IS-ENES3 Deliverable D3.6

Synthesis on user requirements

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ABSTRACT

As part of WP3-NA2 an overview was made of user requirements related to the services developed within the IS-ENES3 project. The set-up of the project is largely based on earlier user requirements or user wishes. The progress on these requirements/wishes is described in the deliverables and milestones of the IS-ENES3 project. In this report a short summary of the progress and remaining user requirements is presented. Besides, some new user requirements were identified in M3.1. If possible these were included in the work of IS-ENES3. For the remaining user requirements it is described whether they can be included in follow-up projects or whether it is hard to do so.

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Executive Summary

Target users of the services and tools developed in IS-ENES3 are the climate researchers, the Vulnerability, Impacts and Adaptation (VIA) researchers, and climate service providers. The idea is that when the services and tools meet the requirements in a better way, they will be used more widely. Therefore, an overview of the progress on user requirements and possible remaining requirements is made at the end of this project, as part of WP3-NA2.

Many requirements from the climate research community related to services and tools for climate modeling and evaluation, as well as tools and services for climate data access and use, were included from the start of the project and most of these requirements have been reached, although further developments are still possible. The progress on these requirements/wishes is described in the deliverables and milestones of the IS-ENES3 project, and this report provides a synthesis of the progress and possible remaining user requirements.

Besides, some new user requirements were identified in M3.1, especially from other potential user groups. If possible these were included in the work of IS-ENES3. Also for these new user requirements the progress is described. Since these were not included from the start of the project, it was more difficult to develop these new services or tools. Also, considerable background knowledge of climate data is required to be able to get access to the data, to process the data, etc. Although it can be made easier to do this up to a certain level (e.g. standardizing file names, indices, making information from the ESMValTool available to select climate models, etc.) not all user requirements from the VIA-community and climate service community can be met, at least not at the moment. For these cases, easy to access and understand background information and tailored training can help these groups.

For the remaining user requirements, it is described whether they can be included in follow-up projects or explained why it is hard to do so.

1. Introduction and objectives

In order to work on widening the user base, nurturing existing users/stakeholder communities, improving mutual understanding between users and developers and expanding community standards, information on user requirements for the various services and tools developed by IS-ENES3 are needed. Target users are the climate researchers and the Vulnerability, Impacts and Adaptation (VIA) researchers. WP3/NA2 also targets societal innovation through the emerging climate service providers. When the services and tools meet the requirements in a better way, they will be used more widely. Therefore, collection of user requirements, both scientific and technical, is an important task in this project (WP3/Task 4). This includes project wide user requirements (information from other WPs and from the activities in the other tasks within WP3/NA2) and more specific requirements. Within tasks 1, 2, 3 in WP3 and through interactions with users in other WPs (e.g. access activities), feedback/user requirements were collected. They were supplemented with desk research on information from other projects or from institutional sources. Specific information on user requirements related to model evaluation and CMIP documentation for climate modeling were also collected through a specific survey (D3.1 & D3.4 respectively).

The set-up of the WPs and tasks in IS-ENES3 is based largely on known requirements for the climate research infrastructure and experience from previous IS-ENES projects. The developments on these user requirements are described in other IS-ENES3 reports. Here only a summary will be given from these reports. In M3.1 a first inventory of additional user requirements was presented. This report D3.6 extends this first inventory and describes the level of answers to the requirements: actions achieved within IS-ENES3, requirements that can be taken into account in future projects/activities, or requirements that cannot be solved. This report also includes some information on the user requirements that were the starting point for the IS-ENES3 project and that were included in the project set-up.

2. Methodology

2.1 Description of the potential users of the results of IS-ENES3

The potential user groups of the services and tools of the IS-ENES3 project are very diverse and not every group is interested in all services and tools provided. To keep the requirements of all these users in mind, we first give a short overview of the potential users we have in mind (based also on the groups identified in the CLIPC[1] project (Bennett & Groot, 2015). It is important to distinguish between different user categories as each has its specific requirements and preferences and they may need different forms and levels of guidance (Petrie et al., 2016).

Climate scientists (including students)

- Climate modelers work on the improvement of climate models. They need among others software tools to develop the climate models, tools to exchange data between modules, to evaluate or calibrate models with observational data, or against other models, etc[2]. They also design and make specific climate model simulations, following common protocols that can be used for climate services
- Climate scientists analyzing climate (model) data need tools to select data, to process data, to visualize climate data, to download large amounts of climate data, to evaluate climate model data (determine skill/bias), etc[3]. Flexibility with many choices in examining the data is key from these climate scientists' point of view. They also wish opportunities to easily share data files. Key for them are clear conventions on data file formats, naming of climate data and indices, together with complete documentation and provenance information. Regularly, results from the analysis are used for climate services, e.g. climate scenarios, analysis of the change in global temperature under specific SSP-RCPs

Vulnerability, impacts and adaptation (VIA[4]) researchers (including students)

- This is a very broad group of users from many different sectors/disciplines who use climate data (observations and climate model data) for VIA studies
- As with climate scientists there are VIA-researchers that focus more on the development of models (impacts, to test various adaptation measures, etc.). These researchers may rather use observational climate data or reanalysis to calibrate their models. Others focus more on the analysis of vulnerability, impacts and adaptation measures. These researchers are more

[1] Climate Information Platform for Copernicus 2013-2016: http://www.clipc.eu/;

[2] Within the IS-ENES projects among others tools for coupling modules, Input/Output, workflow management, evaluation of climate model data were developed or further improved;

[3] Within the IS-ENES projects among others CDO (Climate Data Processing), ICCLIM and the Climate4Impact portal were developed or further improved;

[4] For types of VIA see Hinkel et al. (2012)

likely to use data from climate models to calculate vulnerability, impact and adaptation options under future climate change. Climate data are often used as input for such models, although in most cases a correction for the bias in climate model data is needed

- The spatial and temporal resolution, the domain, the format, etc. may differ a lot between the various disciplines, but also within. They need tools to select data, to process data, to visualize climate data to download large amounts of climate data, to evaluate climate model data (determine skill/bias), etc. These impact scientists benefit from partly preprocessed data and indices (e.g. bias-corrected). They need clear conventions on data file formats, naming of climate data variables and indices, documentation and provenance, etc.
- The level of background knowledge on climate data differs a lot between the various sectors/disciplines. In general researchers on water management are more used to working with climate data than users from e.g. financial/economic research who will need more guidance for the use and selection of climate data
- These groups use climate data and information, but they also often serve as climate service providers further in the chain

Climate service providers (or intermediaries; Bennett & Groot, 2015)

- Very diverse group, but IS-ENES3 focuses only on those climate services providers that use climate model data
- As mentioned above, institutes for climate research often also provide themselves climate services to society. This can be in the form of climate data that others can use (e.g. for vulnerability and impact assessments), information on the state of the current climate and what can happen in the future (e.g. climate scenarios), information on what the impact of mitigation measures can be on the future climate, information on adaptation measures and the effect of these measures, etc.
- As mentioned above, institutes for VIA research often also provide some climate services to society. This can be in the form of data and information on the impacts of climate change and vulnerability in many different sectors. This can also include risk analysis and options to adapt to climate change
- Commercial climate services providers often use data from e.g. climate research and VIA research. They may use the 'raw' data (directly from climate models) or already processed data (climate indices, bias-corrected datasets, etc.). They process the data into products that are tailored to specific user groups. They profit from preprocessed datasets and tools to process climate data into tailored data sets. Commercial providers may also help with decision support related to mitigation and adaptation to climate change (e.g. consultancy companies). Then the provision of climate services is an element of their wider services. IS-ENES3 does not develop services for decision support

- Governmental organisations at different levels (national, regional, municipal, etc.) may also serve as climate service providers. They often use information from research institutes (may also be governmental organisations) or commercial providers
- NGO's may also serve as climate service providers. They often use information from research institutes or commercial providers, sometimes with their specific expertise or data added
- All climate service providers benefit from clear conventions on data file formats, naming of climate data and indices, documentation and provenance, etc.
- Providers that use climate data will need tools to select data, to process data, to visualize climate data, to download large amounts of climate data, to evaluate climate model data (determine skill/bias), etc.

Other potential user groups

- Companies such as reinsurance companies, may use the basic/raw climate data themselves to process them into the information that they require (they are their own climate service provider). They may need tools to select data, to process data, to visualize climate data, to download large amounts of climate data, to evaluate climate model data (determine skill/bias), etc. although they may have developed their own tools. They also need clear conventions on data file formats, naming of climate variables and indices, documentation and provenance, etc.
- Other societal users (or societal end users; Bennett & Groot, 2015): everyone interested and able to use climate data. This could be an NGO that wants to create more awareness of climate change impacts. The expectation is that if they use tools from IS-ENES3, it will be the Climate4Impact portal. However, they may find the C3S CDS and Toolbox more adequate / helpful
- New users from interdisciplinary research fields, attracted by inclusion of climate data in interdisciplinary search catalogs e.g. in the b2find catalog in the context of the EOSC[5]. For most of these users it is important that they can get access to the most up-to-date information through tools that work easily and that will continue to exist for many years

2.2 Models, services and tools developed within IS-ENES3

We shortly list the tools and services provided within the IS-ENES3 project. The services mentioned under Models and tools are used especially by climate modelers and some also by other climate scientists. The services and tools mentioned under data and tools are for all users, although some are used or could be used more by specific groups.

[5] European Open Science Cloud, https://eosc-portal.eu/

Tools for models access and use

- Unified NEMO sea ice model
- Infrastructure tools:
    - OASIS3-MCT coupler (synchronized exchanges of information between different components of the climate system in climate models)
    - XIOS (data flow infrastructure for climate models)
    - Cylc/Rose (for cycling workflows)
    - ESMValTool (model evaluation)
- Framework for coding standards and improving code efficiency (exploit option of ML and AI)
- Common standards for European data sharing, scientific provenance of model evaluation, services on documentation of models and experiments and errata services
- Earth System Model services (HadGEM/UKESM, EC-Earth, NorESM, NEMO): Regular updates, Documentation and Issue tracking

Tools for data access and use

- ENES CDI data distribution (ESGF) and data archival (WDCC)
- Transnational access mechanism (TNA) and VA access to compute resources
- Common standards for European data sharing, scientific provenance of model evaluation
- ES-DOC services on documentation of models and experiments and errata services (for data users)
- Climate4Impact portal (including access to other types of data sets, especially VIA researchers and CS providers)
- CDO data post-processing (climate data operators; for analyzing gridded data)
- Indices and indicators, including standards for names
- Derived data: climate model evaluation data products based on the ESMValTool

2.3 Methods and sources

The following methods and sources are used for collecting information on user requirements for this report:

- During WP3 tasks 1, 2, 3 and other interactions with users in other WPs feedback has been collected (e.g. working with the C4I portal in tasks 1 and 2 provides indirect information about requirements, challenges and questions from various user groups)
- Literature review and other desk research: reports and articles that report on challenges and requirements in other projects

- Feedback and questions from (potential) users of the tools and services during e.g. short trainings, demonstrations or in webinars and during the schools that will be organized in IS-ENES3 (e.g. feedback on the C4I portal)
- Information from other WPs (workshops, reports)

2.4 Delimitation

As indicated in the section on the objectives, the set-up of the work packages and tasks in IS-ENES3 is based largely on known requirements for the climate research infrastructure. In this report we will only shortly report on the progress for these specific requirements and refer to the reports for more detailed information. Known user requirements related to both tools and climate data included in the set-up of the project can be summarized with:

- Unification/standardization, consistency, interoperability, compatibility (with different programming languages and different configurations)
- Scalable, modular and containerization, easy to extend
- Technically robust and reliable/secure
- Easy to maintain
- Efficient/fast/work smoothly/problems solved fast
- Up-to-date (data; coding and design standards; technologies)
- Sustainable (will continue to exist)
- Flexible
- Transparency, provenance, reproducibility
- User friendly, usable
- Quality

Several of these requirements are mentioned also in Milestone 10.1 on technical requirements on the software stack for the Climate Model Data Infrastructure of IS-ENES3. In general, the requirements focusing on users of data and tools aim at making data, models and tools easier to find, easier to use and interpret correctly and to widen the use of them. If these requirements are not met, users may start looking for alternative services and tools.

In M3.2, in the first inventory of additional user requirements, no judgment was made whether all wishes/requirements can or should be implemented. In this deliverable we indicate what can and cannot be implemented.

3. Results

3.1 Sustainability

Sustainability addresses how the community can establish and maintain an infrastructure which can evolve in response to requirements without exclusive project funding such as that delivered via I3 investments from the European commission, such as the IS-ENES funded projects. Within the WP2 task on sustainability a clearer understanding was developed of what needs to be sustained, how it might be done, and what are the needed initial steps towards the implementation of an ENES-Research Infrastructure (ENES-RI). A thorough, iterative analysis of scientific needs and corresponding technical requirements and solutions was done. At the same time the possible legal and organizational opportunities and solutions were evaluated alongside possible governance structures. This resulted in a feasible contour (Sustainability Scoping Report, M2.3), identifying who needs to be involved in delivering the foundational infrastructure, and a proposal and sustainability plan (D2.2). The plan for an ENES-RI (D2.2) sustains some main services and is expected to address the need of users for sustainability.

User interaction: Through bilateral and multilateral exchanges, survey, workshops and discussions in project workshops and general assemblies with the partners, Advisory Board and the likely funders (host institutions, national agencies etc.).

Relevant WPs and tasks

- WP2/NA1, Task 3: Sustainability

Relevant IS-ENES3 documents

- M2.3 Sustainability Scoping Report
- D2.2 ENES-RI Sustainability Plan

3.2 Services related to climate models and tools

The figure below gives an overview of the different services related to climate models and tools and shows where they are used in the infrastructure. The various services and user requirements are described in the following paragraphs.

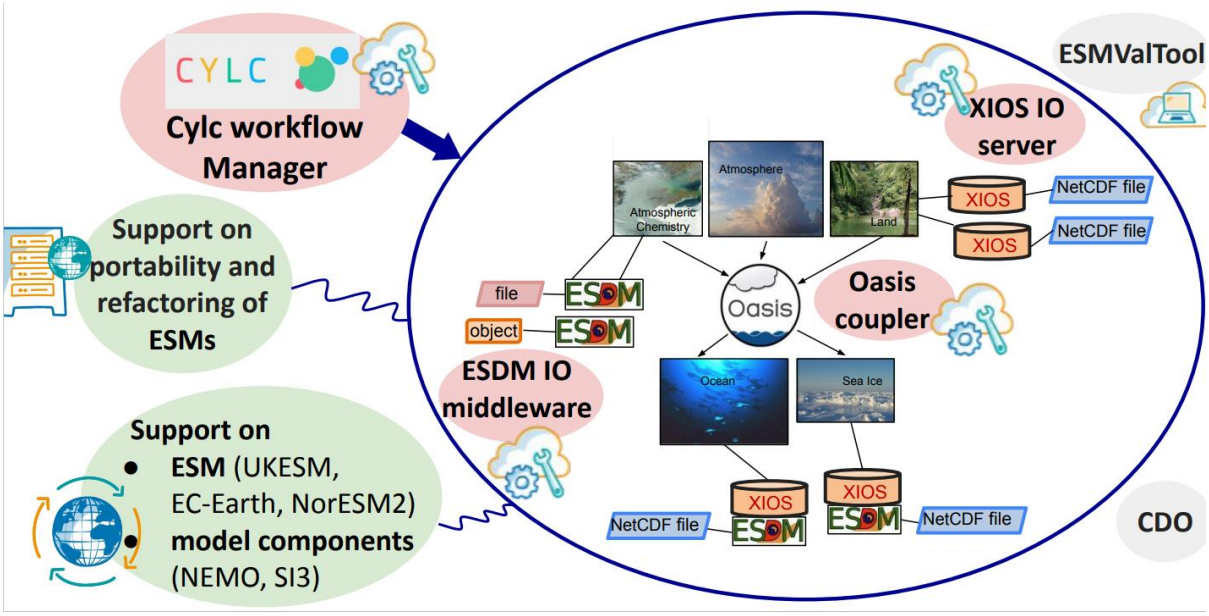

Figure 1. Overview of services and tools in the infrastructure around climate models (source: modified after M2.3).

3.2.1 Unified NEMO sea ice model

The workshop on 'the future of sea ice modeling', held 23-26 September 2019 in Laugarvatn, Iceland (M4.1) brought together many sea ice model developers and expert users to discuss some of the big questions in sea ice modeling. Discussion themes and conclusions from this workshop, published in BAMS (Blockley et al., 2020), were subsequently used within D4.2 'Development strategy for sea ice modeling in NEMO', which also included an update of the sea ice chapter of the 2018 NEMO Development Strategy (NDS). The updated strategy from D4.2 was used as the first draft of the sea ice chapter within the 2022 NDS refresh, which was released on 4th November 2022 following review from NEMO's Scientific Advisory Committee.

Progress on user requirements

At the end of the IS-ENES3 project, a NEMO Development strategy for 2023-2027 version 3.0 (2022) was published. This document contains a section on user requirements (2.1). There are several user requirements that IS-ENES3 has contributed towards. In particular, NEMO requires an integrated sea ice model and that the code should be robust, well-maintained and readable, and HPC compliant (requirements 4, 8,9). IS-ENES3 has supported the development and release of the NEMO's new sea ice model component, Sea Ice modeling Integrated Initiative (SI3) in which several of the user requirements are included (D8.1). In IS-ENES3 also work has been done on the requirement that the code is supported by documentation and peer-reviewed publications (M8.5).

Further user requirements

In November 2022 an updated NEMO Development strategy for 2023-2027 (version 3.0, 2022) was published, including many contributions from the IS-ENES3 project.

User interaction: Participation in workshops/annual meetings, list of who downloaded, ticketing system for support

Links: https://is.enes.org/smt-european-ocean-platform/, https://www.nemo-ocean.eu/, https://forge.nemo-ocean.eu/nemo

Relevant WPs and tasks

- WP4 Task 1: Development of a new Quality assurance approach for the NEMO consortium
- WP4 Task 2: Building a new community around a European Platform for Sea Ice modeling in NEMO
- WP8 Task 1: Improving Nemo computational performance
- WP8 Task 2: Developing the unified European platform for sea ice modeling

Relevant IS-ENES3 documents

- M4.1 Development strategy workshop for European Platform for Sea Ice modeling (2019).
- D4.2 Development strategy for sea ice modeling toolset (2022)
- D4.4 NEMO Quality Assurance update (2023)
- D4.5 White paper on innovation on tools, platforms and techniques (2023)
- M8.4 Definition of NEMO optimization strategy (2020)
- M8.5 Documentation of the NEMO sea ice model (2023)
- D8.1 NEMO sea ice model code (2020)
- D8.5 Update of NEMO code (2022)

3.2.2 Infrastructure tools

3.2.2.1 OASIS3-MCT coupler

This coupler allows synchronized exchanges of coupling information between numerical codes representing different components of the climate system in climate models.

Progress on user requirements

The following user requirements were addressed within IS-ENES3:

- A complete benchmark of SCRIP, ESMF, XIOS and YAC regridding functionality
- A unified scripting environment to calculate the regridding weights with SCRIP, ESMF and XIOS

- A new load balance analysis tool
- Development of Python bindings
- New diagnostics and field combination
- Migration from SVN to GIT for the source management
- New website
- New Short Private Online Course (SPOC)

From the scalability tests done with OASIS3-MCT at high number of cores and the fact that it supports unstructured grids, it can be concluded that this coupler offers today a fully parallel and efficient coupling solution answering the short- and mid-term needs of the European climate modeling community

Further user requirements

The following could not be addressed within IS-ENES3, but can be solved in future projects or activities:

- evaluate the scalability of the regridding weight calculation for SCRIP, ESMF and XIOS and possibly YAC for a number of cores higher than 2000 to produce a more complete performance analysis
- facilitate the use of the unified scripting environment including SCRIP, ESMF and XIOS by delivering the whole environment using a container technology such as Docker or Sarus
- evaluate the behaviour of the coupler on heterogeneous hardware, e.g. CPU-GPU systems
- on the longer term consider the support of vertical interpolation and the modernization and extension of namcouple syntax

User interaction: The page on governance describes how users are included in the user and advisory board (https://oasis.cerfacs.fr/en/governance/). In 2017 and 2019 user surveys were held and the findings were included in the development plans (https://oasis.cerfacs.fr/wp-content/uploads/sites/114/2021/03/GlobC-TR-164-202011_OASIS3-MCT_development_plan_final.pdf). Five categories of developments are distinguished: Interpolation & transformations, Communication, Configuration, Other functionalities, Support & training (for more information see development plan). The forum on the OASIS website gives an overview of user support, issues, bugs, etc.

Links: https://is.enes.org/smt-common-software-tools/; https://oasis.cerfacs.fr/en/

Relevant WPs and tasks

- WP4, Task 3: Complex Coupled Systems HPC performance evaluation (integrate LUCIA (Load-balancing Utility and Coupling Implementation Appraisal) performance tool in the OASIS3-MCT coupler)

- WP6, Task 3: Services for European infrastructure tools (Active user support (AUS), including web services (e.g. on-line download, installation information, tutorial, FAQs, hints for best practices, forum) and assistance through e-mails)
- WP8, Task 3: OASIS3-MCT development

Relevant IS-ENES3 documents

- D4.1 Coupling workshop report (2020)
- D6.4 Report on new OASIS coupled models/interface (2022)
- M8.3: Final list of development for OASIS3-MCT_5.0 (2020)
- D8.2: OASIS3-MCT_5.0 release (2021)

3.2.2.2 XIOS

XIOS is a tool offering a full and efficient data flow infrastructure for climate models that combines parallel online data treatment and data input/output from/to files.

Progress on user requirements

The following user requirements were addressed within IS-ENES3:

- Complete rewriting to improve code performance, readability, reliability and evolutivity
- New client/server protocols for increased performance
- Rationalization and improvement of the grid distribution for lower memory consumption
- New HPC service-oriented infrastructure opening the door to future climate modeling, ensuring improved support of large ensembles and coupling
- A set of automated unit tests based on continuous integration concept https://forge.ipsl.jussieu.fr/ioserver/chrome/site/XIOS_TEST_SUITE/xios_report.html)
- More explicit error diagnostics for easier resolution of problems
- Graphic representation of the XIOS work for better debugging and tuning
- Additional internal output timers to refine the performance profiling of the workflow.
- Internal tracking of the memory to diagnose memory leaks and overall consumption.
- Extension of the dr2xml, a python package written to exploit the CMIP6 Data Request API, to other simulation contexts (dr2xml V3.0)

Further requirements

The following user requirements could not be achieved within IS-ENES3, but can be addressed in future projects or activities:

- The possibility of restarting a model using XIOS at any time without losing part of information (may be done before the end of the project)
- Additional spatial transformations: bilinear or nearest-neighbour interpolations, and more complex operators, such as curl or divergence

- Time interpolation (to ensure, for example, that a monthly file could be read in and will automatically provide interpolated daily values)
- Multi-threading: the technique implemented in ESiWACE still needs to be revised

User interaction: Information on user needs collected from users and through the Active User Support

Links: https://is.enes.org/smt-common-software-tools/, https://forge.ipsl.jussieu.fr/ioserver

Relevant WPs and tasks

- WP6, Task 3: Services for European infrastructure tools (Active user support (AUS), including web services (e.g. on-line download, installation information, tutorial, FAQs, hints for best practices, forum) and assistance through e-mails)
- WP8, Task 4: XIOS development

Relevant IS-ENES3 documents:

- M8.1: A set of unit tests for XIOS (2020)
- D8.3: XIOS new release (2022)

3.2.2.3 Cylc/Rose

Cylc is a general-purpose workflow engine that orchestrates cycling workflows very efficiently. It was designed for use in production weather, climate, and environmental forecasting systems, but it is not specialized to those domains and is agnostic to the applications it manages. Rose is designed for use with Cylc and is primarily a toolkit for writing, editing, and running application configurations.

Progress on user requirements

Cylc and Rose were further developed, increasing their usability, responding to changing technologies and improving performance.

- Improvements to the performance and scalability of Cylc to address the needs of increasingly complex workflows. This was achieved primarily via the new scheduling algorithm described in D8.4
- Adoption of new GUI technologies to replace the deprecated GTK+ 2 based GUIs. This has been achieved for Cylc, but for Rose this will not be completed before the end of IS-ENES3
- Implement the 'graph view' (a widely used feature of the Cylc 7 GUI) and add support for viewing job log files (including historical tasks). These requirements both refer to missing

features from the new Cylc GUI (they are part of 'Adoption of new GUI technologies'). Both will be delivered before the end of IS-ENES3

- Migration from Python 2 to 3. With the end of life of python 2 expected in 2020 this work is essential to ensure long term support (completed)
- M8.2 also identified 'Migrate the Rose functionality for running Cylc workflows ('rose suite-run') into Cylc' as a key priority (completed)

Further user requirements

And the following could not be solved within IS-ENES3, but can be solved in future projects or activities:

- Some enhancements were identified in the agreed development priorities (M8.2), for example improved housekeeping and support for running multiple tasks in a single job. These were identified in M8.2 as priorities beyond Cylc 8 & Rose 2, but they haven't been addressed because the work on Cylc 8 & Rose 2 is not yet complete

User interaction: Development priorities are community driven, supported by the governance activities in WP2/NA1 and informed by the service activity in WP6/VA1. Priorities for development are described in M8.2. A distinction is made between the highest priorities and immediate priorities beyond Cylc 8 and Rose 2. Priorities were constantly reviewed based on progress and user feedback.

Links: https://is.enes.org/smt-common-software-tools/, https://cylc.github.io/

Relevant WPs and tasks

- WP6, Task 3: Services for European infrastructure tools (Active user support (AUS), including web services (e.g. on-line download, installation information, tutorial, FAQs, hints for best practices, forum) and assistance through e-mails)
- WP8, Task 5: Cylc/Rose development

Relevant IS-ENES3 documents

- M8.2: Cycl/Rose development priorities agreed (2020)
- D8.4: Cylc/Rose development summary (2022)

3.2.2.4 ESMValTool (standardized model evaluation)

ESMValTool is a community diagnostic and performance metrics tool for routine evaluation of Earth system models, originally designed to process output provided by large model intercomparison projects, like CMIP. A survey was executed among (potential) users in the months of June to October 2020 (WP3, task 4.2) by Assimila Limited about the services and technical

requirements. The roadmap (https://www.esmvaltool.org/roadmap.html) outlines the ESMValTool developments that are planned until the end of 2022 and which are based on experienced user requirements.

Until now, the results of ESMValTool have been used mainly for model evaluation, to check whether they perform well against observations/re-analysis, to check how they differ from earlier model versions, to check what is the projected change in the future, etc. Efforts are being devoted to coupling ESMValTool to diverse computational platforms, data sources and model development workflows in order to address user requirements. However, results of the model evaluation (e.g. of all CMIP6 or CORDEX) may also be useful for impact research or climate service providers. Several of the requirements that are needed for these applications are included already in the current tool (Eyring et al., 2019; Righi et al., 2020), but these new users often do not know how to access ESMValTool model evaluation products or reproduce those products using the tool.

Progress on user requirements

- free download of up-to-date versions: published on conda-forge, PyPI, dockerhub, and via GitHub. The download statistics can be viewed on these platforms
- enhanced and automated documentation via SPHINX: is available at https://docs.esmvaltool.org and automatically kept up-to-date. The documentation contains detailed instructions on how to install, configure, and run ESMValTool. It also contains extensive documentation on recipes and diagnostic scripts published in ESMValTool releases. The documentation also contains links to additional sources of information: tutorial, FAQ, mailing-list, public monthly meetings, contact information
- tutorial that can be taken online independently is available at https://esmvalgroup.github.io/ESMValTool_Tutorial/ . The tutorial has also been used for trainings taught by instructors
- provide a FAQ is available on GitHub: https://github.com/ESMValGroup/ESMValTool/discussions with different categories of topics
- personal help to efficiently use the software: support is possible through: 1. direct interactions with developers on GitHub (issues and discussions), 2. Monthly ESMValTool community meeting open to all users, see announcements here, 3. the ESMValTool mailing-list
- Set up a diagnostics portal that facilitates the display of results of ESMValTool recipes: is available https://esmvaltool.dkrz.de/shared/esmvaltool/ . Results produced with each new released version of ESMValTool are uploaded there
- Automate the process of observational data acquisition and reformatting in ESMValTool: Was delivered with ESMValTool 2.5.0 (March 2022). The Tool provides scripts to automatically download observational data from about 50 different sources. A second set

of scripts is available to reformat about 75 observational datasets to the CMOR standards so these can be used in model evaluation

- Develop a new component for the coupling scheme that allows the application of ESMValTool as an online analysis tool. This so-called 'Quicklook' capability was delivered in ESMValTool 2.3.0 and enables users to monitor simulations while they are running in the machine
- Incorporation of ESMValTool into modeling or stand-alone workflow: was delivered in ESMValTool 2.3.0 and subsequent releases. A set of monitoring recipes and diagnostics is available for online analysis of model runs. Also, support for 5 different native model output has been added to ESMValTool: CESM2 (experimental support), EC-Earth3, EMAC, ICON, and IPSL-CM6. Output from these models can be 'CMORized' during model evaluation runs without needs to store formatted copies of the output
- Coupling ESMValTool to ESGF data nodes: the Tool searches for data first on the local ESGF node (if access possible from the HPC cluster) and then downloads missing data from all other nodes. The implementation uses ESGF-Pyclient and is documented here
- Deployment on HPC clusters: a module is available on CEDA-Jasmin and a module and a Jupyter Kernel on DKRZ-Levante
- Distributing tasks across compute nodes of different machines: preprocessing tasks can be split across machines. This can significantly reduce the volume of input data for the diagnostics. Preprocessed data from different machines can be downloaded to the end machine where the diagnostics are computed. This feature would allow setting up a WPS
- Support data from the decadal climate prediction project (DCPP[6]) activity: DCPP data is now supported in ESMValTool through a more flexible handling of the time coordinate
- Support data from the CORDEX project: CORDEX data can be loaded, addition of metadata fixes is still ongoing
- Improving the performance of the ESMValTool backend: ongoing until the end of the project
- Containerization: docker containers and Singularity are supported, enabling users to run ESMValTool on HPC clusters. This is particularly convenient for users of clusters where other installation methods are disabled and significantly lowers the barrier to deploy ESMValTool on these clusters
- Implementation of standard interfaces, provenance and coding guidelines for the inclusion of external diagnostic packages': done following recommendations from D5.2 and D5.5

As indicated many analyses could already be executed with ESMValTool, but not all potential users are aware of this. For this purpose a webinar and trainings were organized (in June 2022), and an introduction to ESMValTool was given during the Impact Schools. Also a lot of tutorial material is available on the ESMValTool website.

[6] https://www.wcrp-climate.org/dcp-overview

Further user requirements

- ESMValTool is widely used and has a considerable user community that is involved also in the development teams and workshops. Although the current roadmap does not go further than the end of 2022, further user requirements will be identified and included in the future roadmap (https://www.esmvaltool.org/roadmap.html). The roadmap will be overseen and updated by the future Steering Group as part of the ESMValTool governance for which a consortium agreement has been prepared
- Improved support for irregular and unstructured grids is ongoing: it requires a long process of discussion between modelers and tool community

User interaction: In the development teams many of the users are represented (https://www.esmvaltool.org/team.html). Also regular meetings were held to discuss future strategies and provide updates on progress (https://www.esmvaltool.org/meetings.html). Besides, presentations and training are provided on ESMValTool (e.g. in Oct 2021). However, it is difficult to know all users, since the tool can be downloaded in various ways.

Links: https://www.esmvaltool.org/, https://is.enes.org/smt-common-software-tools/

Relevant WPs and tasks

- WP5, Task 5: Technical standards and an architecture for plugin diagnostic tools
- WP9: Earth System Model Evaluation developments (all 8 tasks)
- WP3, Task 4.2: Specific user requirements (the survey conducted by Assimilia Limited)
- WP6, Task 3: Services for European infrastructure tools (active user support)
- WP7, Task 2: Compute services (recipe portal hosted at DKRZ)

Relevant IS-ENES3 documents

- M5.3 Requirements for technical standards for diagnostic tools (2020)
- D5.2 Technical standards for diagnostic tools (2021)
- M9.1 Release of enhanced ESMValTool documentation for VA1 Activity (2021)
- M9.2 Release of enhanced ESMValTool documentation for VA2 Activity (2021)
- D9.1 ESMValTool version supporting irregular and unstructured grids (2020)
- D9.2 ESMValTool version enabling model development usage (2021)
- D9.3 ESMValTool version with ESGF coupling and distributed computation (2021)
- D9.4 ESMValTool version supporting reginal climate models and different timescales (2021)
- D9.5 ESMValTool version (2023)
- D3.1 Initial requirements on model evaluation (2021) (the survey conducted by Assimilia)

3.2.2.5 New technical opportunities and tools

During the project a complete computational and energy performance analysis of CMIP6 was performed. This is required to reduce the cost of each component independently and as a whole. Machine learning, artificial intelligence and big data together represent an area with a wealth of specialist hardware platforms available that are likely to prove useful to the climate community to improve code efficiency and analysis of large datasets.

Progress on user requirements

The computational and energy performance analysis of CMIP6 is described in D4.3 and this document also contains advice on how to reduce computational and energy costs. During the IS-ENES3 project the options of machine learning and artificial intelligence were explored and the results are described in M4.2, M4.3 and D4.5.

Further user requirements:

- The adoption of machine learning by the climate modeling community is still in its early stages. Most of the work in IS-ENES3 was based on information exchange about exploratory projects. It is too early to clearly elicit user requirements in that area
- The HPC performance work will continue. Some particular areas of improvements are better metrics and tools for energy consumption of models on HPC. More advanced automatic load balancing tools are also an active area of research with demand from modeling centers for better algorithms

User interaction: HPC workshop and other interactions with HPC, Data School

Links: https://is.enes.org/workshops/ (HPC workshops), https://www.iit.demokritos.gr/is-enes-summer-school/ (lectures Data Science School)

Relevant WPs and tasks

- WP4, Task 3: Complex Coupled Systems HPC performance evaluation
- WP4, Task 4: Machine Learning and Technology Tracking
- WP4, Task 5: Community Workshops
- WP4, Task 6: Innovating with software and HPC industry
- WP8: Models & Tools developments

Relevant IS-ENES3 documents

- M4.2 New technical opportunities workshop in ML and AI (2021)
- M4.3 HPC workshop report (2022)
- D4.3. CMIP performance metrics and community advice (2021)

- D4.5 White paper on innovation on tools, platforms and techniques (2023)

3.2.3 Standards on climate models

Standards in Earth system science are numerous and it is key to evaluate which can be used or adapted for IS-ENES use and which need to be developed. The existing standards used by ENES are not necessarily the same as the standards in user communities (e.g. impacts) and a venue for exchanging on these standards is needed to collect user requirements and provide training. Within IS-ENES3, a series of workshops was organized (or IS-ENES3 contributed to these workshops) for different areas of standards development and addressed areas of work which were associated with bottlenecks in operational procedures (M3.4 and D3.3). D3.3 mentions the following streams of activities related to standards:

- Vocabularies and Standards for Climate Model Data
  - Earth System Model Documentation (ES-DOC)
  - CMIP Data Request
  - Exploiting CMIP6 Data Request tools for additional MIPs
  - Climate and Forecast Convention (CF)
  - file naming convention for climate model output (see also par. 3.3.5)
  - vocabulary metadata (for climate indices see par. 3.3.4)
- Standards Supporting data Exploitation Services
  - FAIR Data
  - Licensing
  - Citation
- Standards for Trust
  - Propagation of documentation and provenance information
  - Long Term Preservation and Trust

Progress on user requirements (based largely on D3.3):

- The process of enabling flow of information from ES-DOC, through the Copernicus Climate Change Service (C3S) platform and into the European Climate Data Explorer (ECDE) portal, combined with the reverse process of updating ES-DOC to match the end-user requirements, has shown how a vertically integrated workflow from modeling community to end-users can give feedback to enhancements in the core services
- Vocabularies and standards for CMIP: data request of the Coupled Model Intercomparison Project Phase 6 (CMIP6) defined all the quantities from CMIP6 simulations that should be archived. The complexity of the data request has increased from the early days of model

intercomparisons, as has the data volume. In contrast with CMIP5, CMIP6 required distinct sets of highly tailored variables to be saved from each of the more than 200 experiments. This placed new demands on the data request information base and led to a new requirement for development of software that facilitates automated interrogation of the request and retrieval of its technical specifications. Building on the CMIP6 data request combined requirements the challenges and achievements of CMIP6 were reviewed and recommendations were provided for CMIP7 (M3.4 and D3.3). M10.2 CMIP data request schema 2.0 sets out the strategic and technical requirements for a revised request designed to support future model intercomparison work. In D3.3 the issues and solutions with the data request are described

- Climate and Forecast Convention (CF, https://is.enes.org/sdm-access-metadata/): this standard underpins interoperability of climate model data by providing a rich framework for detailed, machine-operable, technical information about the data products. The CF Convention is maintained by a community network to support the international climate research community. This CF Convention is also reviewed and recommendations are formulated (M3.4 and D3.3)
- File naming convention (http://cfconventions.org/standard_name_rules.html): IS-ENES3 partners are contributing to two ongoing discussions about evolving metadata standards which are being led within the WGCM Infrastructure Panel on Harmonizing Metadata and Filenames Across CMIP Eras and WCRP Activities and Climate experimentation beyond CMIP6
- Vocabulary metadata: CEDA (UKRI) contributed to the RDA 'InteroperAble Descriptions of Observable Property Terminologies (I-ADOPT) WG Outputs and Recommendations' which set out an ontology for describing parameter vocabulary metadata. That is, a means of describing the terms used to identify parameters in different vocabularies is set out as a means to enhance interoperability between vocabularies.
- FAIR Data: IS-ENES members worked with TG-DATA and the IPCC WG1 Technical Support Unit to design and implement FAIR Data Guidelines for the IPCC 6th Assessment Report (Pirani, 2022). Implementation of these guidelines results in direct links from the IPCC 6th Assessment Report to standards compliant catalog entries in the CEDA catalog
- Licensing: IS-ENES3 partners contributed to productive and influential discussions about the CMIP and IPCC licensing frameworks, leading to agreement on licenses which enables a balance between flexible exploitation of CMIP data and protection of the rights of the data creators. Licensing is a crucial aspect of distribution that allows for the wide-spread use of products with legal security. The CMIP6 data is covered, for the first time, by a standard license which gives clarity about the legal status of the data
- Citation: The Citation Service (https://doi.org/10.5281/zenodo.35178) is based on existing standards and recommendations of the data publishing community. Citation links are

provided in the ESGF search results and the CMIP6 citation search (http://bit.ly/CMIP6_Citation_Search with export possibility in csv). They can also be provided in the ES-DOC system

- Scientific provenance of model evaluation: Documenting and providing information on the origin and post-processing stages of model evaluation is key to build trust, allow for a consistent scrutiny and comparison of evaluation products and increase use of a model evaluation software (data provenance) for users. It also provides a framework for climate expert groups to provide and govern the complete definition of metrics and diagnostics (computation, observations used, documentation, etc). A user requirements inventory was done (D3.1) and a framework was defined for the propagation of documentation and provenance information, in order to ensure that the evaluation process is traceable and fully reproducible (Andela et al., 2021)
- Coding standards and improving code efficiency of the Earth System Model Evaluation Tool (ESMValTool, https://www.esmvaltool.org/): see section 3.2.2.4 on ESMValTool for progress on coupling, data acquisition, unstructured/irregular grids, display, containerization, etc.
- It is important for their long term traceability and trust to preserve core climate data as well as core components of the ENES Research Infrastructure (ENES-RI) for the long-term. Standards for climate data, climate models, climate model evaluation, etc. are the basis for this traceability

Further user requirements:
The 'IS-ENES3 White Paper Framework for the propagation of documentation and provenance information in the model evaluation process' (https://zenodo.org/record/5759571#.Y4naMFLMIdqand) provides a general set-up for the framework for the propagation of documentation and provenance information in the model evaluation. The implementation may result in further user requirements.

User interaction: workshops on vocabularies and standards for CMIP, CF- conventions, survey on ESM evaluation, etc. (see also M3.4 for an overview of workshops related to standards).

Links: see in the text above and in D3.3 for the various subjects.

Relevant WPs and tasks

- WP3, Task 3: Community standards
- WP5: Networking on data and model evaluation
- WP7, Task 4: Support for CF convention and Data Request - 'CFDR'
- WP9, Earth System Model Evaluation developments

Relevant IS-ENES3 documents

- M3.4 Summary of workshops on standards (2023)
- D3.1 Initial requirements on model evaluation (2021)
- D3.3 Standards synthesis (part on provenance) (2023)
- D3.4 CMIP documentation requirements (ES-DOC services) (2021)
- D5.6 ES-DOC governance (2023)
- M7.3 Improved version of evaluation portal (2021)
- D7.1 First KPI and TNA report for ENES CDI services (2020)
- D7.3 : Second KPI and TNA report for ENES CDI services (2022)
- D7.6 : Third KPI an TNA report for ENES CDI services (2023)
- D9.1 ESMValTool version supporting irregular and unstructured grids (2020)
- D9.2 ESMValTool version enabling model development usage (2020)
- D9.3 ESMValTool version with ESGF coupling and distributed computation (2021)
- D9.4 ESMValTool version supporting reginal climate models and different timescales (2021)

3.2.4. ESM services

Services around the main European ESMs, and the NEMO ocean model, have been further maintained, extended and improved during the IS-ENES3 project. The overarching objectives for all services are to give easy access to information (level 1 for all the main European ESMs in CMIP6), to provide interfaces between ESM developers and users, and to define processes (such as for feedback) for model development and usage (level 2 for the ESMs HadGEM/UKESM, EC-Earth, NorESM and NEMO). Beside the climate models, a number of critical infrastructure software tools have been identified in previous IS-ENES projects and by the community at large (the user requirements and activities around these are described in section 3.2.2). Model and tool development groups provide updated versions of their respective software, documentation, contact information and user feedback channels. Particularly for ESMs, updated information for CMIP6 model versions and links to in-depth documentation on ES-DOC is provided.

Progress on user requirements

- Minimal set of information for CMIP5 and CMIP6 ESMs easily and centrally accessible for the whole community: Model description, contact, link to website available for all ESMs at https://is.enes.org/smt-european-esms/ ES-DOC information and links for CMIP5 and CMIP6 available for all models except for NorESM, where CMIP6 is missing (only CMIP5)

- Advanced set of services (level 2) to allow researchers to make effective and efficient use of a subset of ESMs and the NEMO ocean platform: access to up-to-date model versions and associated documentation, functional communication channels between model users and developers. service provided as described for all level-2 models and tools. Quantitative level-2 results (KPIs) reported in D6.1 and D6.3, last report upcoming with D6.6

All ESMs and tools have maintained a high level of service activities (D6.2). At the end of the external review, a decision was taken to entirely rewrite the ENES portal pages, following the external review recommendations for the Services section. The update of the website has been completed and the latest information is available for all ESMs (D6.5).

User interaction: User requirements are typically received via the information on the Portal, or directly through the communication channels (e.g. issue tracking and the Active User Support) linked.

Links: https://is.enes.org/smt-european-esms/

Relevant WPs and tasks

- WP6: Services on European ESMs and Software Tools

Relevant IS-ENES3 documents

- M6.1 ENES ESM resources updated (2020)
- M6.3 ENES ESM resources updated RP2 (2021)
- M6.4 ENES ESM resources updated RP3 (2022)
- D6.1 First Periodical report on service statistics for models and tools (2020)
- D6.2 First external review of model and tools services (2020)
- D6.3 Second periodical report on service statistics for models and tools (2022)
- D6.4 Report on new OASIS coupled models/interface (2022)
- D6.5 Second external review of model and tools services (2022)
- D6.6 Third periodical report on service statistics for models and tools (2023)

3.3 Services related to tools for data access and use

Several of the services mentioned under 3.2 are also relevant for tools and data access and use, since many climate data are based on climate models: such as standards, ESMValTool and sustainability. These will not be treated again in this paragraph unless this concerns new services.

3.3.1 ENES CDI data distribution (ESGF) and data archival (WDCC)

Climate models can produce a large amount of data nowadays, but the storage capacity, processing capacity and access is not always in line with what users would like to have. In IS-ENES3, key software components related to the data infrastructure like data distribution, processing, vocabulary management, documentation based on standards and impact study tools (e.g. Climate4Impact, access through C3S CDS, CDO) were considered (partly discussed in other paragraphs). Technical requirements for these services and the software stack were explored.

User requirements

- Implementation of technical requirements: A core user requirement is associated with the stability and resilience of the ESGF based data delivery. This was addressed at several levels in IS-ENES3:
  - IS-ENES3 user support addressed the majority of ESGF related user interaction
  - IS-ENES3 contributed to a more reliable and sustainable deployment possibility of ESGF data nodes (based on docker containers), which improves stable data distribution service operations
- ENES Climate Analytics Service (ECAS): To exploit the ECAS service users often need to include external data in their analysis which is not yet available in the ECAS associated data pools. Users are supported in this and important data sets are replicated and thus included in the ECAS service offering
- Indice Calculation CLIMate (icclim): see par. 3.3.8
- The IPCC Data Distribution Centre (IPCC-DDC) provides: 1) Data used as input to the Second, Third, Fourth, and Fifth IPCC Assessment Report (long time archival); 2) Socio-economic data and scenarios for the impact community: population, economic development, technology, and natural resources; 3) Visualization service
- The World Data Center for Climate (WDCC) is hosted at DKRZ in Germany and provides curated data for storage periods longer than 10 years and the technical quality checks and data publication service grants permanent accessibility by assigning unique persistent identifier DOI to data and metadata. Core CMIP6 data collections were added (these include CMIP6 IPCC-DDC related data as well as other oftenly requested CMIP6 data collections)
- Specific quality controlled CMIP and CORDEX data collections are stored separately at DKRZ and CNRS-IPSL and exposed to the CDS

Further user requirements

The complete replication of CMIP6 to Europe as well as the archival of the majority of CMIP6 is not easy to realize, because of the huge data volume and the limited storage resources in the ENES CDI. Additionally, the overall CMIP6 data collection is still constantly changing (removal of erroneous data, update of new versions, adding new simulation etc.). Thus users are constantly supported in on demand replication of needed data collections to the ENES CDI data pools. This can be taken up partly in new projects and in the ENES-RI (sustainability plan).

User interaction: Info on type of questions to CDI helpdesk, use cases for CDI, most user interactions are related to data access problems often related to temporarily unavailable data servers. For scientific questions (this e.g. also includes the detection of erroneous data) users were directed to the specific climate model related science contacts.

Link How to Access and Use Model Data: https://is.enes.org/sdm-access-use-data/

Relevant WPs and tasks

- WP5, Task 3: Defining and communicating European priorities for ESGF
- WP7 Task 1: ESGF Data Dissemination, Long Term Archival and User Support (VA) – 'ESGF-WDCC-C4I
- WP7, Task 3: Virtual workspaces (TNA) - 'Comp2'
- WP10: ENES Climate Data Infrastructure software stack developments

Relevant documents:

- M5.1 Draft Architecture Design (2020)
- M5.2 ESGF CMIP6 Summary (2020)
- M5.4 Compute service roadmap (2021)
- D5.1 Compute service requirements and state of the art approaches (2019)
- D5.4 IS-ENES3 involvement in ESGF (2021)
- M7.1 ENES CDI help desk (2019)
- M7.2 Complete ENES-CDI long term archival for CMIP6 (2023)
- D7.1 First KPI and TNA report for ENES CDI services (2020)
- D7.2 First external review report for ENES CDI services (2020)
- D7.3 Second KPI and TNA report for ENES CDI services (2021)
- D7.4 Second external review report for ENES CDI services (2022)
- D7.6 Third KPI an TNA report for ENES CDI services (2023)
- M10.1 Technical requirements on the software stack (2020)
- M10.2 CMIP Data Request Schema 2.0 (2020)
- D10.1 Architectural document of the ENES CDI software stack (2020)
- D10.2 First release of the ENES CDI software stack (2020)
- D10.3 Second release of the ENES CDI software stack (2021)
- D10.4 CMIP6 documentation (2022)

3.3.2 Access to other (types of) data sets

Impact researchers often use high spatial resolution climate data for the past and future climate. Therefore, the observational data, reanalysis data and (EURO-) CORDEX data available are very helpful, especially for a large part of this user group. As many impact models are calibrated with observational data and since these models often contain non-linear relations, bias-adjustment has to take place before the climate model data can be used in these impact models. Many of these

impact researchers have limited knowledge on how to perform a bias adjustment. Bias-adjusted EURO-CORDEX runs save them a lot of work.

It would be interesting in some cases to combine climate variables with non-atmospheric climate variables (e.g. land cover or leaf area index (Hall, 2019), or to determine impacts, and vulnerability (UNEP, 2013; EEA, 2017)). Carter and Makinen (2011) compiled several publications with indicators and composite indices of vulnerability and the sectoral information systems of C3S also combine climate information with other variables to calculate impacts of climate change.

Progress on user requirements

- Through the Climate4Impact portal, now users have easier access also to CMIP6, EUROCORDEX (also high resolution), Bias-adjusted EUROCORDEX (only courser resolution)
- A clinic on bias-adjustment was organized with many links to methods and tools to perform bias-adjustments if no bias-adjusted datasets are available

Further user requirements

- Other CORDEX data (from other regions) not yet available through the main menu of C4I. Since these CORDEX datasets for other regions exist (but no large data sets with bias-adjusted data), in principle it should be possible to include them in the future in a relatively easy way. However, producing bias-adjusted datasets for these CORDEX datasets requires a lot of effort, also because good quality reference datasets (based on observations or reanalysis) are not always available. Maybe this could be (partly) included in future projects focussing on regions outside Europe, however, this may not be the first priority of the EC and the ENES-RI
- Easier access to station data: in general the access to station data is outside the scope of (EU-)projects, since the institutes and governments that collect these data, decide themselves whether the station data become freely available. However, products such as E-OBS are based on station data and are more widely available. Through the Climate Explorer many station data that are freely available can be accessed and downloaded
- In principle also access to non-climatic data is possible through ESGF, but not through the main menu of C4I. Due to the diversity of non-climatic datasets and the challenges combining them in a correct way with climate data this seems also difficult to do in the future. For the C3S CDS several datasets have been developed that combine climate and non-climate data, but they may not be in a format that is useful for all users or in the combinations with climate model data that are required by all users

User interaction: during the short trainings and schools organized within WP3

Relevant WPs and tasks

- WP3, tasks 1 and 2 (on training and schools)

Relevant IS-ENES3 documents

- M3.5 Workshop on climate indices (2021)
- D3.2: Synthesis on climate and impact and climate data schools (2023)

3.3.3 Transnational access mechanism (TNA) and VA access to compute services

Because of the large increase in scientific data volumes in all scientific domains, the need for compute services to enable data processing as close as possible to data storage are needed. This is one of the ideas behind the TNA and VA compute service offerings in IS-ENES3. 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 are crucial to support this service, and also the functionalities that are provided. A basic layer of generic services laying the foundation of tailored services should be able to provide needed functionalities for users (D5.1). Sustainability aspects of the compute services are agreed and discussed further as part of the sustainability work in WP2/NA1. Compute services are part of the future ENES-RI services portfolio (D2.2).

Progress on user requirements

- The user requirement for a generic user interface which is aligned with the evolving broader community software ecosystem (e.g. the PANGEO software stack) lead to a consistent support of jupyter-hub interfaces at the ENES compute service providers. The harmonization of data access (e.g. through the shared support of data catalogs) as well as available processing libraries and tools enabled the development of consistent training material (e.g. in the form of jupyter notebooks)
- The additional requirement for the support of data near data reduction and transformation operations lead to the inclusion of web processing services (WPS) into the VA service offerings. These services also supporting the integration of the Climate4Impact portal as well as Copernicus are thus also directly exploitable by users (initially at one computer service provider - DKRZ, but will be offered by additional centers in the future)

Further user requirements

In the future there may be additional user requirements related to access to climate model data and compute services. Climate Data Infrastructure, including compute services are part of the future ENES-RI services portfolio (D2.2). Probably at least part of the additional user requirements can be included in this.

User interaction: people can apply for the TNA and VA services. TNA applications are reviewed and require a detailed work description, whereas VA services are associated with a light-weight application procedure managed by the individual service providers. In both cases, granted users get personal support to exploit the service offering. This gave direct information on challenges

accessing and processing climate data, including e.g. information on needed additional external data to be replicated and made accessible as part of the ENES data pools which are associated to the compute service offerings.

Link: https://is.enes.org/sdm-climate-analytics-data/

Relevant WPs and tasks

- WP7 Task2: Compute Services (VA) - 'Comp1'
- WP7 Task 3: Virtual workspaces (TNA) - 'Comp2'

Relevant IS-ENES3 documents

- D7.1 1st KPI and TNA report for ENES CDI services (2020)
- D7.3 Second KPI and TNA report for ENES CDI data services (2021)
- D7.6 Third KPI and TNA report for ENES CDI data services (2023)

3.3.4 Standards for names of climate variables and indices and metadata

To make it easier for users to find climate variables, climate indices and derived data, it is important to well define the name and abbreviation of the variable, index or derived variableEspecially for new users, the abbreviations used are often difficult (e.g. Tas and Tg or Tmean) to recognize or they don't realize that indices that appear the same may be calculated in a slightly different way (e.g. different threshold temperatures, 17 or 18 ºC, may be used for heating degree days). This is confusing for users and can lead to errors/misunderstandings. To avoid this, an inventory was made of existing climate indices and their metadata for climate indices and standards for climate index naming are proposed. Consistent naming may help (CF-conventions) as well as a good overview of metadata of all used climate variables, indices and other derived data. For climate indices and derived data, it would be useful to have a similar documentation as for climate model data, accessible in a similar way as e.g. the ES-DOC information.

Also for indices and other derived data it is useful to have information on quality and uncertainties. The metadata for uncertainties across datasets is not yet consistent (Petri et al., 2016) or missing.

Progress on user requirements

- Improved documentation on indices definition, more metadata available: Inventory of existing climate indices definitions/metadata and proposal for standardization of indices within IS-ENES3 in the public repository CLIX-META (https://github.com/clix-meta/clix-meta) (reports M3.4 and D3.3). Information from this repository is used by the icclim software
- During the schools on 'climate data for impact assessments' background information was provided on the standards for climate data and climate indices

- The community uses the netcdf data standard and applies the Climate Forecast (CF) conventions, providing standard names for variables and common rules for data standardisation (e.g. units, geographical location information on data)
- The list of variables to be provided for each CMIP6 experiment is described in the Data Request

Further user requirements

- Consistent information on uncertainties and quality of climate variables and indices
- Interactive traceability chains and efficient tools for data users to obtain confidence in the quality, robustness, and limitations of data

Since these are relevant points for the use of climate information, we expect that these can be incorporated in future projects.

User interaction:

- Workshops/interviews/online documents for the inventory of climate indices definitions
- During the online workshops on climate indices for Eastern Europe the results of the inventory were presented and discussed

Relevant link: https://is.enes.org/sdm-access-metadata/, http://cfconventions.org/Data/cf-standard-names/79/build/cf-standard-name-table.html

Relevant WPs and tasks

- WP3 Community engagement
- WP10, Task 6: Tools, services, information models for data standards

Relevant documents:

- M3.4 Summary of workshops on standards (2023)
- M10.3 - Climate indicators/indices and file metadata specifications and tools (2021)
- M10.4 Update of the climate indicators/indices and file metadata specifications and tools (February 2023)

3.3.5 Standards for names of climate data files

For users with relatively little background on climate modeling, it is often difficult to understand the naming of climate data files. When they try to find climate data in the various portals, the results of their search show the various climate data files. However, without knowledge on the naming standards, these users do not know how to find the climate data files that they need.

Progress on user requirements

- See par. 3.2.3 on 'file naming convention for climate model output'

- During the schools on 'climate data for impact assessments' background information was provided on the standards for climate data file names

Further user requirements
- See also par 3.2.3
- Information on file names may be included in e.g. the guidance material of the Climate4Impact portal, which would make it easier for new users to find information on these standards. This can easily be done with a short explanation and providing links with more detailed information

User interaction: During the schools on 'climate data for impact assessments' background it became clear that, especially for VIA researchers, the climate data file names are often a challenge. Through various portals they can get access to climate data files, but they often do not understand what information the file names provide.

Relevant links:
https://wcrp-cmip.github.io/WGCM_Infrastructure_Panel//Papers/CMIP6_global_attributes_filenames_CVs_v6.2.7.pdf, https://github.com/WCRP-CMIP/CMIP6_CVs, https://pcmdi.llnl.gov/CMIP6/Guide/dataUsers.html

Relevant WPs and tasks
- WP3 Community engagement

Relevant documents:
- D3.3 Standards synthesis (2023)
- M3.4 Summary of workshops on standards (2023)

3.3.6 Climate4Impact portal

The Climate4Impact portal is intended for a broad range of users, with a broad range of background knowledge. The challenge is to keep the user interface as simple as possible. However, simple for people with a lot of background knowledge on climate data is generally by far not simple enough for (first time) users (Bennett & Groot, 2015). The Climate4Impact portal has been rebuilt with new techniques, making it work better/faster and making it more future proof. However, the new version uses Python notebooks, which are not common to all potential new users. Some training is needed for those not familiar with Python notebooks, but after training it can offer a research-ready environment on searchable and focussed datasets[7].

[7] After the training in Delft, a Phd candidate is already using the Python notebooks in his teaching to illustrate how the climate model data is organised.

Progress on user requirements:

Easier data search

- Attempts made to improve the menu for data search. Scoped variables interface to focus on more commonly used ones organised by type. Optionally users can switch an extended interface to allow searches on a wider set of variables
- Better descriptions or names for the variables under the scoped variables interface will be included in the manual for the portal
- Updated and improved guidance, including information on biases and changes for several CMIP6 models (D5.1; M10.1). The manual is under development, but not yet linked to the C4I portal 2.0 (will be added after the end of IS-ENES3)

Access to data

- Access to CMIP6, EUROCORDEX (2 spatial resolutions) and EUROCORDEX-biasadjusted. The latter will be managed via the new authorisation infrastructure developed at CEDA (IdeA). User identities are already managed through the new system. Ongoing development at CEDA includes access control to CORDEX. This is likely to be finalized after the end of IS-ENES3

Access to metadata

- ES-DOC: information about evaluation, quality and uncertainties on data sets, e.g. with link to ESMValTool results: updated information. In the portal there is a link to WDC with some climate model data, and in the data result files there are links to ES-DOC
- Information on provenance, uncertainties, biases in climate model data to determine quality of the data

Processing of data

- New versions of icclim to calculate climate indices, validated against Climdex and xclim, with addition of a large number of functionalities (icclim v5 then v6)
    - Releases information: https://github.com/cerfacs-globc/icclim/releases
    - Complete refactor of icclim v4 now using xarray and dask exclusively
    - Units check for input data
    - Unit tests to check code functions in new releases
    - Fix to many event-based climate indices
    - One function per index along with a generic function
    - Generic indices, complex thresholds, generic operators
    - Adds the possibility to give percentiles as an input instead of computing them.
    - Seasons between 2 exact dates
    - New wind-based and humidity-based ECA&D climate indices added
- Option to make spatial and temporal selection is now available via the subsetting functionality. This feature can be used in combination with the analytical workspaces and is supported on those ESGF nodes exposing WPS subsetting services on the hosted data. The availability of such service at the remote site is made explicit to users who can choose to focus their search on the particular node.

- integrate ESMValTool data: concept version with information on annual biases and changes in temperature and precipitation (D5.1)

Guidance:

- Guidance on how to use the C4I portal and workspaces is provided through two dedicated help pages, which we link below.
  - https://www.climate4impact.eu/c4i-frontend/helpC4I
  - https://www.climate4impact.eu/c4i-frontend/helpSwirrl
- Also guidance for other than GCMs (will be added after the end of IS-ENES3)
- Some notebooks with examples are available on GitLab.
  - https://gitlab.com/is-enes-cdi-c4i/notebooks

Information on progress during processing:

- More information is given on the estimate of the data requested from the remote node, and the effects of subsetting on data reduction. The workflows used to stage and subset the data to the workspace show their status and error messages are available in the provenance. Although they could be more detailed.

Further user requirements

- Many users indicate that information on uncertainties is important for them. Currently there don't seem to be parameters related to uncertainty or error, which makes it impossible to search for this information in e.g. satellite data files
- Many people state that uncertainty information is important, but they use this information not very often. Guidance and examples on how to calculate and/or use the various types of uncertainty information may help them to use it more (Bessembinder, 2017). Also the information from the ESMValTool on model biases and changes in various climate models may help with this. It can be included in training material and in the guidance material
- The service could benefit from additional guidance to take into account the wide diversity of users, their objectives, interests and skills (Swart et al., 2017), in order to provide usable information.
- Continued support for users: support after the IS-ENES3 project is limited unless this can be included in new projects
- It is unavoidable that many abbreviations and specific terminology are used, but more explanation on the names of e.g. the climate data file names could be useful for new users. It would be good to provide links to further background information from the new C4I portal
- More options to transform the format of the climate data into the required format for VIA researchers
- In order to guide users, there is a need to reflect on what limitations should be built into the toolbox that would stop users from creating combinations and analyses that are scientifically unjustified and potentially misleading (Petrie et al., 2016)

- Tool for calendar harmonization would be useful for users. In climate models sometimes different lengths of years are used than in real life
- Information from ESMValTool for bias-adjustments: There are other tools available which can help with doing bias-adjustments. It does not seem logical to include this all in the C4I portal. However, some background information on Bias adjustments and tools for this would be interesting to have in the C4I portal It would be good to provide links to further background information on bias adjustments and tools from the new C4I portal

User interaction: with the new version of C4I users were asked to give some information so we understand who is using C4I (see also D7.6). There were some Alpha users and in February 2023 some short trainings were organized.

Links: https://is.enes.org/sdm-c4i-portal/, https://www.climate4impact.eu

Relevant WPs and tasks

- WP3, Task1: Widening the user base for science and societal innovation
- WP3, Task 2: Training and resources: nurturing the community
- WP7, Task 2: Compute Services (VA) - 'Comp1' (to make ESMValTool info available)
- WP10: Task 3: Improve the user interface and functionalities of the climate4impact platform for the impact communities
- WP10, Task 4: Integrate the newly developed data compute services for data analytics into the climate4impact platform

Relevant IS-ENES3 documents

- M3.1 Report on user requirements (2020)
- M7.3 Improved version of evaluation portal (2020)
- D7.6 Third KPI and TNA report for ENES CDI services (2023)
- M10.3 Climate indicators/indices and file metadata specifications and tools (2021)
- M10.4 Update of the climate indicators/indices and file metadata specifications and tools (2023)

3.3.7 CDO data post-processing

CDO is not only used by scientists with focus on climate, but also weather services (production + development), data services (like Copernicus for server-side processing), private companies that deal with weather/climate data (local weather prediction, shipping) and the military. CDO has a public website with a ticket system and forum. Users can submit their wishes and requests. There are regularly new requirements from the users. Most of them are implemented quickly. No list of

remaining wishes is kept for further development. The general requirement is the availability of consistent, flexible, easy to use and performant data analysis framework.

Progress on user requirements:

- During several schools and shorter activities training sessions on CDO were organized (see D3.5)
- Support for the use through the support services (Info on required help around CDO)
- In 2019, when more CMIP6 data became available, some new operators have been implemented for CMIP6 compliant processing and calculation of climate extremes indices (Wachsmann & Schupfner, 2019). This was done without financial support from IS-ENES3

Further user requirements

No list of remaining wishes is kept for further development, but continued support for CDO through a support service is desirable. No support can be provided 'at no cost', so new funding is needed for this.

User interaction: through the support services and during the trainings within the IS-ENES3 project

Links: https://is.enes.org/smt-common-software-tools-detailed/, https://code.mpimet.mpg.de/projects/cdo/wiki

Relevant WPs and tasks

- WP3, tasks 1 (Widening the user base for science and societal innovation) and task 2 (Training and resources: nurturing the community)
- WP6, Task 3: Services for European infrastructure tools

Relevant IS-ENES3 documents

- M3.1 Report on user requirements (2020)
- D6.1 First periodical report on service statistics for models and tools (2020)
- D6.2 First external review of model and tools services (2020)
- D6.3 Second periodical report on service statistics for models and tools (2022)
- D6.5 Second external review of model and tools services (2022)
- D6.6 Third periodical report on service statistics for models and tools (2023)

3.3.8 Indices and indicators

Several lists of indices were developed by WMO, WCRP Expert Teams (ETCCDI and ET-SCI), as well as European initiatives (ECA&D) and more recently EU Horizon 2020 projects and Copernicus C3S activities. These indices/indicators are often used to estimate impact of climate and climate change.

Progress on user requirements

Within this project a workshop was organized to see whether in Eastern Europe there are other additional indices required (M3.5). Some of the most important requirements/wishes are on options to calculate trends, combine various climate variables in one climate index (multivariate indices)[8], flexibility in choosing the threshold for a climate index, combining climate variables with non-climate variables, easier access to observational data and data of climate models (e.g. CORDEX) to calculate climate indices. Many of these were mentioned already in the first inventory on user requirements. Part of these requirements has been included in a new version of the icclim tool (Improved software, documentation and user guides; https://icclim.readthedocs.io/en/latest/) to access and calculate climate indices by now:

- icclim 5.0 was re-written from scratch, moving from a C-language core to an xarray and dask core. Usability, code structure and architecture, flexibility and a modular approach guarantee the sustainability of the codebase. Strong cooperation with the xclim[9] development team was also initiated and pursued
- icclim 6.0 (https://github.com/cerfacs-globc/icclim/releases?q=6.0&expanded=true) introduced the concept of generic indices that can be defined using one or several variables combined with one or several operations and thresholds. Some operations available are: Count occurrences where threshold(s) are met, Count the maximum number of consecutive occurrences when threshold(s) are met, Sum the lengths of each consecutive occurrence spell when threshold(s) are met, etc. A large number of operations https://icclim.readthedocs.io/en/latest/references/generic_functions_api.html# and thresholds https://icclim.readthedocs.io/en/latest/references/threshold.html#module-icclim.generic_indices.threshold are available and are documented. This feature was the most liked by students in schools and trainings since the release of icclim 6.0
- Performance of icclim was improved, especially for percentile-based climate indices
- Several missing climate indices in icclim 4.x were added. Notably wind-related climate indices from ECA&D were added in icclim 6.1.2 along with some other indices related to humidity
- More quality control on datasets used to calculate indices: within IS-ENES3 the documentation of climate models has improved (ES-DOC) and during the schools on

[8] E.g. for agriculture and ecosystems climate indices that combine information about temperature and precipitation are often relevant to either indicate good growing conditions or conditions that could cause damage. Some combined indices are included in the list of indices and are evaluated in the ESMValTool

[9] https://xclim.readthedocs.io/en/latest/

'Climate data for impact assessments' special attention was paid to where this information can be found (many new users are not aware of the availability of these metadata)

- More detailed description of potential application and/or on index interpretation: some examples were provided during the schools/trainings, especially some example notebooks: https://gitlab.com/is-enes-cdi-c4i/notebooks
- Training to use available tools for climate indices calculation: During various schools training was provided on various tools/portals. During the Romania school specific attention was given to icclim and CDO

Further user requirements (not included in IS-ENES3)

Not all requirements could be included in this project, but several can probably be included in other projects/follow-up projects:

- indices on changes or trends in climate variables: in principal not that difficult to determine if at the same time indices can be determined for various time periods
- indices for variables such as radiation, soil moisture/groundwater, indices based on satellite products and indices at sub-daily level: more and more of such data become available. They often require the same type of processing as indices related to temperature and precipitation, however, often the problem is the supply of data (few observed data, inhomogeneities, large uncertainties, etc.). Model data is in some sense 'less well researched in general' in particular with relation to observations. Satellite data typically cover a comparatively short period from a 'climate perspective' and share some other problems with model data, but on the other hand offers unique and very interesting prospects regarding spatial coverage
- Improvement in graphical products and visualization tools/software/libraries: this can often also be solved with other tools
- calculation over custom season/period in the year: The diversity of users and approaches and the different levels of community organisation complicate the identification of such indices or may lead to a large number of closely related ones. Therefore a tool with flexibility in the definition of the custom period is required. In icclim, and especially the new version, several flexible option are available, but more can be developed
- combine various climate variables in one climate index: This is already available for some climate indexes, but here the possibilities (and user requirements?) are infinite, and there are practical limitations. Would be good if developers together with users determine what are the most important multi variable climate indexes
- Climate indices that are combined with non-climate variables: not easy to implement, especially in terms of finding reliable long-term non-climate data. Maybe this can be taken up in a special project and in collaboration with those who produce the non-climate variables

- Information on uncertainties in climate variables: first requires to determine which types of uncertainties have to be quantified (e.g. natural variability, model uncertainty or scenario uncertainty), then which datasets can be used for this. Seems more complicated, since for e.g. model and scenario uncertainties large datasets have to be used. Another complicating factor is that the scientific understanding of factors contributing to uncertainty is not necessarily what is most relevant to users. There sometimes is a mismatch in terminology as well as in expectations
- More quality control on datasets used to calculate indices: IS-ENES3 worked on more consistency and better description of the definitions of indices, but more can be done on this is further projects
- More detailed description of potential application and/or on index interpretation: more guidance needed

User interaction: workshops, interviews, inventory, schools

Links: https://is.enes.org/sdm-c4i-portal/, https://icclim.readthedocs.io/en/latest/

Relevant WPs and tasks

- WP3, Task 3: Community standards
- WP10, Task 4: Integrate the newly developed data compute services for data analytics into the climate4impact platform

Relevant IS-ENES3 documents

- M3.4 Summary of workshops on standards (2023)
- M3.5 Workshop on climate indices (2021)
- D3.3 Standards synthesis (2023)
- M10.3 - Climate indicators/indices and file metadata specifications and tools (2020)
- M10.4 Update of the climate indicators/indices and file metadata specifications and tools (2023)

3.3.9 Derived data: climate model evaluation data products

As a result of the ESMValTool a lot of climate model evaluation data becomes available which is useful for climate modelers to evaluate the climate models. However, other groups of climate data users may profit also from the information that the ESMValTool can provide. The information can be used for example for two other purposes:

- For selection of climate model runs for climate model analysis or for impact analysis. Many impact researchers do not have the time and resources to use a large ensemble of climate

model runs for their impact analysis. To get an idea of the range of impacts of climate change it also suffices to use a small number of climate model runs
- For bias adjustment of climate model data

Progress on user requirements

For the selection of climate models: A first concept was made in which the bias and projected change for annual temperature and precipitation of many CMIP6 models was presented visually (https://esmvaltool.dkrz.de/shared/esmvaltool/climate4impact/) and this is accessible through the Climate4Impact portal from the model selection interface, where the preselected models are highlighted to help the user comparing their performance with the others. The current implementation shows how a particular model foresees a change in the temperature and precipitation variables compared to the past, which, in combination with the bias, gives some confidence on the model performance (https://esmvaltool.dkrz.de/shared/esmvaltool/climate4impact/?project=CMIP6). There is no time to further develop this within IS-ENES3, but this could potentially be done in other projects.

Further user requirements

- For the selection of climate models: it would be interesting to further develop the first concept mentioned above also for e.g. CORDEX data and for a much wider range of climate variables, also for different seasons. In principle this can be included in other projects
- For bias-adjustments: no specific adaptations were made to ESMValTool for this purpose, but in principle much of the required information on biases can be generated with ESMValTool. However, it is not as easy as for the model selection to visualize the information for bias-adjustments, since the biases vary over the year, over regions, etc. Several of the developments around ESMValTool make it easier to use it for bias-adjustments, however. Training on ESMValTool may help to profit from this

User interaction: online trainings on ESMValTool were provided in the past years and also an online workshop/clinic was organized on bias adjustments, Attention was paid to bias-adjustments and ESMValTool during the online schools.

Links: https://esmvaltool.dkrz.de/shared/esmvaltool/climate4impact/

Relevant WPs and tasks

- WP3, community engagement
- WP7, Task 2: Compute Services (VA) - 'Comp1'
- WP9, Task 3: Data preprocessing and reformatting
- WP9, Task 5: Enhancing the use of the ESMValTool for model development

Relevant IS-ENES3 documents

- M3.1 Report on user requirements
- M7.3 Improved version of evaluation portal (2021)

4. Synthesis and recommendations

4.1 Challenges experienced

Achieving clarity on the requirements for standards in sufficient details to enable reliable implementation is an enduring problem. The desired outcome, in the form of frictionless exchange of information, is clear, but few users are able to engage constructively with the level of technical detail required (D3.3).

It is more difficult to reach commercial organisations, or organizations outside research, compared to users within the climate research community and these users may have difficulties describing their exact requirements/wishes. Working together with these users in case studies, in schools, helps to get a clearer understanding of their requirements (D3.5, D3.2). Due to COVID19 there were no physical meetings during about 2 years. This made working together at location more difficult. Face-to-face meetings probably give more opportunities to see what are the obstacles accessing and using climate data.

4.2. Objectives reached and recommendations

Target users of the services and tools developed in IS-ENES3 are the climate researchers, the Vulnerability, Impacts and Adaptation (VIA) researchers, and climate service providers. The idea is that when the services and tools meet the requirements in a better way, they will be used more widely.

Many requirements from the climate research community were included from the start of the project and most of these requirements have been reached, although often further developments are possible.

For other user groups, also several improvements were made, however, considerable background knowledge of climate data is required for them to be able to get access to the data, to process the data, etc. Although it can be made easier to do this up to a certain level (e.g. standardizing file names, indices, making information from the ESMValTool available to select climate models, etc.) not all user requirements can be met, at least not at the moment, although a large part can potentially be included in further project (see paragraphs in chapter 3). For these cases, easy to access and understand background information and tailored training can help these groups. Also further development of the connections between climate researchers and the VIA researchers and Climate service providers will help so they can help each other with access and processing of climate data and doing impact/adaptation assessments.

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Apart from the project documents mentioned in the text. Those publicly available, can be found at the IS-ENES3 website (https://is.enes.org/deliverables-milestones/).

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