D8.3 – ACROSS integration products and EuroHPC cross-project collaboration benefits

Deliverable ID	D8.3
Deliverable Title	ACROSS integration products and EuroHPC cross-project collaboration benefits
Work Package	WP8
Dissemination Level	PUBLIC
Version	0.7
Date	2022 - 02 - 28
Status	Submitted
Deliverable Leader	LINKS
Main Contributors	LINKS, AVIO, SINTEF, ECMWF, CINI

Disclaimer: All information provided reflects the status of the ACROSS project at the time of writing and may be subject to change. This document reflects only the ACROSS partners' view and the European Commission is not responsible for any use that may be made of the information it contains.

The ACROSS project has received funding from the European High-Performance Computing Joint Undertaking (JU) under grant agreement No 955648. The JU receives support from the European Union's Horizon 2020 research and innovation programme and Italy, France, Czech Republic, United Kingdom, Greece, Netherlands, Germany, Norway.

Published by the ACROSS Consortium

Document History

Version	Date	Author(s)	Description
0.1	2021-12-07	LINKS Foundation	First version ToC
0.2	2022-01-07	LINKS Foundation	In review
0.3	2022-02-10	ATOS	Reviewed by ATOS
0.4	2022-02-14	IT4I	Reviewed by IT4I
0.5	2022-02-22	LINKS, AVIO, ECMF, SINTEF	Changes related to the reviewers comments
0.6	2022-02-25	LINKS	Pre submission
0.7	2022-02-28	LINKS	Submitted

Table of Contents

Glossary

Acronym	Explanation
AI	Artificial Intelligence
CDO	Climate Data Operators
CFD	Computational Fluid Dynamics
DL	Deep Learning
DS	Design System
FPGA	Field-Programmable Gate Array
GPU	Graphics Processing Unit
HPC	High Performance Computing
HPDA	High Performance Data Analytics
IFS	Integrated Forecasting System
LES	Large Eddy Simulation
MPI	Message Passing Interface
ML	Machine Learning
NWP	Numerical Weather Prediction
RANS	Reynolds Averaged Navier Stokes
URANS	Unsteady Reynolds Averaged Navier Stokes

List of figures

List of tables

Executive Summary

ACROSS has started on 01/03/2021 and will end on 29/02/2024. it is a EuroHPC -JU project funded under the topic EuroHPC-02-2019 “HPC and data centric environments and application platforms” [1]. ACROSS will collaborate with the funded projects of the same topic for not only the activities related to the dissemination and communication but also to more specific and technical activities so that co-design deployment and innovation will be put in place. ACROSS will also collaborate related to the dissemination and communication activities with some projects of the funded under the topic EuroHPC-01-2019 “Extreme scale computing and data driven technologies” [2] that has been identified so far.
This deliverable will present the initial plans for collaboration activities with EuroHPC-JU projects. The first steps towards collaboration with six EuroHPC projects and one H2020 project have already been taken. Events, and activities, information exchange, joint use of EC services, information sharing and cooperation on the projects' accessible communication channels are among the domains of potential collaboration foreseen by ACROSS.
The next relevant deliverable D8.7, "ACROSS integration products and EuroHPC cross-project collaboration benefits (Intermediate version)" is due in month 24 and will expand on the projects' outcomes, and prospective contributions from other projects.

Position of the deliverable in the whole project context

Deliverable D8.3 “ACROSS integration products and EuroHPC cross-project collaboration benefits” is linked to WP8 “Enabling Integrated Validation and Value Creation Adoption” dedicated to promote the ACROSS project, engage target-sector stakeholders and enable value creation adoption for strengthening EU’s capacity related to HPC, Big Data and AI Integration. It is related to Task 8.2 “Strategic integration boosting synergies with EuroHPC projects” which has the objective to strategically integrate the project’s key results in order to develop “lighthouse” examples and then cross-collaborate with other EuroHPC projects for supporting new knowledge and technology creation. This task has the objective to enable cross-collaboration with other EuroHPC projects so that co-design deployment and innovation actions will be put in place.

Description of the deliverable

The deliverable is organized as follows; Section 1 gives a brief introduction of the context and the scope of the deliverable. Section 2 will describe the most prominent envisaged results at pilot level and at technological level of ACROSS. In Section 3 will be listed the identified projects and the possible collaboration points including the first initiatives started and the next steps. Section 4 provides Conclusions.

1 Introduction

The Deliverable D8.3 summarizes the identified EuroHPC-JU funded projects for the collaboration and the future steps and activities that are foreseen.
The structure of the Deliverable 8.3 is organised in the following way:

- The Scope and methodology of the deliverable is described in subsection 1.1 and 1.3.
- The most prominent envisioned results of the ACROSS are described in Section 2. Are reported
  - the pilot envisioned results
  - the technological envisioned results
- In section 3 are defined the cross project collaboration goals and the identified projects for the collaboration.

1.1 Scope

The scope of this deliverable is clearly described in the project proposal as follows:

"*This activity will enable cross-collaboration with other EuroHPC projects so that co-designed deployment and innovation actions will be put in place. Creating synergies and liaising with other EuroHPC projects will allow to:*

- *leverage on their lessons-learnt;*
- *establish contact and share information;*
- *foster innovation through inter-project new knowledge creation, validation and exploitation of key findings.*"

The work done in this first deliverable consists of defining prospective collaboration strategies, providing a general overview of relevant identified projects, and reporting on the first contacts made.
For the collaboration will be considered to be held the following activities:

- Projects' social media channels linked and mutually promoted.
- High-level workshops (e.g. Coordinators' meetings, Technical groups' meetings)
- Joint activities (e.g. common (final) events, webinars, policy sessions
- Validation and exploitation of the key results..

Nevertheless, another set of possibilities will be elaborated and, in the future will be discussed with each of the identified projects. Specifically, will be evaluated the following organisational and performance options:

- definition of a short roadmap and particularly specific collaboration goals.
- specification a wider set of joint activities.
- definition of collaboration output indicators and result indicators (tangible/measurable results).

1.2 Related documents

ID	Title	Reference	Version	Date
[RD.1]	D8.4 "Dissemination, Exploitation and Communication (DEC) plan"	Envisioned results	0.6	31/08/2021
[RD.2]	D2.1 "Summary of pilots co-design requirements"	Pilot KPIs	3.0	31/08/2021
[RD.3]	D2.2 – Description of key technologies and platform design	Pilot KPIs technologic tools and software that will be used	0.8	30/11/2021

1.3 Methodology

The methodology that will be used in this deliverable is the follow:

1. In the first release (M12) will map and list relevant former and current EuroHPC-JU and H2020 funded projects.
2. In the second release (M24) will be reported the active dialogue (sharing content and lessons learned) with the identified projects.
3. In the third release (M36) will be reported the integrated validation and exploitation of shared key findings.

2 ACROSS envisaged results

ACROSS Project is a complex project, which involves thirteen partners, three pilots and foresees seventeen exploitable results that can be classified as tools, products, open source software, methodology, pilot demonstrators and knowledge. The overall ACROSS fact sheet is shown in Figure 1.

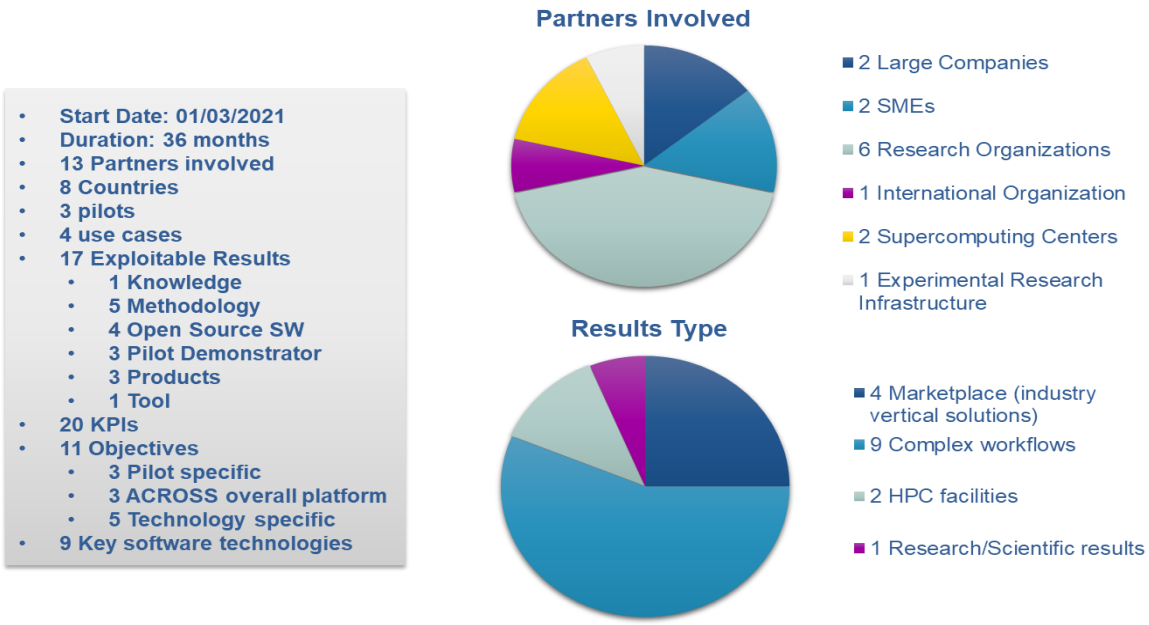

Figure 1 ACROSS Project Factsheet

In the following subsections will be described the technological and pilot related envisioned most prominent results and the KPIs.

2.1 Pilots envisaged results

2.1.1 Greener aero-engine modules optimization pilot envisaged results

This pilot includes two aeronautical engineering case studies: one regarding the combustor and the one referring to aeronautical Low-pressure turbines design. Numerical investigations are based on complex CFD analyses and rely on CPU-intensive and time consuming routines. The objectives of this pilots are:

- Introduce new, complex design workflows for the design of key aeronautical engines components, fully exploiting HPC capabilities, driven by AI and leveraging state-of-the-art HPDA to handle the huge amount of data involved.
- Innovate the existing Combustor design process by introducing a multi-physics unsteady approach to improve flow performance prediction and product durability/Life Cycle Cost, both aimed at developing safety aspects, with an eco-friendly vision in line with society needs.
- Innovate aeronautical turbine design by introducing HPC driven optimization systems, aimed at improving efficiency of the low-pressure modules and consequently markedly reduce planes' fuel consumption. This research task is fully coping with Clean Aviation vision and agenda.

In the following table are included the KPIs of the pilot.

KPIs	Description
Turbine use case KPI 1	The overall KPI of the WP5 pilot is an expected time reduction (~50%) of the design procedure related to the introduction of the new DS as a whole into the Avio Aero industrial design procedure
Turbine use case KPI 2	A speed-up of at least 20% is expected for the introduction of GPU's for the AI models. Even more marked improvements (speed up > 50%) appear necessary looking to more advanced HW (FPGA,

	neuromorphic systems, etc.), to justify their introduction in daily usage of the DS.
Turbine use case KPI 3	For the improved workflow on LES/HPDA, a time reduction at least of 30% is expected. Moreover, it is important to underline that it will also ensure a more homogeneous database in terms of LES convergence.
Combustor use case KPI 1	Productivity target (time-to-design reduction with regards to current situation) for both aeronautical test cases. At least 30%, acting on both the modelling aspects and the improvement brought by (new) hardware resources
Combustor use case KPI 2	Combustor metal temperature prediction with regards to experiments. Target reduction of uncertainty margin to ±30K by acting on the modelling aspects used within the simulation

Table 1 Greener aero-engine modules optimization pilot KPIs

The envisaged results related to this pilot are included in the following table. These envisioned results are part of the exploitable results (ER) listed in D8.3.

#ER	Envisaged results	Description	Type
ER10	Design System	Foster extensive use of state-of-art HPC solutions to sustain and support Avio Aero products excellence that means, specifically for Across project, aeronautical combustor and turbine design systems. Aim is to develop advanced modelling and, at the same time, reduce the required computational efforts and time. Expected KPI's for the aeronautical use-cases developed inside the ACROSS project will be: Combustor: Key objective is to develop Multi-physics/multi-scale framework in ANSYS Fluent with 3 different simulations performed in parallel independently. KPI's target are listed in terms of: • *accuracy: reduction of uncertainty margin of temperature prediction to ±30 K wrt experiments acting on the numerical modelling practices optimization* • *Time-to-analysis reduction -> - 30%. This will be achieved through* – *Procedure automation: eliminate waiting time associated with data exchange information among different solvers* – *Frequency of data exchange to be sorted out. Best practice to be defined in terms of accuracy / computing time balance* – *Fluid domain mesh benchmark* Turbine: Expected KPI's of this activity are related to the change of paradigm provided by the new DS, based on meta-models that will leverage on the generation of a large numerical database treated by means of HPDA and AI. They are summarized hereafter: • *Time-to-design > -50% wrt current* • *turbine aero design efficiency gain: +0,30%* *LES / HPDA analysis time > -30% wrt current (1 week)*	Marketplace (industry vertical solutions)

ER14	Design System	Innovative Design approach CFD based leveraging on AI/HPC. The Pilot in the ACROSS project will provide an example of the potential innovation of such an approach. This methodology will be adopted as a very powerful approach for facing complex design phases, when multidisciplinary aspects are involved and multi-fidelity analysis are available. The methodology behind the new Design System developed in ACROSS will open important possibilities in several other fields of application in which CAE and AI tools can be combined and exploited leveraging on HPC resources. In ACROSS project, partners have jointly identified how to improve this work flow, that is a combination of different in-cascade steps based on standard CFD RANS and HI-FI ones finally post-processed by HPDA dedicated routines. In the improved vision, HPDA as well as some other performance evaluations will be carried out while LES is still running, and the convergence of this co-processing will be adopted as a new, more effective, stopping criterion for the calculations. Moreover, all the results will be directly available at the end of the calculation, as post-processing is performed concurrently with the calculation. Details of this new approach is presented in the ACROSS deliverable 2.1. *Multi-fidelity CFD Database creation of Optimal Geometries and Aero-engine Turbine aerodynamic design pilot Demo*	Complex workflows
ER15	License Agreement	Internalisation and implementation of the U-THERM3D procedure in Avio Aero practices for the design of aeronautical combustors. The optimised tool within the ACROSS project will allow a much faster design of combustors without loss of quality due to steady simulations or where certain effects are neglected for the calculation of thermal loads (standard practice in the early stages of design). In ACROSS project, partners have jointly identified how to improve this work flow, that is a combination of simultaneous CFD simulations, evolving in the time domain and solving fluid, solid and radiative domains of a combustor chamber. The work-flow of the novel designed procedure will be aimed to avoid as much as possible the write/read files exchanged among the different domains in the time domain. This will allow an important time saving, in line with KPI's objectives defined for this use-case. Details of this new approach is presented in the ACROSS deliverable 2.1. *Standardisation of the optimized U-THERM3d tool for implementation in Avio Aero's internal combustor design procedure.*	Complex workflows

Table 2 Greener aero-engine modules optimization pilot envisioned results

In the Figure 2 is shown a fact sheet of the Greener aero-engine modules optimization pilot.

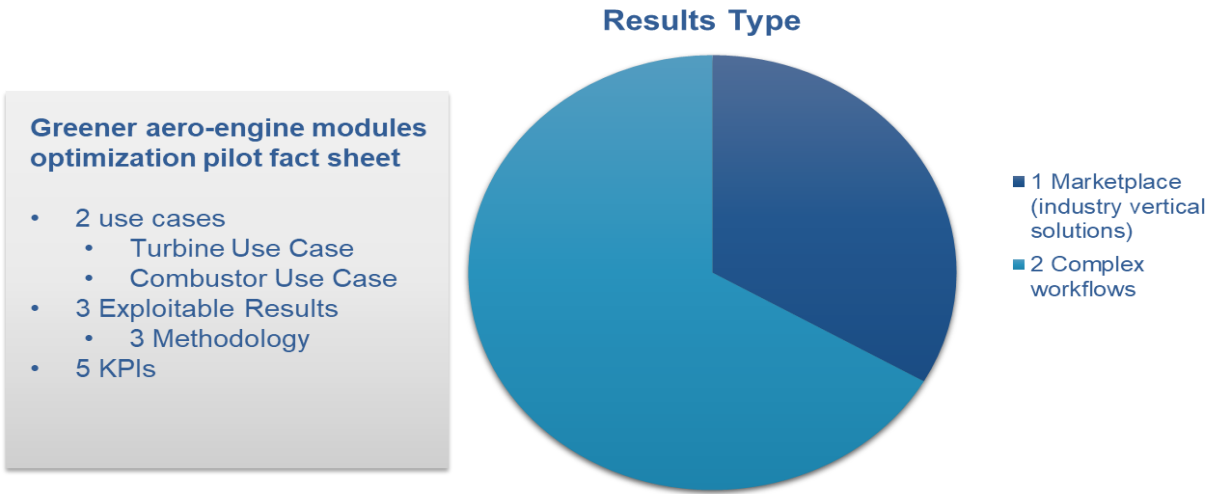

Figure 2 Greener aero-engine modules optimization pilot fact sheet

The demo tools, factsheets currently available for WP 5 are summarized in the followings subsections (see subsection 2.1.1.1 and 2.1.1.2) for the two uses cases.

2.1.1.1 Turbine Use Case

The demo-tools under development in the turbine use cases are at the present state the AI tools that will be used for the analysis of the database and the HPDA routines that will be used to extract the most important information from the hi-fidelity simulations and reducing the dimensionality of the database. These two demo tools are the fundamental requirements for the development of the new DS. Workflows, use-cases, and software tools are described in the table below:

Workflows	1. The baseline workflow includes: the generation of the URANS database by means of URANS and AI tools, the computation of hi-fidelity simulations for some of the blade configurations identified from the URANS database, the HPDA of the LES simulation. The two databases are then analyzed to identify the optimal design condition. 2. The improved workflow will include the automatic execution of HPDA routines while the LES simulation is running, thus providing a 30% reduction of the execution time of the two workflows. AI tools will be improved to jointly analyze the URANS database and the hi-fidelity simuations results for an improved and more efficient automatic identification of the optimal engineering solution. More information and a block diagram for a better understanding of the workflows are described in Deliverable 2.1.
Use-Cases	Within the new DS it is possible to identify several use-cases, namely: 1.The URANS database that constitute a large database with the variation of several parameters that are relevant for Aero-engine design. Restriction due to proprietary information may be applied (not open) 2. Each LES hi-fidelity simulation is an use case for HPDA routines. About 20 simulations will be performed, and some of them may be available as demo-tools of a complete data analytics procedure. 3. The inclusion of the LES simulation results in the URANS data base jointly with the AI tools developed in the project will represent the final use case of the DS. More details on the use-case can be found in Deliverable 2.1.

Software	The database will be created by means of the CFD commercial software STAR-CCM+ solver. The prominent innovation on the software side will not be related to the commercial software but to the AI tools and HPDA routines. Namely, the AI tools are currently based on Fortran, and are being ported to Python-Keras in order to exploit heterogeneous and innovative HPC hardware. The HPDA tools are currently written and deployed in Fortran and MATLAB using MPI and LAPACK libraries. They are currently being ported to python for a more efficient implementation on HPC and easy porting to GPUs.

Table 3 Turbine use case summary

2.1.1.2 Combustor Use Case

The objective of the combustor task is to optimize the multi-scale, multi-physics simulations with which aero-engine combustion chambers are currently designed. The U-THERM3D procedure is a customization of the ANSYS Fluent commercial CFD solver, which is used extensively in both research and industrial applications. Now, however, U-THERM3D, although extensively validated, is not sufficiently automated to be used in industrial environments, but one of the objectives of the project is to make the instrument more automated and user-friendly to simplify its use. The optimized tool will guarantee accurate results with a reduced calculation time and, at the same time, the setup procedure will be automated and made more user-friendly for industrial environments. At the moment a new workflow for a more efficient data management is being implemented, this optimization will ensure the achievement of the technical KPIs set in Table 1 and at the same time guarantee a setup phase more suitable for the internalization of Avio Aero's aeronautical combustor design procedure, as reported in the exploitable results in Table 2.

Workflows	1. The baseline workflow includes: the generation of the URANS database by means of URANS and AI tools, the computation of hi-fidelity simulations for some of the blade configurations identified from the URANS database, the HPDA of the LES simulation. The two databases are then analyzed to identify the optimal design condition. 2. The improved workflow will include the automatic execution of HPDA routines while the LES simulation is running, thus providing a 30% reduction of the execution time of the two workflows. AI tools will be improved to jointly analyze the URANS database and the hi-fidelity simuations results for an improved and more efficient automatic identification of the optimal engineering solution. More information and a block diagram for a better understanding of the workflows are described in Deliverable 2.1.
Use-Cases	Within the new DS it is possible to identify several use-cases, namely: 1.The URANS database that constitute a large database with the variation of several parameters that are relevant for Aero-engine design. Restriction due to proprietary information may be applied (not open) 2. Each LES hi-fidelity simulation is an use case for HPDA routines. About 20 simulations will be performed, and some of them may be available as demo-tools of a complete data analytics procedure. 3. The inclusion of the LES simulation results in the URANS data base jointly with the AI tools developed in the project will represent the final use case of the DS. More details on the use-case can be found in Deliverable 2.1.
Software	The database will be created by means of the CFD commercial software STAR-CCM+ solver. The prominent innovation on the software side will not be related to the commercial software but to the AI tools and HPDA routines. Namely, the AI tools are currently based on Fortran, and are being ported to Python-Keras in order to exploit heterogeneous and innovative HPC hardware. The HPDA

	tools are currently written and deployed in Fortran and MATLAB using MPI and LAPACK libraries. They are currently being ported to python for a more efficient implementation on HPC and easy porting to GPUs.

Table 4 Combustor use case summary

2.1.2 Weather, Climate, Hydrological and Farming pilot envisaged results

This pilot aims to demonstrate pre-exascale scalability of state-of-the-art meteorological and climatological models developed by ECMWF and MPI-M research centres. In particular, it targets numerical weather prediction ensemble at 5km on a global-scale and Grand-Ensemble climatological simulations.
The objectives of the pilot are:

- Improve the existing operational system for global numerical weather prediction, post-processing and data delivery by exploiting hardware-acceleration and data streaming/object store techniques to demonstrate exascale scalability.
- Enable low-latency exploitation of climate simulations by integrating data delivery trough domain-specific object store
- Develop and demonstrate an environment for user-defined in-situ data processing. The system will enable HPDA on multi-petabyte meteorological and climatological archives and data streams to enable data analytic workflows that improve insight to data.

In the following table are included the KPIs of the pilot.

KPIs	Description
KPI 1	Demonstrate Numerical Weather Predictions (NWP) workflow with IFS model resolution improved from the current 9.0km operational resolution to 5.0km.
KPI 2	Improve WFLOW (hydrological application) runtime performance when compared to today's capabilities at least factor 5, to enable full ensemble simulation
KPI 3	Demonstrate hydrological simulations over Rhine and Meuse basins (220.000 km2 area) adopting 1.0km model resolution

Table 5 Weather, Climate, Hydrological and Farming pilot KPIs

The envisaged results related to this pilot are include in the following table. These envisioned results are part of the exploitable results (ER) listed in D8.3

#ER	Envisaged results	Description	Type
ER2	Parallellized adopted for operation forecasting	Reach the point where the tested speed-up version of the wflow_sbm model will be passed on to the Dutch operational water authorities to be tested within operational setting and ultimately incorporated as part of the national hydrological forecasting suite for flood and drought forecasting and monitoring within the Netherlands. *Updated model delivered to operational authorities where will be evaluated and considered for operations.*	Marketplace (industry vertical solutions)
ER8	IFS global NWP model working at 5km	We will demonstrate the IFS global NWP model working at 5km resolution and adopted as input model for downstream applications (hydrological simulation and mesoscale downscaling). *Exploitation by downstream application in WP6 workflows and/or external applications. Output data archived and available on MARS or CDS archive.*	Marketplace (industry vertical solutions)

ER11	Parallellized open-source software version	The multi-threated and parrallized version of the wflow_sbm Julia software developed on a GitHub branch, once tested and evaluated becomes merged with the main branch to become publically available. *Updated and tested code added to main branch on GitHub page*	Complex workflows
ER12	Mesoscale weather simulations & forecasts	Downscaled weather simulations & forecasts will be conducted over Greek Peninsula in the context of smart farming applications Public demonstration in relevant environment (smart farming applications)	Marketplace (industry vertical solutions)
ER16	CDO-FDB-Connector	To allow the climate model ICON to directly write to the DB FDB the central MPI-M I/O library libcdl is extended to copy data via the climate data operators (CDO) application to an FDB DB instance. *Optimized Object Store, handling of all data sets of the pilot, support of complex WFs using semantic queries*	Complex workflows

Table 6 Weather, Climate, Hydrological and Farming pilot envisioned results

In the Figure 3 is shown a fact sheet of the Weather, Climate, Hydrological and Farming pilot.

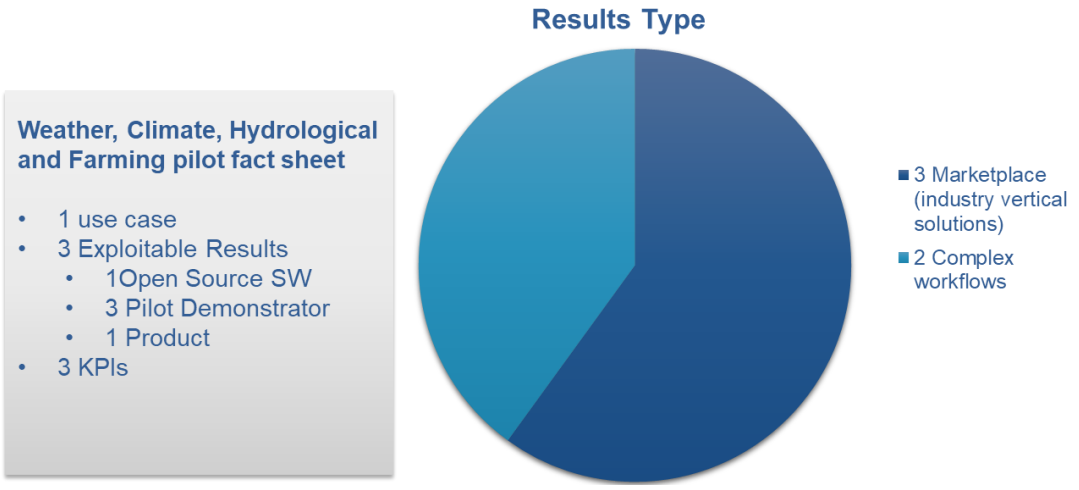

Figure 3 Weather, Climate, Hydrological and Farming pilot fact sheet

2.1.3 Energy and Carbon Sequestration pilot envisaged results

This pilot aims to transform the open-source subsurface simulator OPM Flow towards becoming a truly high-performance computing tool capable to address large-scale CO2 storage scenarios. OPM Flow includes MPI parallelization of the most important parts of the simulator, but currently with limited scalability. In this pilot ACROSS aims to build on OPM Flow to achieve:

- flexible, high-performance and massively parallel simulations of large scale CO2 storage in an open-source program;
- Achieving robust, high-performance and adaptive reservoir simulation on geo-models extracted automatically from seismic data (thereby reducing the need for expensive model-building steps);
- Performing in-situ (real time) analysis and visualisation workflows on large result sets;
- Defining new workflows for analysis and assessment of reservoirs that are supported by machine learning and artificial intelligence tools.

In the following table are included the KPIs of the pilot.

KPIs	Description
KPI 1	Improving OPM Flow runtime performance scaling when compared to today's parallel capabilities, scaling to 1000 processes with reasonable efficiency.
KPI 2	Carrying out flow simulations on large grids for long term migration scenarios (> 1000 years), on models with up to 100M cells.
KPI 3	Running direct flow simulation on models consisting solely of processed seismic data, at high resolution, with automatic and dynamic coarsening/refinement, on models with up to 100M cells.
KPI 4	Demonstrating analysis of simulation results in-situ using methods from the AI spectrum in 3 new workflows. Increase by 50% the overall data processing throughput (i.e., the number of scenarios evaluated per unit of time and the requests per second served in extreme cases).

Table 7 Energy and Carbon Sequestration pilot KPIs

In the following table are included the envisaged results related to this pilot.

#ER	Envisaged results	Description	Type
ER4	OPM Flow for carbon sequestration	The OPM Flow software can be used by stakeholders in industry, academia and public sector to perform assessments and studies of large-scale carbon sequestration scenarios and strategies, and drive decisions on such. *New improved capabilities merged into OPM Flow main branch, accessible by stakeholders outside the ACROSS consortium.*	Complex workflows
ER5	Damaris Analytics Plugin	Damaris in-situ/in-transit plug-in to enable analytics of streaming data being received from one or more simulations. *Public release of plug-in enabled Damaris software*	Research/Scientific results

Table 8 Energy and Carbon Sequestration pilot envisioned results

In the Figure 4 is shown a fact sheet of the Energy and Carbon Sequestration pilot fact sheet:

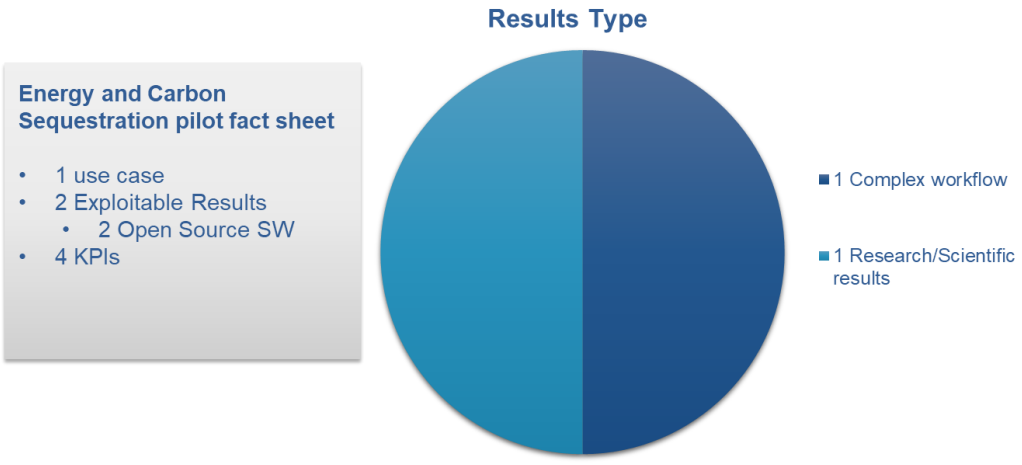

Figure 4 Energy and Carbon Sequestration pilot fact sheet

2.2 Technological envisaged results

At the present state of the project from the technological point of view, the envisaged exploitable results identified are:

#ER	Envisaged results	Description	Relevant WPs	Type
ER1	FastML	FastML is a component of the Atos CODEX AI Suite product. Its goal is to facilitate the ML/DL operation (ML Ops), by managing AI Models (training…) and hiding infrastructure and deployment concerns to the user. It will be used, adapted and integrated to other components of the ACROSS software stack, to handle HPC/ML/DL workflows. *FastML enhancements resulting from its ACROSS usage will be available in the Atos product.*	WP4	HPC facilities
ER3	YSTIA YORC Orchestrator	YORC is a TOSCA based orchestrator available under open source licence. It manages deployment and execution of software application & workflow on any infrastructure. It will be extended according to ACROSS requirements. *YSTIA/YORC orchestrator is available as open source, it is used within Atos products like Atos CODEX AI Suite, by some external users, and within other collaborative projects. New versions will benefit from the ACROSS related enhancements.*	WP4	Complex workflows
ER6	HyperTools tool chain extension by Pilots requirements	HyperTools is an acronym for a set of software for different users orchestration requirements. We will extend the selected one by the ACROSS requirements. All these software are currently under open source license. *Pilots and external third party - integration the ACROSS extensions into the other SW solutions developed by IT4I for orchestration. The sustainability of this result is key for IT4I for its users.*	WP4	Complex workflows
ER7	AI Acceleration	Hw/Sw extension of HPC architecture to accelerate AI-based applications. *Exploitation by project pilots and/or external applications.*	WP3	HPC facilities
ER9	Dynamic Resource Allocator	Dynamic Resource Allocator will be extended to integrate smart allocation policies targeting heterogeneous systems (both HPC and Cloud) and aiming to energy efficiently use them. *YSTIA Orchestrator Tool*	WP4	Complex workflows
ER13	Queue timing prediction	We will integrate our methodology for analysing and predicting queue waiting time of jobs into the middle-level orchestration layer of the ACROSS orchestration system. *Project pilots and external applications.*	WP4	Complex workflows

Table 9 Envisioned technological results

3 Cross project collaboration plan and goals

3.1 Collaboration goals

The collaboration activities have the goal to foster innovation through inter-projects new knowledge creation, validation and exploitation of key findings.
The collaboration activities lays the foundation for integrating a selection of the results of the pilots delivering the best of the tested HPC-enabled ACROSS solutions.Collaboration will also be pursued in circumstances when merging the experience of other HPC projects will provide new or enhanced insight, findings, or techniques. To this end, the collaboration with other EuroHPC projects will allow to leverage their lessons-learnt, establish contact and share information and foster innovation through inter-project new knowledge creation, validation and exploitation of key findings.

3.2 Collaboration plan with EuroHPC-JU projects

ACROSS has officially started in March 2021 and will end in February 2024. During this period, several other HPC research projects will be actively working on related HPC activities. In the Table 10 are listed the identified EuroHPC-JU projects for possible collaborations.

EuroHPC-JU projects	Partners	Start-End Dates	Collaboration in
eFlows4HPC (Enabling dynamic and Intelligent workflows in the future EuroHPC ecosystem) has been funded under the EuroHPC-02-2019 topic. It aims to deliver a workflow software stack and an additional set of services to enable the integration of HPC simulations and modelling with big data analytics and machine learning in scientific and industrial applications. The software stack will allow creating innovative adaptive workflows that efficiently use the computing resources considering novel storage solutions. The project is coordinated by Barcelona Supercomputing Center (BSC). The project aims to demonstrate the workflow software stack through use cases of three application Pillars with high industrial and social relevance: Manufacturing - construction of DigitalTwins for the prototyping of complex manufactured objects integrating state-of-the-art adaptive solvers with machine learning and data-mining, contributing to the Industry 4.0 vision. Climate - develops innovative adaptive workflows for climate and for the study of Tropical Cyclones (TC) in the context of the CMIP6 experiment, including in-situ analytics. Urgent computing for natural hazards - explores the modelling of natural	Coordinator: Barcelona Supercomputing Center (BSC) Partners: CIMNE, Jülich Supercomputing Centre (JSC), Universitat Politecnica de Valncia, BULL, DtoK LAB, cmcc, Inria, SISSA, PSNC, Universidad de Malaga, Helmholtz Center for Polar and Marine Research, INGV, ETH Zurich, SIEMENS, NGI	01/01/2021 - 29/02/2024	Collaboration related to dissemination and communication activities. The principal foreseen possible collaborations are related principally to WP4 and the orchestration (YSTIA orchestration, FastML etc.)

catastrophes in particular, earthquakes and their associated tsunamis shortly after such an event is recorded.			
HEROES (Hybrid Eco Responsible Optimized European Solution) has been funded under the topic EuroHPC-02-2019. It is a collaborative research and innovative project that aims to strengthen the links between HPC and IA/ML user communities and HPC centres with the objective to reinforce European capacities in terms of innovation. It is coordinated by UCit. The project will focus on a software solution for composable workflows in the renewable energy and manufacturing industries for the development of energy efficient products. By facilitating the creation of HPC marketplaces where end users can connect easily to HPC resources, the HEROES Software Platform will accelerate HPC adoption in scientific and industrial processes and create opportunities for HPC resource providers to publish their services. The HEROES Software Platform includes the following modules: Identity & Security Management; Data Transfer & Storage; User Interfaces & APIs; Application and Container Lifecycle Management; Cloud Cluster Deployment; HPC Centre Cluster Integration; Logging & Accounting Services; Energy Monitoring & Optimisation; Pricing and Cost Management; Workflow & Job Orchestration.	Coordinator: UCit Partners: BSC, Do IT Systems, HPCNow!, Neovia Innovation.	01/03/2021 - 28/02/2023	Collaboration related to dissemination and communication activities. The principal foreseen possible collaboration is related to WP2, WP3, and WP4 activities.
MICROCARD (Numerical modelling of cardiac electrophysiology at the cellular scale) has been funded under the topic EuroHPC-02-2019. It will develop an exascale simulation platform to study the mechanisms of cardiac arrhythmia with models that represent the heart cell by cell. It is coordinated by Université de Bordeaux. It will develop numerical schemes suitable for exascale parallelism together with matching linear-system solvers and preconditioners, and a dedicated compiler to translate high level model descriptions into optimized,	Coordinator: Université de Bordeaux Partners: Université de Strasbourg, Simula Research Laboratory AS, Università degli Studi di Pavia USI: Università della Svizzera italiana, KIT - Karlsruhe Institute for Technology , Konrad-Zuse-Zentrum für	01/04/2021 - 30/09/2024	Collaboration related to dissemination and communication activities. Principal foreseen possible collaboration are related to WP4.

energy-efficient system code for heterogeneous computing systems. The code will be resilient to hardware failures and will use an energy-aware task placement strategy. At the same time, they develop highly parallel mesh generation software to build the extremely large and complex models that we will need for the simulations. These meshes will be based on large volumes of confocal microscopy data that were recently acquired with the latest clearing and labelling techniques.	Informationstechnik Berlin, MEGWARE Computer Vertrieb und Service GmbH, NumeriCor GmbH, Orobix srl.		
REGALE (An open architecture to equip next generation HPC applications with exascale capabilities) has been funded under the topic EuroHPC-02-2019. It aims to build a software stack that is not only capable of bringing efficiency to tomorrow's HPC systems. It is coordinated by Institute of Communication and Computer Systems (ICCS). It also will be open and scalable for massive supercomputers. In the race to greater performance using less energy, the focus has often been on hardware. However, system software can now play a crucial role towards a controlled balance between application performance, power constraints and energy consumption, taking advantage of software interfaces for hardware configuration, without neglecting application needs. REGALE intends to realize these benefits under real operational environments by equipping the HPC system software stack with the mechanisms and policies for effective performance, power and energy control and optimization, bridging the gap between research and practice.	Coordinator: Institute of Communication and Computer Systems (ICCS) Partners: Technische Universität München (TUM), Leibniz Supercomputing Centre, ANDRITZ HYDRO GMBH, Université Grenoble Alpes, Atos (Bull SAS), Barcelona Supercomputing Centre (BSC), CINECA, Consorzio Interuniversitario, E4 Computer Engineering SpA, National Technical University of Athens - NTUA, Ryax Technologies, Electricité de France (EDF), Ubitech, SCiO Private Company, TWT GmbH Science & Innovation, Alma Mater Studiorum - Università di Bologna.	01/04/2021 - 31/03/2024	Collaboration related to dissemination and communication activities. The principal foreseen possible collaboration is related to WP2, WP3, and WP4 activities.
RED-SEA (Network Solution for Exascale Architectures) is funded under the topic EuroHPC-01-2019. It will build upon the European	Coordinator: Atos (Bull SAS) Partners: Idryma Technologias Kai Erevnas,	01/04/2021 - 31/03/2024	Collaboration related to dissemination and communication activities.

interconnect BXI (BullSequana eXascale Interconnect), together with standard and mature technology (Ethernet) and previous EU-funded initiatives to provide a competitive and efficient network solution for the exascale era and beyond. It is coordinated by Atos (Bull SAS). RED-SEA supports the Modular Supercomputing Architecture (MSA) that underpins all of the SEA projects. In the MSA, BXI is the HPC fabric within each compute module, delivering low-latency, high bandwidth and all required HPC features, whereas Ethernet is the high-performance federative network that offers interface to storage and with other compute modules. RED-SEA will design a seamless interface between BXI and Ethernet via a new Gateway solution.	Commissariat à l'énergie atomique et aux énergies alternatives (CEA), Forschungszentrum Jülich, EXTOLL GmbH, Eidgenössische Technische Hochschule Zürich, Universitat Politècnica de València, Universidad de Castilla - La Manche, Istituto Nazionale di Fisica Nucleare – INFN, Exapsys - Exascale Performance Systems, eXact lab SRL.		Prototyping the RED-SEA switch design on an acceleration technology FPGA to be investigated together with ACROSS (WP3)
DEEP-SEA (DEEP – SOFTWARE FOR EXASCALE ARCHITECTURES) is funded under the topic EuroHPC-01-2019. It builds upon exascale concepts developed over nearly 10 years. It will build a software stack for heterogeneous compute and memory systems that allows scientists and developers to make best use of all available resources. It is coordinated by Forschungszentrum Jülich (Jülich Supercomputing Centre) and represents the latest undertaking (Phase 4) in the family of DEEP projects. DEEP-SEA is building upon proven software packages to create an open-source environment optimally supporting heterogeneous and modular supercomputers, guided by co-design with applications from seven high-impact scientific fields. Objectives of the project are: Co-design the software and programming environment of the upcoming European exascale systems; Provide tools to map complex applications and non-uniform workflows onto heterogeneous and modular computer architectures; Enhance the system software, programming paradigms, tools, and runtimes in order to extract the maximum performance from heterogeneous computer	Coordinator: Forschungszentrum Jülich (Jülich Supercomputing Centre) Partners: Atos (Bull SAS), Leibniz Supercomputing Centre , Barcelona Supercomputing Centre (BSC), Fraunhofer-Gesellschaft zur Förderung der angewandten Forschung e.V, Katholieke Universiteit (KU) Leuven, Eidgenössische Technische Hochschule (ETH) Zürich, ParTec, Idryma Technologias Kai Erevnas (FORTH), Commissariat à l'énergie atomique et aux énergies alternatives (CEA),	01/04/2021 - 31/03/2024	Collaboration related to dissemination and communication activities.

platforms and improve performance portability; Improve the use and management of new memory technologies and the placement of data in compute devices with deep and heterogeneous memory hierarchies; Release the DEEP-SEA software stack in production-ready quality to enable its operation and exploitation in upcoming European exascale systems.	Technische Universität München, Technische Universität Darmstadt, Kungliga Tekniska Högskolan (KTH), European Centre for Medium-Range Weather Forecasts (ECMWF).		

Table 10 EuroHPC-JU projects

Despite the EuroHPC projects shown above, ACROSS has started the collaboration also with H2020 projects like LEXIS (Large-scale EXecution for Industry & Society) project. LEXIS has built an advanced engineering platform at the confluence of HPC, Cloud and Big Data, which leverages large-scale geographically distributed resources from the existing HPC infrastructure, employs Big Data analytics solutions and augments them with Cloud services. In the context of task 2.4 “Infrastructure Set-up and cross stack convergence integration"” is being evaluated the integration of the ACROSS orchestrator with the LEXIS Platform.

In the Figure 5 are shown the planned collaboration activities for the whole duration of the project.

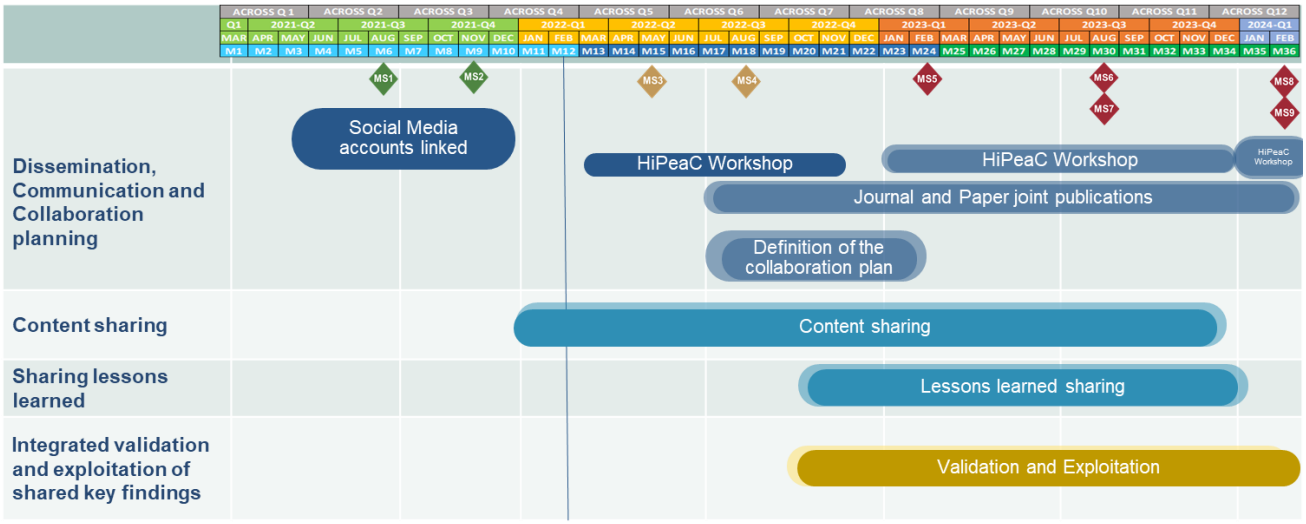

Figure 5 Collaboration Plan

3.3 First Initiatives

The first steps towards the collaboration have been already taken, to this end has been organised a workshop “HeLP-DC: Heterogeneous and Low-Power Data Center technologies in the EuroHPC Projects Context” (https://www.hipeac.net/2022/budapest/#/program/sessions/7930/) that was planned to be held in January 2022 but due to COVID situation has been postponed in June 20 2022 (Budapest, Hungary).
Will participate to this workshop, EuroHPC funded projects, along with other EU projects that strongly rely on the capabilities of newly available supercomputers. The main aim of this workshop is to foster sharing of project results, lesson learned, ideas, and technological solutions, as well as the vision on forefront technologies which are intended to drive HPC systems towards the Exascale and the convergence with AI, Cloud computing and Big-Data domains.
Among the projects that will participate during this workshop are included all the identified EuroHPC projects and this event will serve as a starting point for the discussions related the second step for the collaboration.

This workshop will be dedicated to cross discovery, cross dissemination among the projects and base on progress and results define the basis of collaboration.
The PO has been notified by email about the workshop on September 21st. 2021.
By the end of 2021 the ACROSS the social media accounts have been linked to the social media accounts of the identified projects.

3.4 Next Steps

After the workshop the HeLP-DC, that will serve as a starting point to share the main activities, pilots and objectives of each project, will be defined the future steps and the next events Projects Coordinators' meetings to be organised, in order to put in place a collaboration strategy. These meetings will serve to:

- Define the roadmap and particularly specific collaboration goals
- Identify a wider set of joint activities.

The five topic EuroHPC-02-2019 projects will join forces through a series of collaboration activities, which will examine developed software and hardware tools and technologies. Collaborative work in this direction will allow not only to share best practices, but also to take the potential achievements of each individual project well beyond what was originally envisaged.

Moreover, initiatives such as special issues on academic journals, workshops and special sessions at international conferences, and other knowledge transfer efforts, will maximise the potential impact of the collaboration. To this end the workshop "HeLP-DC: Heterogeneous and Low-Power Data Center technologies in the EuroHPC Projects Context" will be held also in 2023 and 2024.

4 Conclusions

The cross collaboration among these projects not only paves the way for sharing of best practises and cutting-edge technologies, but also for the potential outcomes of each project to go far beyond what was originally envisioned. In addition, the organisation of activities such as special issues in academic journals, workshops and special sessions at international conferences, and other knowledge transfer efforts will maximise the potential impact of the joint research.

This document will be updated during the project to reflect any updates or changes that arise during the course of the project. WP8 will focus its efforts in the next months on strengthening relationships with collaboration partners and finalizing a community-building strategy, which will be more detailed in the next deliverable on M24.

References

[1] EuroHPC-JU, “HPC and data centric environments and application platforms,” [Online]. Available: https://ec.europa.eu/info/funding-tenders/opportunities/portal/screen/opportunities/topic-details/eurohpc-02-2019;callCode=H2020-JTI-EuroHPC-2019-1;freeTextSearchKeyword=;matchWholeText=true;typeCodes=1;statusCodes=31094501,31094502,31094503;programmePeri.

[2] EuroHPC-JU, “Extreme scale computing and data driven technologies,” [Online]. Available: https://ec.europa.eu/info/funding-tenders/opportunities/portal/screen/opportunities/topic-details/eurohpc-01-2019;callCode=H2020-JTI-EuroHPC-2019-1;freeTextSearchKeyword=;matchWholeText=true;typeCodes=1;statusCodes=31094501,31094502,31094503;programmePeri.