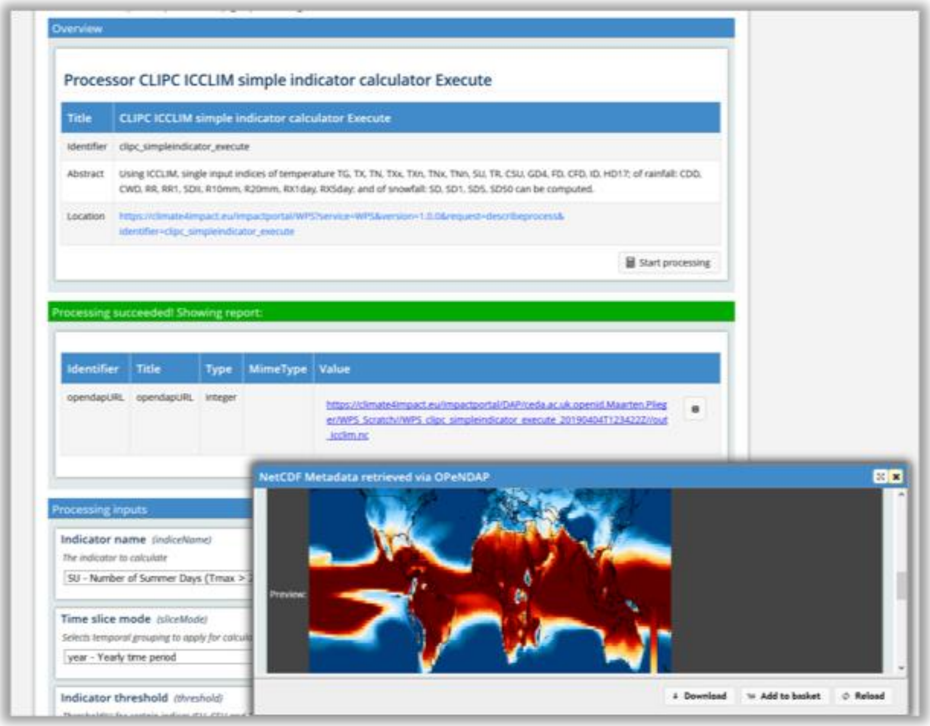

Figure 1.1: C4I Processing Services Interface

The current front-end is written using the Drupal CMS for the static part, and Java for the interface part. The processing is interfaced with a pyWPS 3.2 instance supporting the OGC WPS 1.0.0 standard. In the processing backend, several tools are leveraged: icclim for calculating climate indices and indicators, CLIPC libraries for advanced functions, and the Birdhouse suite for a large range of functionalities.

Several issues are present for the operational version, currently deployed on Amazon Web Services (AWS). The data processing services, excluding statistical downscaling, are performed on the portal server itself, which is not scalable and could bring down the server if calculations are too large. The interface is often non-intuitive even if it has improved over the years. The code of the portal is not modular. There is a lot of help and guidance, but more guidance (especially dynamic guidance) is needed to support end users. Concurrent WPS Solutions such as the Birdhouse should be better integrated and used in place of the current pyWPS specific implementation.

The IS-ENES3 project gives an opportunity to redesign and restructure the whole portal and platform. C4I 2.0 will be rewritten in ReactJS, using MarkDown format for the static documentation, stored in S3 Bucket. A micro-services approach is expected to be developed, probably based on Python/Flask. Those micro-services will provide APIs, such as a MyCollection for the Basket features, another one using the WPS Birdhouse framework. Some old Java code from the previous version could be reused in that framework.
All components will be deployed using docker-compose, and all source code and documentation will be stored in Gitlab.

DKRZ compute services

DKRZ acts as a national compute and storage provider for the German climate research community and is closely integrated in European and international collaborations supporting the wider international climate community. As part of this DKRZ provides different types of compute services and maintains large collections of climate model data in a data pool which is efficiently accessible for data analysis activities. This 5 PByte data pool currently provides popular CMIP5, CMIP6 and CORDEX data collections. The following data pool associated compute services are provided:

- *Direct access to DKRZ compute resources (interactive and batch)*
  User groups can apply for projects at the DKRZ HPC system and a Committee is deciding on the grant of associated compute and storage resources[1]. Users in selected projects can directly access interactive data analysis nodes and also submit batch jobs to the HPC system. Data managed in the data pool is directly accessible as part of the overall parallel Lustre file system.
- *Jupyter hub based interactive analysis environment*
  Authorised project users can also use the Jupyter-hub environment deployed at DKRZ[2] to run Python notebooks on HPC resources. Users can reserve different amounts of resources for dedicated time frames, which are used to run the notebooks. Different pre-defined environments are available and users can also extend their environments to include specific python package dependencies they require in their data analysis programs.
- *Web accessible processing services and associated support framework*
  Some projects have the requirement to host dedicated interfaces to their processing backends using DKRZ resources. For this currently two options are provided: a hosting service for virtual machines (VMs), which can be configured according to user's requirements. These VMs can e.g. host specific portal functionality like e.g. the CMIP6

[1] Application for compute resources at DKRZ: https://www.dkrz.de/services/bereitstellung-von-rechenleistung?set_language=en&cl=en
[2] Juypter-hub at DKRZ: https://www.dkrz.de/up/systems/mistral/programming/jupyter-notebook

ESMValTool portal hosted at DKRZ[3]. The other option is the deployment of a web service interface to specific processing functionality which users want to trigger via the web (e.g. from remote portals). For this a framework is provided supporting the easy packaging and deployment of OGC WPS (Web processing service) standard conforming web services[4]. This framework is currently being applied within a Copernicus project (C3S_34e) involving DKRZ and STFC to implement and support a specific set of processing options (subsetting, averaging and basic regridding) for CMIP/CORDEX data.

- *Integration of services*

  As part of the EOSC-hub project DKRZ worked on the integration of a dedicated JupyterHub deployment (as part of the ECAS EOSC service, which is provided together with CMCC) with EOSC data sharing and AAI components. The overall architecture is illustrated in the following picture

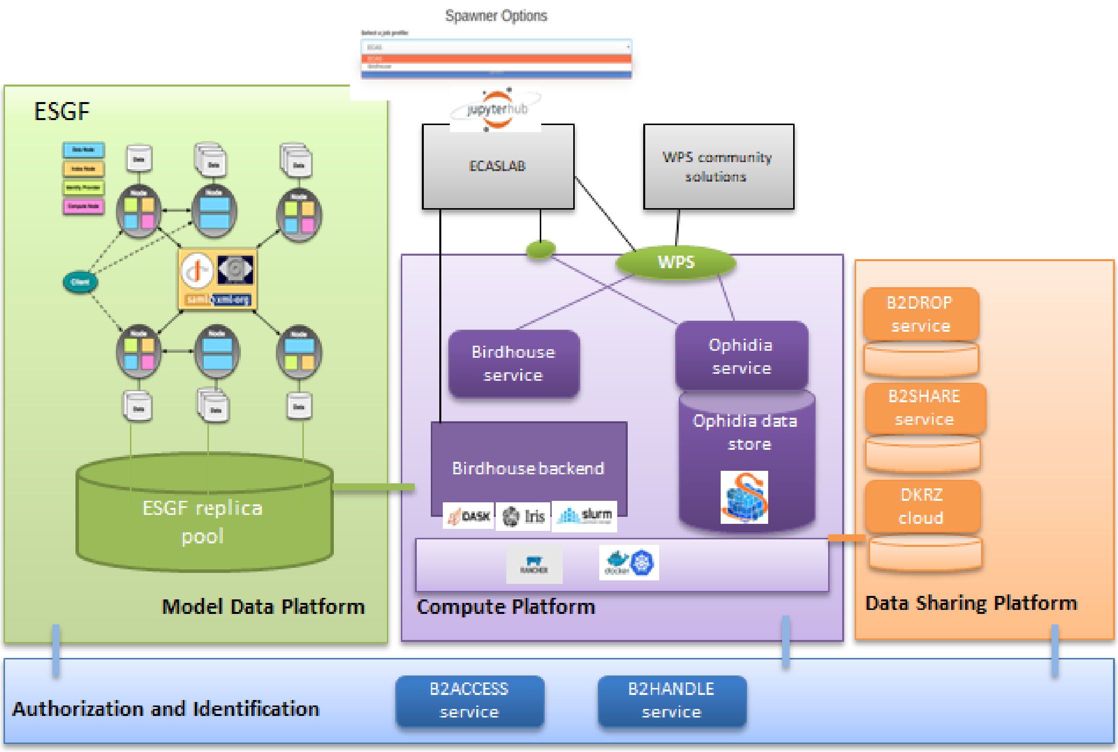

Figure 1.2: DKRZ Compute Service Architecture

The EUDAT EOSC data sharing services integrations (B2Drop and B2Share) enable researchers to upload input data and share data results as part of the European Open Science cloud. Additionally different compute backends are supported to be able to address specific user requirements. On one hand side a Ophidia backend supports Ophidia-operator and workflow based data cube processing. On the other hand generic e.g. cdo and xarray based computations are also supported.

[3] The CMIP6 evaluation portal at DKRZ. https://cmip-esmvaltool.dkrz.de/
[4] The Birdhouse WPS service framework: https://birdhouse.readthedocs.io/en/latest/

IPSL compute services

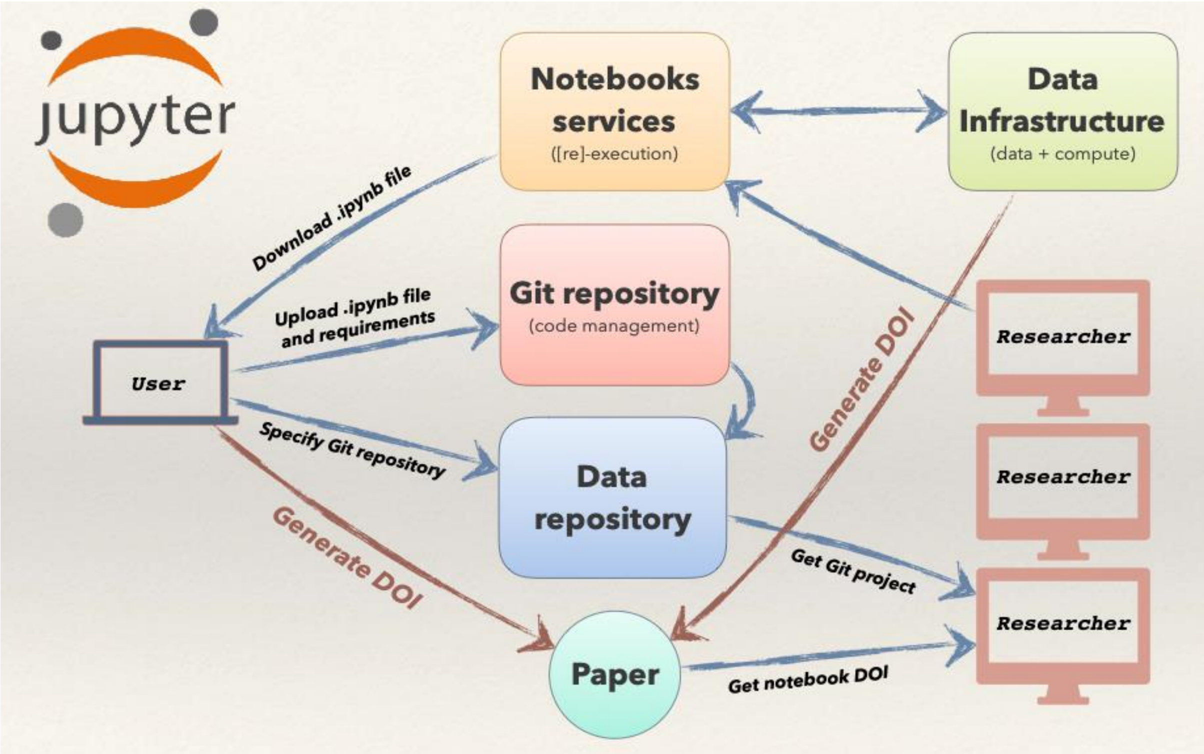

Figure 1.3: IPSL Proof of Concept for compute traceability and reproducibility

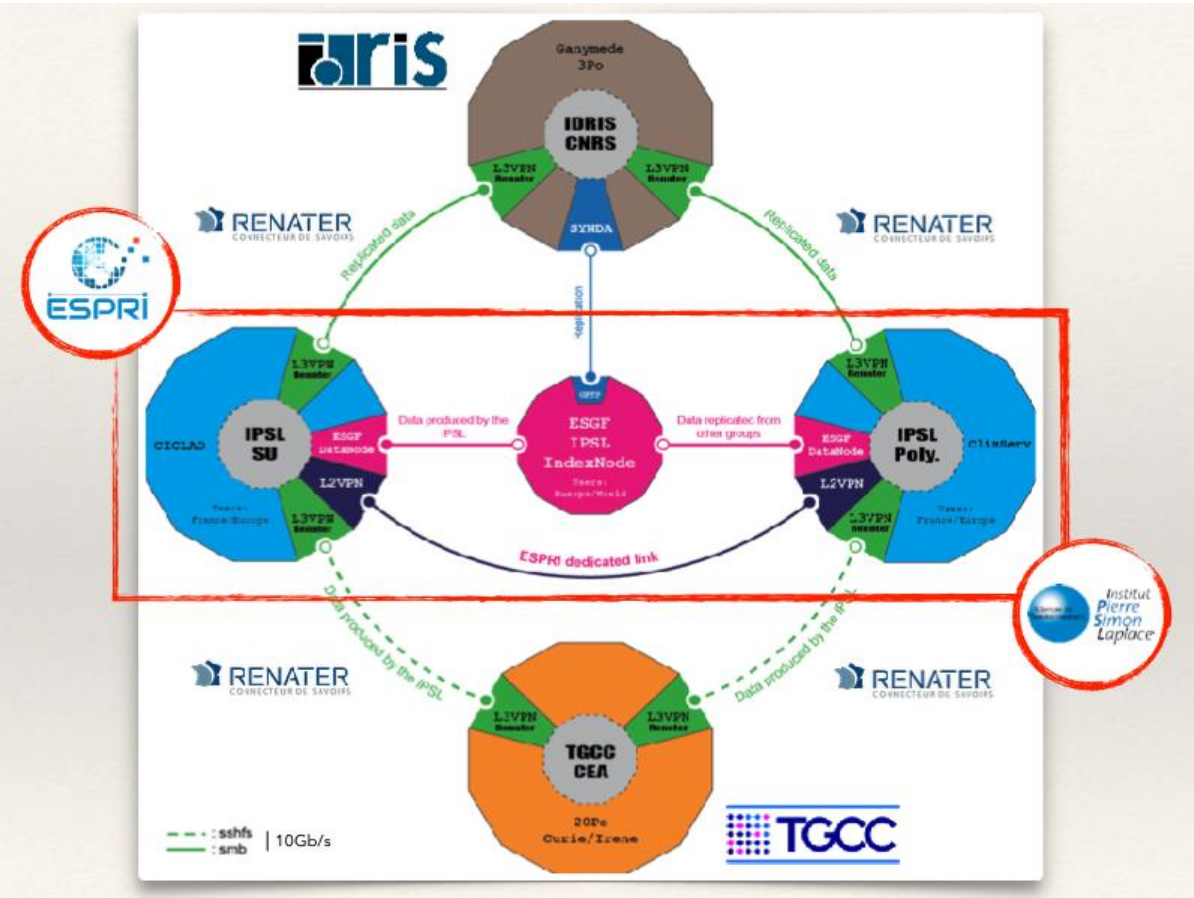

Figure 1.4: IPSL multi-model infrastructure

The IPSL formed the ESPRI ("Ensemble de services pour la recherche à l'IPSL") platform to gather all common services for research at IPSL. The ESPRI mission is to design, develop and deploy applications to support the scientific climate community and ease the distribution, access and analysis of international climate data. ESPRI acts as a national research infrastructure called CLIMERI-France and provides compute and storage facilities for the French climate research community. As one of the IS-ENES partners, it is closely integrated in European and international collaborations providing basic compute services and maintains 10PB of large collections of climate model data and observations through an open analysis platform efficiently accessible.
The ESPRI analysis platform provides the following compute services:

- Direct access to ESPRI cluster (1,200 cores and 3TB RAM, virtualization servers). User groups can apply for projects. Users in selected projects can directly access interactive data analysis nodes and also submit batch jobs. Data pools managed by ESPRI are directly accessible as part of the overall parallel Lustre file system and from our HPC centers remotely mounted in a read-only mode.
- A Jupyter hub based interactive analysis environment is being deployed on ESPRI relying on a Kubernetes orchestrator.
- Different pre-defined environments will be available through the notebooks and direct access ("module load" command) and users can also extend their environments to include specific python package dependencies they require in their data analysis programs:
    - Python libraries as xarray or Dask with access the ESPRI cluster for native and user-friendly parallel analysis.
    - CliMAF (already available) is an open source software that aims to ease the common steps that separate scientists from their diagnostics. CliMAF is able to deal with several data structures, plug and play with homemade scripts, usual data treatments (subsetting, regridding, ensemble mean, etc.), cache mechanism to not recompute a whole treatment chain.
- A new CEPHFS storage is being installed with a few TB which will soon be ready as "object-store" storage.
- ESPRI is also studying another option of deploying more Web Processing Service. Currently WPS are only deployed in the context of climate service (Copernicus and internal pricing) to provide standard post-processing on climate data. As part of Copernicus project ESPRI deployed a WPS instance based on the "Birdhouse" solution from DKRZ, in a load-balanced infrastructure (AWS Route 53) with CEDA and DKRZ.

Except for direct access to the ESPRI cluster, other compute services currently lack documentation as they are still in the process of being deployed or still in their testing phase.

CMCC Compute Service

The ENES Climate Analytics Service (ECAS) represents the compute service solution deployed at CMCC for the IS-ENES3 project. It enables climate end-users to perform data analysis on large volumes of NetCDF data by exploiting a server-side, declarative, in-memory and parallel approach. ECAS consists of multiple integrated components, centered around the Ophidia Big Data Analytics framework, which has been integrated with JupyterHub and WPS services and the ECASLab web portal[5].

Ophidia represents the core engine of ECAS. It supports parallel data analysis, jointly with an internal storage model able to efficiently deal with multidimensional data and a hierarchical data organization to manage large data volumes. From a physical point of view, the data is partitioned in fragments consisting of multidimensional binary arrays and distributed over multiple nodes. Ophidia also provides a native analytics workflow engine to define processing chains and workflows with tens to hundreds of data analytics operators to build real scientific use cases. It provides about 100 array-based functions and more than 50 datacube-based operators[6] to enable OLAP tasks.

From a web-service front-end perspective, ECAS offers the Web Processing Service (WPS) standard interface through the PyWPS component. Such an endpoint exposes a set of processes, one for each operator, which enables WPS-based client-server interactions and also facilitates interoperability with ESGF. Additionally, ECAS implements the ESGF-CWT specification with a set of interoperable operators (e.g. subsetting, max, min, avg, ...).

From a client-side perspective, ECAS provides a CLI, a Python module and a JupyterHub front-end to run interactive or batch analysis sessions.

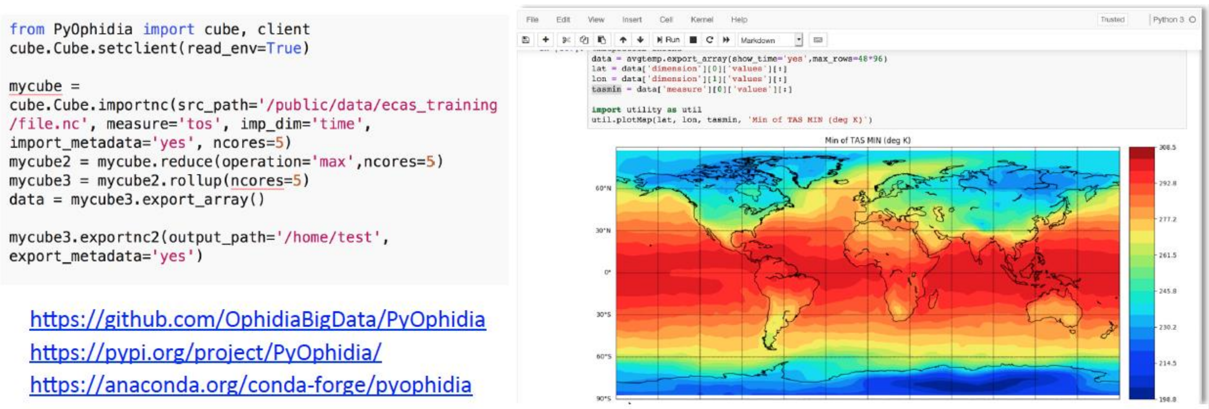

Figure 1.5: ECASLab - a ready-to-use environment based on Ophidia and JupyterHub

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[5] https://ecaslab.cmcc.it/web/home.html

[6] http://ophidia.cmcc.it/documentation/users/index.html

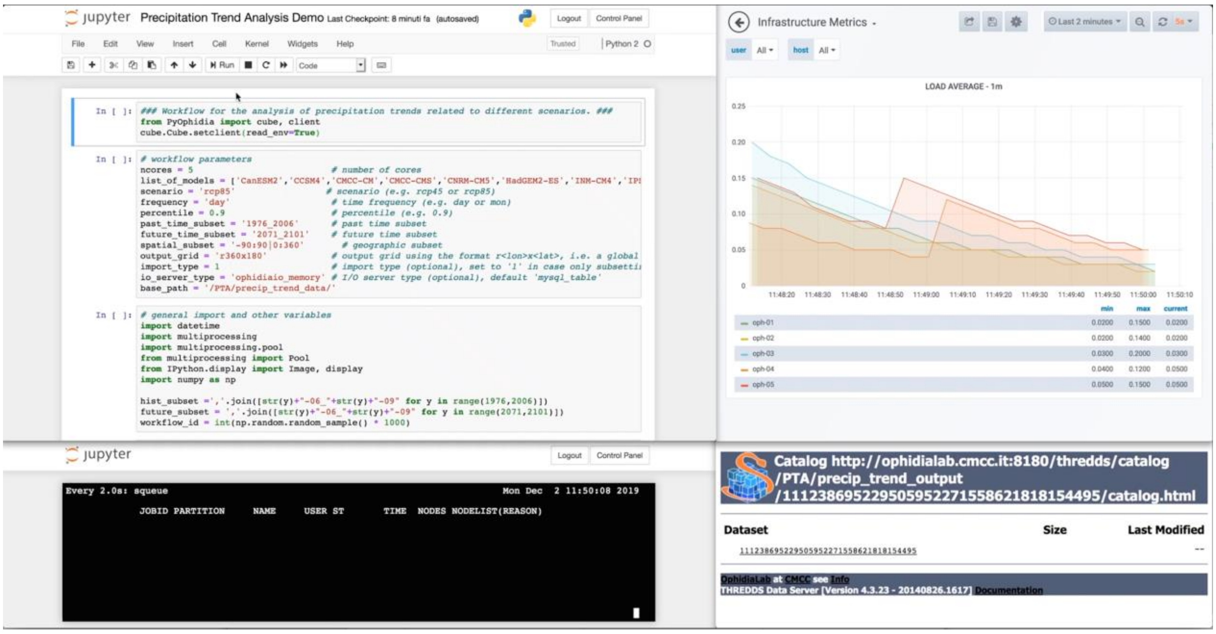

Figure 1.6: a multi-model experiment demo on ECASLab

A dissemination portal[7], providing information about the infrastructure available for the end-users, has been created in the IS-ENES3 project to address Virtual Access and Trans-National Access needs. The dissemination portal is an informative web site with the description of the provided compute service, a quick start guide for using the available JupyterHub instance, additional material jointly with the github link to some climate workflows and the registration form. It also includes a link to get access to the JupyterHub endpoint.

Besides ESGF and the ENES community, ECAS provides a strong link with the European Open Science Cloud. Indeed, it is one of the Thematic Services selected (as a result of an open call at EU level) in the context of the EOSC-hub project. Such connection is very important as it represents a strong bridge towards the EOSC services and infrastructure, as well as additional user communities.

It is worthwhile to mention that the ECAS instance running at CMCC in the context of ESGF/IS-ENES3 implements the Climate Analytics Hub concept. As reported in the paper[8], a Climate Analytics Hub is a specialized compute service implemented on top of the existing ESGF data nodes backbone to support the execution of multi-model climate analysis on a single location. It is responsible for providing analytics capabilities on top of a data collection layer, which both (i) pre-stages and caches the data relevant to the analyses from the different ESGF data nodes and (ii) keeps the local copy of data synchronised with the remote copy available in the ESGF infrastructure.

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[7] https://ophidialab.cmcc.it/is-enes/

[8] S. Fiore *et al.*, "Towards an Open (Data) Science Analytics-Hub for Reproducible Multi-Model Climate Analysis at Scale," *2018 IEEE International Conference on Big Data (Big Data)*, Seattle, WA, USA, 2018, pp. 3226-3234. doi: 10.1109/BigData.2018.8622205

Of course, a centralized storage location, like in the Analytics Hub, cannot represent a scalable solution for the whole CMIP data archive (approximately 20PB expected for CMIP6), but it can be considered as a suitable approach for the analysis of one or more selected variables (depending on storage availability).

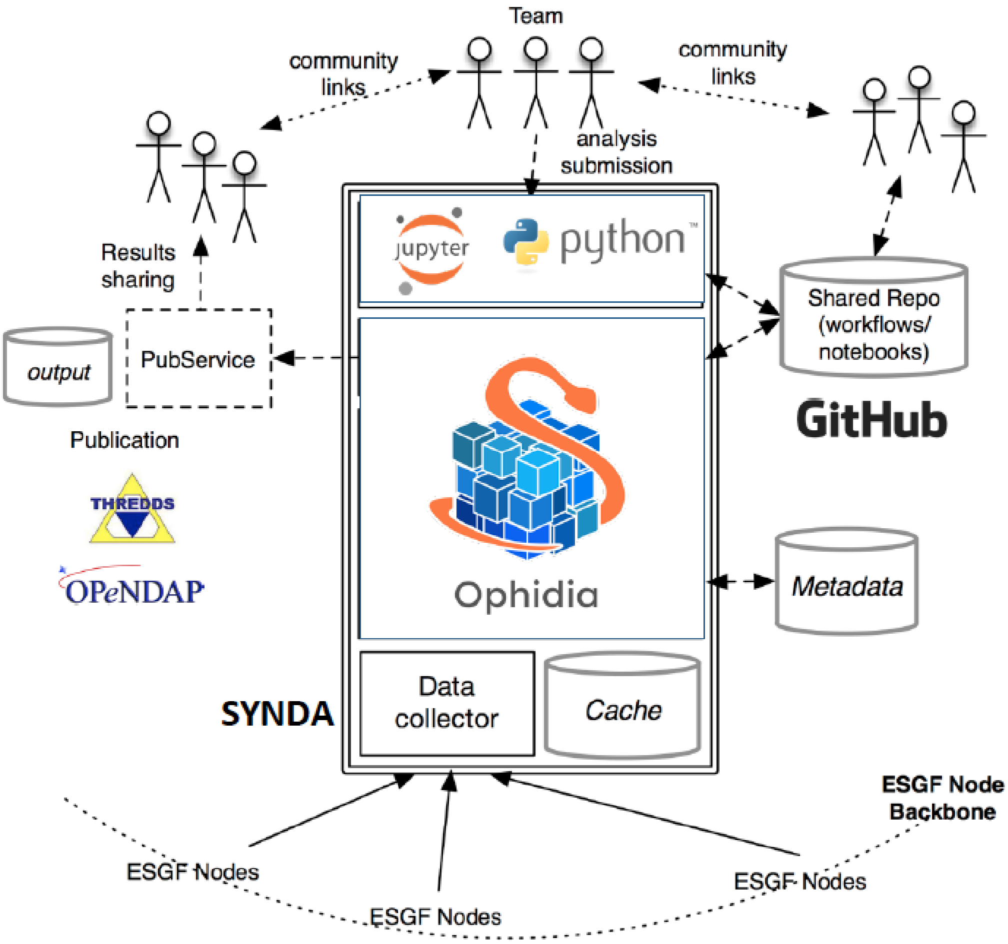

Figure 1.7: The CMCC Climate Analytics Hub

Such approach is the one envisaged at CMCC for ESGF/IS-ENES3 as it allows end-users to find at the same place: (i) a set of relevant (from a community perspective) variable-centric collections from ESGF/CMIP, (ii) data analytics workflows/notebooks, (iii) an interactive and user-friendly environment, (iv) a compute service solution deployed on (v) a dedicated infrastructure.

ESMValTool

The Earth System Model Evaluation Tool (ESMValTool) is a community diagnostics and performance metrics tool designed to improve comprehensive and routine evaluation of Earth System Models (ESMs) participating in the Coupled Model Intercomparison Project (CMIP). It has undergone rapid development since the first release in 2016 and is now a well-tested tool that provides end-to-end provenance tracking to ensure reproducibility. It consists of an easy-to-install, well documented Python package providing the core functionalities (ESMValCore) that performs common pre-processing operations and a diagnostic part that includes tailored diagnostics and performance metrics for specific scientific applications.

It provides:

- *provenance*
  - following the international PROV w3c standard
  - keeps a detailed trace of all steps that led to a resulting graphic of data file
  - ensures reproducibility
- *complex pre-processing of input data*
  - for data of simulations, observations and reanalysis
  - optimized for computational performance
- *well established diagnostics*
  - implementation of diagnostics established in peer reviewed literature
  - well tested implementations by the community
- *convenient configuration and control by the user*
  - easy-to-use configuration and control files that can be configured directly by the user
  - configuration via external web service interfaces is straight forward
- *public API for pre-processor functionality*
  - see https://esmvaltool.readthedocs.io
- *easy installation*
  - conda based installation
  - focus on Linux (eg. for web service application or HPC environments)
- *computational performance optimized by the underlying numerical software stack*
  - numerical intense computations are realised by using iris/scitools that is build on dask

Problems solved for user:

- takes the burden of tedious manual pre-processing from the user
- offers well tested and established diagnostics
- ensures reproducibility and traceability via recorded provenance information
- offers computational performance out of the reach of standard scientific user implementations

The development of the ESMValTool is done in public and open-source in a joint international effort of more than 60 institutions of the climate research community, see links below.

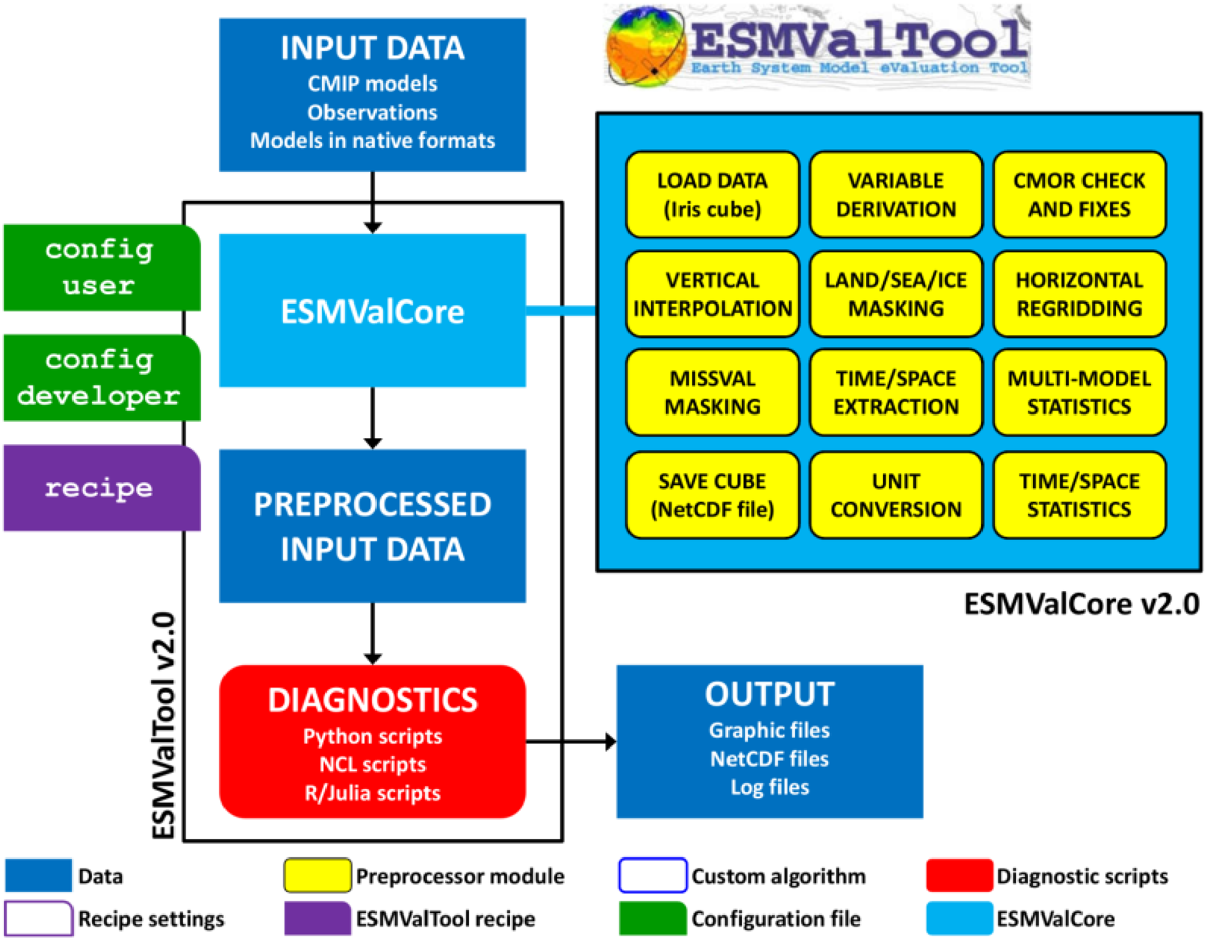

Figure 1.8: Schematic representation of ESMValTool v2.0 workflow (adapted from Righi et al. (accepted))

Figure 1.8 shows the design layout of the ESMValTool. The ESMValCore module is shown expanded picturing the individual pre-processor functions available. Under the configuration and control of the user the flow of the various input data is directed into the pre-processing in the ESMValCore module. The diagnostics chosen by the user are then applied to the pre-processed data and the results of the computations (graphics, data files, etc.) are stored under the control of the user. All user interactions could be abstracted via external web services if desired.

ESMValTool References

- Eyring, V., Bock, L., Lauer, A., Righi, M., Schlund, M., Andela, B., Arnone, E., Bellprat, O., Brötz, B., Caron, L.-P., Carvalhais, N., Cionni, I., Cortesi, N., Crezee, B., Davin, E., Davini, P., Debeire, K., de Mora, L., Deser, C., Docquier, D., Earnshaw, P., Ehbrecht, C., Gier, B. K., Gonzalez-Reviriego, N., Goodman, P., Hagemann, S., Hardiman, S., Hassler, B., Hunter, A., Kadow, C., Kindermann, S., Koirala, S., Koldunov, N. V., Lejeune, Q., Lembo, V., Lovato, T., Lucarini, V., Massonnet, F., Müller, B., Pandde, A., Pérez-Zanón, N., Phillips, A., Predoi, V., Russell, J., Sellar, A., Serva, F., Stacke, T., Swaminathan, R., Torralba, V., Vegas-Regidor, J., von

Hardenberg, J., Weigel, K., and Zimmermann, K.: ESMValTool v2.0 – Extended set of large-scale diagnostics for quasi-operational and comprehensive evaluation of Earth system models in CMIP, Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2019-291, in review, 2019.

- Righi, M., Andela, B., Eyring, V., Lauer, A., Predoi, V., Schlund, M., Vegas-Regidor, J., Bock, L., Brötz, B., de Mora, L., Diblen, F., Dreyer, L., Drost, N., Earnshaw, P., Hassler, B., Koldunov, N., Little, B., Loosveldt Tomas, S., and Zimmermann, K.: ESMValTool v2.0 – Technical overview, Geosci. Model Dev. Discuss., https://doi.org/10.5194/gmd-2019-226, in review, 2019.

ESMValTool Links

- https://www.esmvaltool.org
- https://github.com/ESMValGroup/ESMValTool (Source code)
- https://github.com/ESMValGroup/ESMValCore (Source code)
- https://esmvaltool.readthedocs.io (documentation)

User Requirements

During the FP7-IS-ENES2 Project, an assessment of impact communities' requirements with respect to processing services was performed. The conclusions were:
A number of processing tools are already offered on the climate4impact portal, but both their functionality and how-to are not easily grasped (except perhaps for the sub-setting tool). Better guidance on which to use for what and especially detailed how-to's need to be provided. In addition to the tools already available high priority should be given to fool-proof bias correction and downscaling tools (and associated documentation and guidance) as support for these processing steps appear most on the end user wish lists. This also requires that observed data (CRU, ECA-D, etc.) should be searchable and accessible through the climate4impact portal (including an observation filter/facet in the data search page).

The IS-ENES future Compute Services will have to target several user categories, ranging from climate impact modellers with heterogeneous expertises and working in several scientific domains, to practitioners, and climate researchers (seniors, post-docs, PhD students). The major challenge is to provide Compute Services that can be used properly by users having a large range of both technical and climate science knowledge, with a proper intuitive user interface. Guidance and help will be crucial to support this service, and the functionalities that it provides have to be carefully chosen. A basic layer of generic services laying the foundation of tailored services will be able to provide needed functionalities for users.

Concerning more specifically impact and adaptation users, an in-depth requirements study has been done, and the outcome are the following specific requirements. It also includes some questions users often have, which highlights the needed guidance that must accompany any compute service. The evaluation has been done using the C4I portal, so there are some specific requirements related to the C4I interface itself.

- For impact and adaptation studies at national or sub-national level often relatively high **spatial resolutions** are required. The impacts are determined by local relief, local groundwater management, local activities and population, etc. Climate change adaptation often takes place at the local level, therefore local information is needed. EUROCORDEX now contains the highest spatial resolution, and is a Europe wide dataset. Besides, the runs also have been **bias corrected**, and impact models generally need bias corrected data as input. Impact/adaptation researchers are often not able to do a good bias correction themselves. It would be interesting to make the data from EUROCORDEX (high resolution and bias-corrected) available through the C4I-portal

- For impact and adaptation research often not enough resources (time and financial) are available to take into account a whole ensemble of climate models. In most cases, however, 2 and sometimes up to 4 climate model runs can be used in the analysis. **How to select 2 model runs** (or a few more) that show the range of impacts? To make a selection information on changes under the various RCPs for a large range of climate variables (not just averages, also extremes, variability) and biases is needed. With the ESMValTool data from multiple climate model runs can be analysed. It would be interesting to make the results of these analyses available to other users such as impact researchers in an easy way. Currently there is a CMIP6 evaluation portal at DKRZ[9] where the CMIP6-results of ESMValTool are currently presented.

- **Terminology** in climate science is often a problem for impact researchers. They sometimes use the same terms, but with a different meaning in their discipline, they may have limited background knowledge on climate data, etc. In the C4I portal there are many options/filters of which many aren't that clear for impact/adaptation researchers. Some filters could be formulated in a different way, such that it is clearer for a broader range of users' way (e.g. "frequency" could be named "temporal resolution" or "time step"). Furthermore, more guidance/explanation can also help and in some cases it may be useful to use default options that are most commonly used. E.g. most impact researchers do not understand the names of the files or they do not know what e.g. "Tasmax" means. For the spatial resolution e.g. daily data could be used as default

- Many impact/adaptation researchers have problems with large **amounts of data and the NetCDF format**. Therefore the possibilities to "cut out" certain regions, time periods within the C4I is very useful for them. Also the various options to **process the data online** without the need to download first the complete dataset is very useful. This means that they don't need that much storage capacity and they don't have to program themselves for processing or visualizing the data. It would be good to look whether

[9] https://cmip-esmvaltool.dkrz.de

some more often used processing options could be added to the C4I portal.

- At the moment the C4I portal regularly gives **error messages**, takes **extremely long times for processing** (with regularly error messages at the end). We hope that the updated version of the C4I-portal which is under development will be faster and give less errors. However, it may be useful if some more feedback can be given on the C4I-portal on the time required for e.g. processing and on indications on what is the problem in the case of error messages.

- If we want a broader group to use the C4I portal, **more guidance** material is needed and more training. People from the broader group often do not have much background knowledge on climate data and on how to use the portal. To use the C4I-portal well, one needs a considerable level of knowledge on climate data. For this the guidance material of the portal is now under revision and use will be made of already existing material (e.g. from the C3S User Learning Services).

1.2 Current and Upcoming Challenges

In the current climate research infrastructure, there is a landscape of solutions involving compute services, such as the ESGF CWT https://github.com/ESGF/esgf-compute-api , Ophidia http://ophidia.cmcc.it , the ENES Climate Analytics Service (ECAS) https://ecaslab.dkrz.de/home.html , C4I https://climate4impact.eu/ , the Birdhouse System http://bird-house.github.io . There is also the operational Copernicus Service for climate data, the C3S (Climate Data Store): https://climate.copernicus.eu providing interactive and computing services.

There are also generic infrastructures providing services to scientific researchers, such as the EUDAT CDI https://www.eudat.eu/eudat-collaborative-data-infrastructure-cdi , the European Open Science Cloud (EOSC) https://www.eosc-portal.eu and emerging platforms such as the DARE Platform http://project-dare.eu .

There is already some integration between the Climate RI and the more generic European RIs:

- ECAS is available through EOSC-Hub,
- Ophidia is the ECAS core engine and it provides an ESGF CWT API Interface,
- EUDAT CDI Services are available in EOSC-Hub,
- The DARE Platform will be interoperable with EOSC-Hub, and integrates some services from the EUDAT CDI as well as the ESGF Data Nodes,
- Birdhouse is the basis for WPS based compute service integrations with Copernicus at ENES partner sites (DKRZ, IPSL, STFC),
- C4I has some basic interface to Birdhouse, and is being interfaced with the DARE Platform.

Those compute services are using different approaches and technologies. Those approaches can be categorized into a few distinct types. The first type of approach is to use a specific cluster providing compute time and local storage. Using a multi-layered approach combined with parallel processing, it is very efficient and optimized. Another type of approach is to develop containerized tools that can be deployed on demand using workflows, onto clouds or dedicated RIs, public clouds or national clusters. This is the approach used by the EUDAT GEF Prototype Service as well as the DARE Platform. This second type depends on Authentication and Authorization harmonization (AAI) to let users deploy those components onto computing resources they have access to, such as EOSC-Hub or the EUDAT CDI.

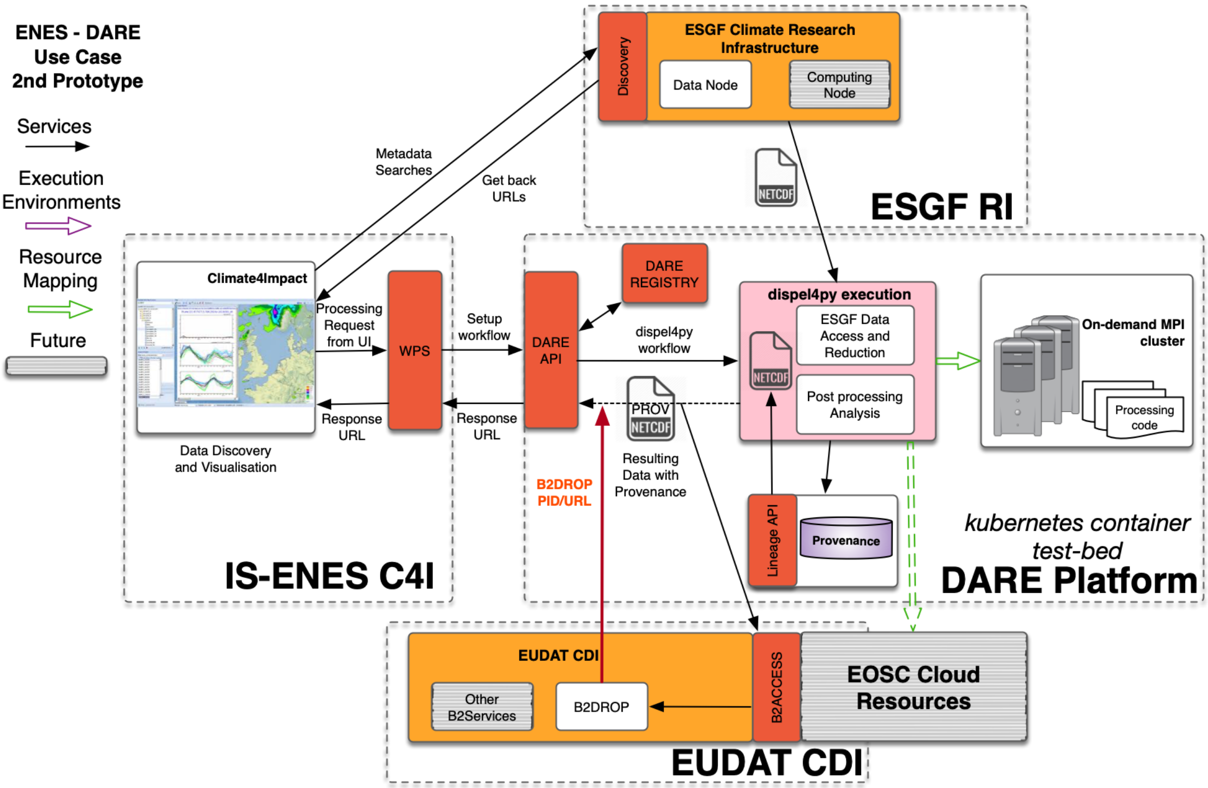

Figure 1.9: Example 1 of integration of RIs: C4I, DARE, EUDAT and ESGF Integration in the context of the H2020-DARE Project.

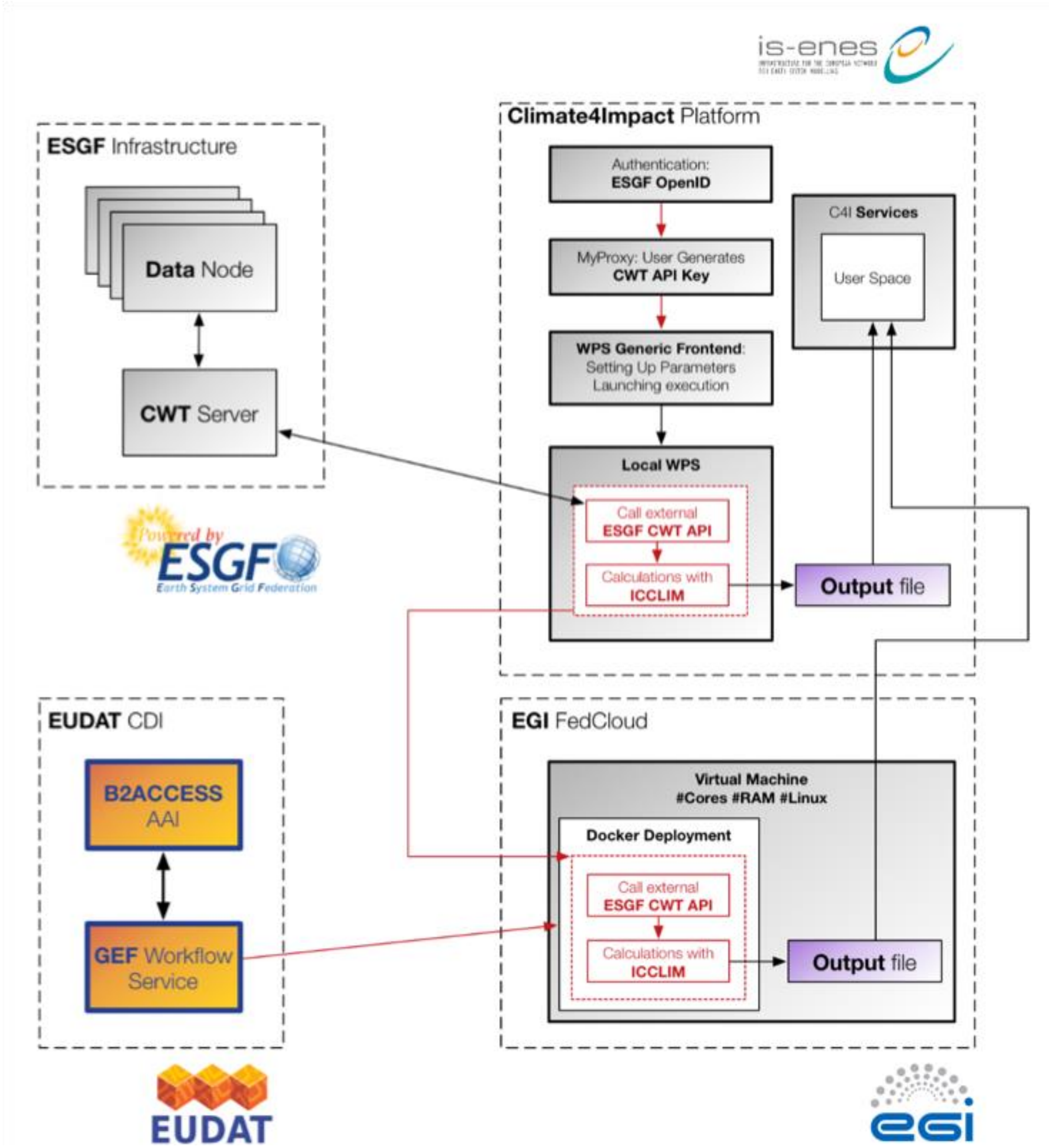

Figure 1.10: Example 2 of RIs integration: C4I, ESGF, EUDAT and EGI in the context of the H2020-EUDAT2020 project.

The added value provided by compute services as part of the ENES e-infrastructure is closely related to the availability of large, efficiently accessible storage pools at sites which can be exploited. Oftenly used data collections (e.g. CMIP5/6 and CORDEX data) are managed as part of these pools, which are also closely associated to ESGF data nodes in many cases, to make the data visible and accessible as part of the ENES ESGF data infrastructure. This required co-location of data and compute services provokes challenges in data management:

- As the overall data volume of e.g. CMIP6 data collections is too large to be stored at one ENES data centre, only parts of these are accessible locally. These parts differ from center to center
- Data collections need to be replicated and synchronized to provide the distributed compute services with an overall consistent data collection.
- Often also non-ESGF accessible data collections are accessible as part of compute services. In contrast to ESGF data there is no consistent overall search service available for these - so site-specific data search and access mechanisms need to be used currently.

A generic challenge for compute services relying on the large climate model data collection stored at ENES data centers is the support of data provenance information for processing results. This on the one hand side requires agreement on standards (e.g. W3C PROV) and the support of these standards as part of the processing framework the specific data analysis code is hosted in. On the other hand side data collections need to be referenced based on persistent identifiers (PID). For CMIP6 ENES partners have established such a PID infrastructure and associated Errata service which can be exploited for future generic data provenance support services.

Data analysis activities often involve large amounts of data and very problem specific amounts of compute resources. Thus users of compute services need to be authenticated and authorized by appropriate AAI infrastructure, and for authorized compute resources have to be scheduled appropriately. On the technical side the core components are present to flexibly support this, yet the organisation of activities at a cross-centre European level is an open issue. First steps are done as part of the compute TNA and VA service offerings supported as part of IS-ENES3, yet this is the very first step with many open sustainability questions.

The evolution of technologies used in platforms, interface and services executing data processing workflows has happened very rapidly during the past few years. This trend is continuing. For example, a few years ago containerization technologies were not mature yet but nowadays they are considered an essential part of infrastructures. It is important to track and consider these developments, with a view to avoiding technology-lockin. Data and metadata standards should also be given consideration, for example the Open Geospatial Consortium (OGC) standards, the CF-Conventions and FAIR data principles.

2. Improving Computing Access for Data Analysis and Processing

2.1 Potential Components for the Compute Architecture

Birdhouse and Twitcher security proxy with Keycloak AAI

The Web Processing Service (WPS) is an OGC interface standard to provide processing tools as web-service. The WPS interface standardizes the way processes and their inputs/outputs are described, how a client can request the execution of a process, and how the output from a process is handled. *Birdhouse* tools enable IT specialists to easily build customised WPS compute service in support of remote climate data analysis. Birdhouse uses the *PyWPS* Python implementation of the Web Processing Service standard. PyWPS is part of the OSGeo project.

Birdhouse offers you:

- A cookiecutter template to build a customised compute service with PyWPS.
- An Ansible playbook to deploy a full-stack PyWPS compute service with Nginx web-server and Postgresql database.
- A Python library, Birdy, suitable for Jupyter notebooks to interact with WPS compute services.
- An OGC security proxy, Twitcher, to provide access control to OGC/WPS compute services.

Twitcher is a security proxy for OWS services like Web Processing Services (WPS). The proxy service uses OAuth2 access tokens to secure OWS services. In addition, one can also use x509 certificates for client authentication. The implementation is not restricted to WPS services. It can also be used for other OWS services like WMS (Web Map Service) and WFS (Web Feature Service).

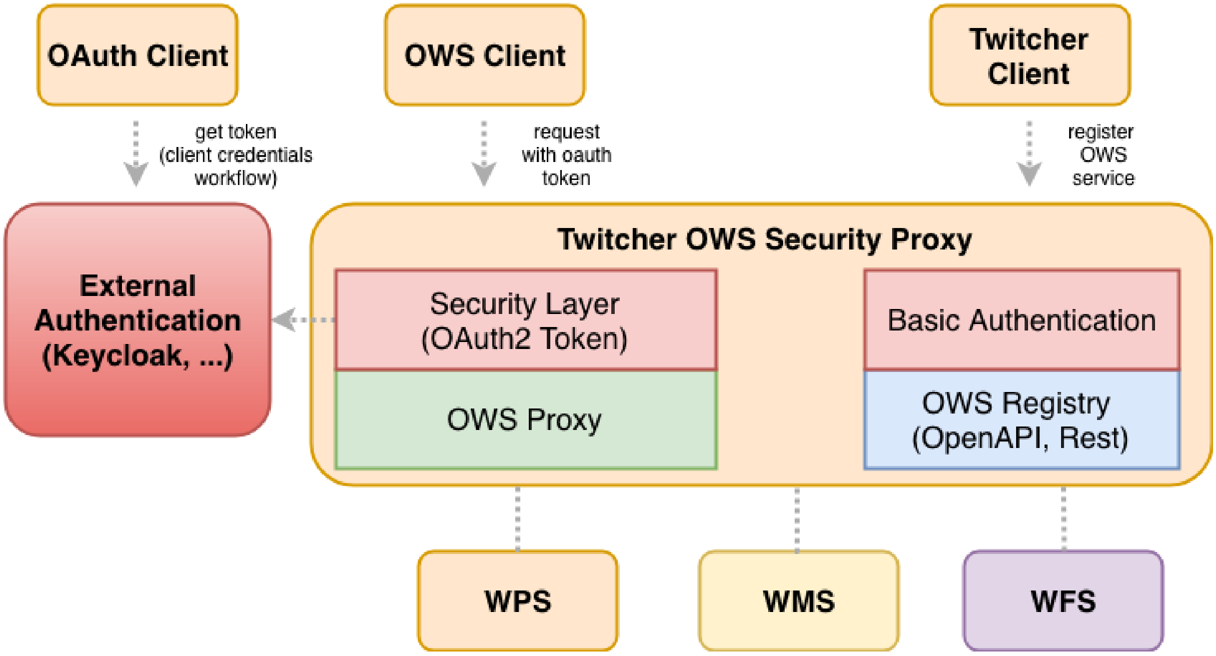

Figure 2.1: Twitcher security Proxy with Keycloak AAI.

Twitcher works together with an external authentication provider service (AAI) like *Keycloak*. Keycloak is an open source implementation for identity and access management. It can be used to secure web services and portals using OAuth2 workflows and access tokens. Keycloak will be used as the AAI component in the future ESGF architecture for a unified identity provider to support data and compute service access.

Birdhouse components are used in the following projects:

- CMCC is using Twitcher/Keycloak to protect the Ophidia PyWPS service.
- The next C4I portal will have access to WPS services protected by Twitcher/Keycloak and will use Keycloak for login.
- In the future ESGF architecture we will use Twitcher/Keycloak to protect the compute service.
- The EU Copernicus project will use a PyWPS compute service deployed with Birdhouse components to provide basic data reduction operations on a CORDEX/CMIP5/CMIP6 data pool.
- The Canadian institution CRIM is using Birdhouse for OGC Testbeds.
- The Canadian climate service centre, Ouranos, is using Birdhouse to deploy PyWPS services for data analysis accessed by Jupyter notebooks (with Birdy).

Components

- *AAI infrastructure*: keycloak, Birdhouse security proxy (“Twitcher”) (see above)
- *Web service endpoints*:
  The approach currently being taken by DKRZ and STFC for Copernicus proposes that the Birdhouse framework is used to provide a single WPS that exposes three main processes:
  1. Subsetting
  2. Averaging (basic fundamental implementation)
  3. Regridding (basic fundamental implementation)

  Since much of this functionality already exists in various code-bases the focus is more on the testing of these operations against a large amount of the relevant "data pools" provided to the Copernicus Climate Data Store (CDS). The heterogeneity of data structures and metadata found within the major MIPs (CMIP5, CORDEX and CMIP6) is a significant barrier to providing generic data processing tools that can operate on a collection of *ESGF Datasets* without errors or inconsistencies. The project aims to generate a database that captures the "character" of the data provided by the MIPs, initially using the subset available to the CDS, which can be mapped to functions that *fix* particular problems. This character will be published to a public register that can be accessed by any tool developers and scientists wishing to work with the data.
  The project will build on existing Python libraries, such as Xarray, and all components will be published in open source repositories. The eventual aim will be to provide an example service that could be easily deployed in a cluster next to an ESGF node.

- *ESGF compute working team specification support*
  As part of ESGF it is planned to expose some processing options in a consistent way to end users. Thus the ESGF compute working team defined on one hand side an API specification[10] (defining a WPS profile) which needs to be supported. On the other hand a server certification document[11] defines requirements on the server backends which ensure stable and efficient processing request handling.
  The ENES CDI will support these specifications for compute service interfaces, which are in the target area of the ESGF CWT specifications (basic, low level data reduction operations like subsetting, regridding etc. This will enable ENES CDI processing service clients (like the C4I portal and end users) to use the different service endpoints in the same way. Several ENES CDI service providers took part in a first "compute challenge[12]" defining a roadmap of coordinated development, deployment and testing steps to stepwise establish ESGF CWT compute interfaces at (some) European ESGF sites.
- *Data search and data catalog services*
  ENES partner sites maintain and manage large climate data pools and parts of these data pools are exposed via ESGF data nodes and thus are indexed and are searchable in the ESGF index services. However, parts of the data pools contain temporary collections stored in specific time frames where they are needed for data analysis activities. To include them in data analysis scripts a standard search interface would be helpful. One option would be to maintain local search indices (eg. Solr or ElasticSearch based) which are updated automatically based on the data pool contents. This route is currently supported e.g. some ENES data centers (e.g. DKRZ and STFC), yet the interfaces are different. An alternative would provide to maintain intake or intake-esm catalogs for those data pool contents. As this intake route is also followed as part of the Pangeo project, this also supports data collections stored in the cloud (e.g. using zarr). Intake catalogs can in principle be coupled with e.g. a ElasticSearch index backend, which would then provide a viable flexible solution for IS-ENES sites. A discussion with the intake-esm and pangeo group at NCAR started to evaluate the potential sustainability of this solution.
  A major advantage of this solution is that data catalogs can be easily exchanged and synchronized between centers. The generation of intake catalogs is also very lightweight in comparison to ESGF data publication and thus supports standard data search and access on very dynamic data collections.
- *Interactive web interfaces: JupyterHub*
  JupyterHub interfaces will provide a key solution to access compute resources and compute services at IS-ENES data centers. They can easily access and exploit Web Processing Services and data catalogs. Yet current deployments differ largely with

[10] ESGF CWT API: https://github.com/ESGF/esgf-compute-api/blob/devel/docs/source/cwt.compat.rst
[11] ESGF Compute Node certification and service certification document: https://esgf.llnl.gov/esgf-media/pdf/ESGF-Compute-Certification.pdf
[12] see e.g. section 6.3. in the OCG testbed report: http://docs.opengeospatial.org/per/19-003.html#_esgf_compute_working_team_api

respect to the available documentation, data access (and search) as well as compute backend solutions and environments. The pangeo initiative defines a full software deployment stack to support HPC computers as well as cloud providers based on new multidimensional data processing technology (Xarray, Iris, Dask, ..). Thus the pangeo community effort will contribute to define a common compute backend software stack, which can be deployed at different ENES-CDI providers.

- *Pangeo*
  Pangeo is a community platform for Big Data geoscience. It is not a specific software package. A Pangeo environment is made up of many different open-source software packages. Each of these packages has its own repository, documentation, and development team. Pangeo Core Packages are:
    a. Xarray
    b. Iris
    c. Dask
    d. Jupyter

  The basis of Pangeo is those 4 packages, and they are very efficient in accessing and processing data stored in NetCDF files using the CF-Conventions.

Interoperability with European e-infrastructures

Because of the large increase in scientific data volumes in all scientific domains, the need of compute services to enable data processing as close as possible to data storage are needed. Those compute services can be part of specific Research Infrastructures, but generic European e-infrastructures have also been developed to provide services to the scientific communities at large. Some major European scientific research generic e-infrastructures are the European Open Science Cloud (EOSC), the EUDAT CDI, EGI, and those that are part of ESFRI. There also exists some current H2020 Platforms for easily deployment of compute services that are also being developed in several projects. One of them has a Use Case based on climate user stories: it is the DARE platform that interfaces the climate ESGF RI, the IS-ENES CDI, and EUDAT B2 Services. This is a good example on how generic research e-infrastructures can be used to provide researchers data processing capabilities, without re-developing those kind of services for a specific scientific domain, providing a more FAIRness approach as well as the possibility to use data from different scientific domains together. Establishing and ensuring that the future compute service for ENES be interoperable with those e-infrastructures are essential.

3. Upcoming Plan – Perspectives

The current deliverable is an important part of the information that will be used to design the architecture of the future compute service. The purpose of the workshop on compute services was to give the opportunity to several groups to present their views and implementation of compute services, and to discuss the approaches and technologies used. Prior to this workshop, MS18 was delivered to work on a draft of the architecture design.

Another important building block is MS20, a milestone due M20 that will gather requirements for technical standards for diagnostic tools, followed by D5.2 on the same subject. The compute service roadmap will be available at M36 with the release of MS21, which will be finalized into D5.3 at M36.

The compute architecture is an integral part of the ENES CDI Software stack. In parallel to the compute services architecture design (M0 to M36), documents describing the overall architecture of the ENES CDI Software stack are released throughout the project at M18, M24, M36, M48, using as a starting point the technical requirements for the software stack MS37 (M14).

Given those milestones, deliverables, and the development plan, the current deliverable act as a starting point to the design and development of the compute service. With the information provided by the Workshop presenters and participants, we have an overview of some data processing approaches, architectures and technologies, as well as targeted users and their respective requirements. Some gaps and limitations have also been identified.

The future compute service should be generic enough to be able to target a large variety of users from different domains and expertises. The difference will be made through tailored interfaces that will target specific users' groups, using the compute service as a backend layer.
Possible limitations will come from technology as well as integration problems between different e-infrastructures and implementation complexity.

4. Conclusions and Recommendations

Currently there is a clear trend visible toward consolidation and harmonizing the processing services provided by the ENES CDI centers. This on one hand side can be stated for the different interfaces provided by the centers: elementary, direct access to compute resources is currently being aligned as part of the IS-ENES TNA service, for providing web service interfaces the birdhouse component (along with its security proxy and support of the OGC WPS interface standard) are being deployed, and for interactive access jupyterhub environments are accessible at the individual centers. Whereas the clear requirement to provide harmonized processing services associated (and co-located) to the large ENES CDI data repositories persists, there is also a clear trend towards providing such services as part of commercial clouds (see e.g. CMIP6 google cloud data offering[13] and associated processing examples) and the European Open Science Cloud (see e.g. the ENES ECAS service). The quality assurance of the diagnostic software and the reproducibility of the results of the analysis already offered by the ESMValTool are strong requirements of the community. With the pangeo software stack and associated current deployments at HPC centers (e.g. NCAR) as well as the cloud, the support for pangeo will also be a strong requirement for the ENES CDI centers. Besides this requirement to provide "standardized" processing service backend software, the need to support flexible, research project specific processing software environments has to be satisfied. This requires the centers to invest in new containerization and container orchestration approaches (which are also used in cloud based deployment scenarios). So the ENES CDI compute service requirements will need to include discussions and agreements on these lower level deployment frameworks to enable consistent and sustainable compute service offerings of the ENES CDI. Initial work started e.g. with respect to Birdhouse-containerization and the Copernicus compute service offering based on this, will be monitored for its usability in a wider context within ESGF environments. Containerization is used in the context of IS-ENES C4I through the use of the DARE Platform (kubernetes approach), and the use of an external deployment of the birdhouse WPS framework.

A current challenge all ENES CDI compute service providers face is the provisioning of common "public" processing services to be used by the broader European (and international) climate science community, because of the missing cost models to cover the (often extensive) resource usage. The current VA and TNA based schemes of H2020 projects are quite insufficient and cross-institutional agreements need probably to be negotiated, which are closely related to the issue of establishing a sustainable ENES CDI and an organisational legal form for this entity.

[13] CMIP6 pangeo data collection on google cloud: https://console.cloud.google.com/marketplace/details/noaa-public/cmip6