

# D2.6

## EuroHPC Engagement Plan

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## D2.6/ EuroHPC Engagement plan

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### Abstract

Developed under the WP2, Activity 2.2.3 - *Alignment with Strategic Initiatives*, this deliverable outlines the engagement plan of the EOSC Future project towards the European HPC ecosystem and EuroHPC, the current leading (super)-computing initiative which aims at establishing an integrated world-class supercomputing and data infrastructure environment in Europe. It provides an overview of the current high-performance computing landscape in Europe and identifies the relevant areas of collaboration that are key for EOSC Future's engagement goals. The objectives underpinning the engagement with the HPC ecosystem are to facilitate the availability of (Euro)HPC resources through the EOSC Platform (1), coordinate technical choices and align the architectures of the EOSC and EuroHPC federated environments (2) and articulate a value proposition to boost engagement and collaboration between EuroHPC and EOSC Future (3). On that basis, the deliverable details background work and proposes a set of recommendations, priorities and activities that support the engagement goals.

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## Table of Contents

|  |    |
|--|----|
| List of Abbreviations .....  | 4  |
| 1 Executive Summary .....  | 5  |
| 2 Introduction - Overall aim and objectives.....   | 6  |
| 2.1 Scope and structure of this deliverable .....  | 6  |
| 2.2 How this fits within the EOSC Future Engagement strategy .....                             | 6  |
| 3 Stakeholders – EuroHPC, related initiatives and EOSC .....                                   | 8  |
| 3.1 EuroHPC.....   | 8  |
| 3.1.1 Areas of collaboration and alignment   | 8  |
| 3.2 PRACE.....   | 9  |
| 3.2.1 Areas of collaboration and alignment   | 9  |
| 3.3 FENIX .....  | 10 |
| 3.3.1 Areas of collaboration and alignment   | 10 |
| 3.4 Related projects.....  | 11 |
| 3.4.1 DICE - Data Infrastructure Capacity for EOSC   | 11 |
| 3.4.2 EGI-ACE - Advanced Computing for EOSC  | 11 |
| 3.4.3 PHIDIAS - Prototype of HPC/Data Infrastructure for On-demand Services                    | 12 |
| 3.4.4 EOSC-Nordic  | 12 |
| 3.5 Other: HPC Excellence and Competence Centres and data community networks .....             | 13 |
| 3.5.1 HPC Centres of Excellence (CoEs)   | 13 |
| 3.5.2 Centre of Excellence in Simulation of Weather and Climate in Europe (Phase 2) - ESIWACE2 | 13 |
| 3.5.3 Centre of Excellence in Computational Biomedicine - CompBioMed                           | 14 |
| 3.5.4 HPC National Competence Centres (NCCs)   | 14 |
| 3.5.5 Data Community Networks: Leveraging the Research Data Alliance (RDA)                     | 15 |
| 4 Engagement strategy and plan .....   | 16 |
| 4.1 EOSC Future, FENIX and the Science Clusters .....  | 16 |
| 4.1.1 Scoping requirements and areas of collaboration  | 16 |
| 4.2 HPC providers to EOSC - How to make HPC resources part of the EOSC Marketplace .....       | 17 |
| 4.3 EOSC (Future) value proposition for (Euro)HPC .....  | 18 |
| 5 Implementation and monitoring.....   | 21 |
| 6 Conclusions .....  | 23 |
| 7 References.....  | 24 |

## Table of Figures

|  |    |
|--|----|
| Figure 2.1: EOSC Future systematic approach to coordinated engagement and targeted communication ..... | 7  |
| Figure 5.1: EOSC Future (Euro)HPC engagement plan timeline .....                                       | 22 |

## Glossary

EOSC Future project Glossary is incorporated by reference: <https://wiki.eoscfuture.eu/x/JQCK>

## List of Abbreviations

| Acronym                       | Definition  |
|-------------------------------|---|
| <b>BDVA</b>                   | Big Data Value Association  |
| <b>ECAS</b>                   | ENES Climate Analytics Service  |
| <b>EOSC</b>                   | European Open Science Cloud   |
| <b>EOSC SRIA</b>              | European Open Science Cloud Strategic Research and Innovation Agenda                  |
| <b>EuroHPC JU</b>             | EuroHPC Joint Undertaking   |
| <b>ETP<sub>4</sub>HPC</b>     | European Technology Platform for High Performance Computing                           |
| <b>ETP<sub>4</sub>HPC SRA</b> | European Technology Platform for High Performance Computing Strategic Research Agenda |
| <b>ESFRI</b>                  | European Strategy Forum on Research Infrastructures                                   |
| <b>ESGF</b>                   | Earth System Grid Federation  |
| <b>IS-ENES</b>                | Infrastructure for the European Network for Earth System Modelling                    |
| <b>ICEI</b>                   | Interactive Computing E-Infrastructure  |
| <b>PRACE</b>                  | Partnership for Advanced Computing in Europe  |
| <b>QuIC</b>                   | European Quantum Industry Consortium  |

## 1 Executive Summary

Developed under the WP2, Activity 2.2.3 - *Alignment with Strategic Initiatives*, this deliverable outlines the engagement plan of the EOSC Future project towards the European HPC ecosystem and EuroHPC, the current leading (super)-computing initiative which aims at establishing an integrated world-class supercomputing and data infrastructure environment in Europe.

The document provides an overview of the current high-performance computing landscape in Europe and identifies the relevant areas of collaboration that are key for EOSC Future's engagement goals. The objectives underpinning the engagement with the HPC ecosystem are to facilitate the availability of (Euro)HPC resources through the EOSC Platform (1), coordinate technical choices and align the architectures of the EOSC and EuroHPC federated environments (2) and articulate a value proposition to boost engagement and collaboration between EuroHPC and EOSC Future (3). On this basis, the deliverable details background work and proposes a set of priority activities and outputs.

The foreseen level of engagement in this project is primarily at technical level, focusing on how architecture, resource allocation and access management of HPC resources can enrich the EOSC Future offering. The objective is to pilot the integration of HPC sites and EuroHPC installations and resources into the EOSC Future architecture and have some of these resources available through the EOSC Portal by the end of the project. Alignment and convergence with the HPC ecosystem is a natural scale-out, and articulating a clear value proposition to the HPC and EuroHPC stakeholders, and HPC providers particularly, will ensure a meaningful engagement and value-add to both the EOSC and HPC sides.

## 2 Introduction - Overall aim and objectives

Supercomputing and data infrastructures are critical strategic resources for the EU and are key to ensuring that European researchers reap the full benefits of data-driven science and lead the path to grand scientific discoveries. Making these resources available through EOSC can contribute to attracting more researchers to EOSC and to widening HPC access to new research communities and enabling new opportunities for interdisciplinary research.

Indeed, EOSC should become one of the first choices for researchers when it comes to looking for and accessing high quality computing resources, and the success of EOSC in creating a web of data will also depend on the possibility for researchers to easily find and access computing resources of different kinds, leveraging the latest technology developments in high-performance computing, cloud platforms, big data, machine learning and artificial intelligence techniques.

By facilitating access to significant amounts of open scientific data, and effectively mobilising valuable high performance computing resources to exploit this data, EOSC can offer all researchers a unique trustworthy environment that enables them to succeed in the global, data driven innovation system.

In its mission statement, EOSC Future commits to build on top of an existing infrastructural baseline of research and e-infrastructures and connect to other environments, while favouring a common understanding of science and strengthening interoperability across infrastructures and user communities.

By the end of the project, the EOSC Platform aims at offering a full spectrum of the available resources, national and European, as well as access to commercially procured resources and links to other infrastructures (such as EuroHPC). Ideally researchers should also be able to request HPC resources (e.g from EuroHPC) as well as other HPC related services directly through the EOSC Platform.

Therefore, a continuous dialogue between the EOSC Future and the EuroHPC ecosystems is critical to ensure technical choices around architectures, tools and services, and federation efforts are not incompatible.

Furthermore, as EOSC Future and EuroHPC tackle similar or related challenges, establishing areas of synergies and complementarity is beneficial to both. To best map these and efficiently approach collaboration opportunities, EOSC Future also looks at articulating a value proposition for EuroHPC and HPC providers in particular, concentrating on ways to optimise onboarding and connections with the scientific communities.

For EOSC Future the objectives underpinning the engagement with the HPC ecosystem are thus focused around making (Euro)HPC resources available through the EOSC Future marketplace (1), coordinating technical choices and aligning the architectures of the federated infrastructures (2) and articulating a value proposition to boost engagement and collaboration (3).

### 2.1 Scope and structure of this deliverable

Developed under the WP2, Activity 2.2.3 - *Alignment with Strategic Initiatives*, this deliverable outlines the engagement plan of the EOSC Future project towards EuroHPC, the current leading (super)-computing initiative which aims to establish an integrated world-class supercomputing and data infrastructure ecosystem in Europe. It provides an overview of the current high-performance computing landscape in Europe and identifies the relevant areas of collaboration that are key for EOSC Future's engagement objectives. It details background work and proposes a set of recommendations, priorities and activities that support these engagement goals.

Following this brief introduction to set the scene, section 3 of the deliverable looks at the key stakeholders including EuroHPC and connected initiatives. Section 4 outlines the engagement strategy and plan covering the aforementioned recommendations and activities, while section 5 summarises the steps around implementation and monitoring, followed by conclusions (section 6).

### 2.2 How this fits within the EOSC Future Engagement strategy

The EOSC Future engagement and communication activities are performed at different levels in all the EOSC Future work packages. WP10 is responsible for the EOSC Future's engagement strategy, its coordination across



the other work packages, and its implementation. It leverages and incorporates strategic inputs from WP2, mandated to engage with high-level actors like EuroHPC and ensure the alignment with developments on EOSC - Core and EOSC-Exchange and other aspects relative to the federation of services and data.

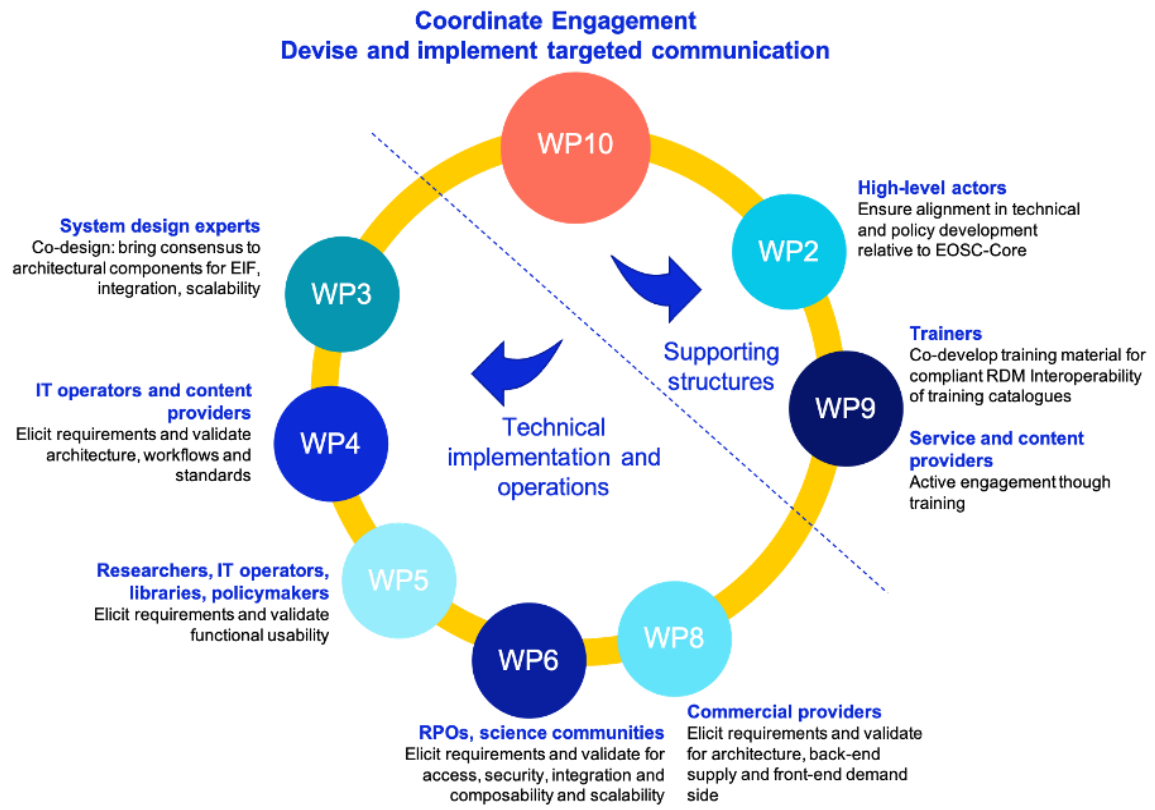


Figure 2.1: EOSC Future systematic approach to coordinated engagement and targeted communication

### 3 Stakeholders – EuroHPC, related initiatives and EOSC

The EuroHPC has “the overall mission to develop, deploy, extend and maintain an integrated world class supercomputing and data infrastructure and to develop and support a highly competitive and innovative High Performance Computing (HPC) ecosystem, extreme scale, power-efficient and highly resilient HPC and data technologies” (EuroHPC Joint Undertaking, 2021, p.5) in close collaboration with scientific communities, public and private organisations, technology platforms, data networks and fora.

Whilst keeping focus on EuroHPC as the flagship stakeholder, this deliverable also looks at other actors in the European HPC ecosystem that are of relevance to EOSC and EOSC Future, detailed in the following section. A number of existing materials presenting the HPC landscape in Europe like the European Technology Platform for High Performance Computing<sup>1</sup>, ETP<sub>4</sub>HPC’s 2021 European HPC Handbook, but also input from networks of the EOSC Future participating partners, public outputs and information from partnering initiatives such as the INFRAEOSC-07-2020 projects (C-SCALE, DICE, EGI-ACE, OpenAIRE-Nexus, RELIANCE), were leveraged in order to identify these additional reference stakeholders and assess activities and the areas of engagement and collaboration.

#### 3.1 EuroHPC

The EuroHPC initiative is a Partnership between the EU and 30 Participating States<sup>2</sup> aiming at establishing an integrated supercomputing and data infrastructure ecosystem in Europe, acquiring leadership-class supercomputers, and deploying HPC services for science, industry and SMEs. The private sector is represented by three partners, the European Technology Platform for High Performance Computing (ETP<sub>4</sub>HPC), the Big Data Value Association (BDVA)<sup>3</sup> and the European Quantum Industry Consortium (QuIC)<sup>4</sup>.

The European High Performance Computing Joint Undertaking (EuroHPC JU) is the legal and funding entity created in 2018 to allow the European Union and the participating countries to coordinate their efforts and pool their resources to make Europe a world leader in supercomputing. This overarching objective is pursued by EuroHPC JU in two pillars, the Research and Innovation pillar and the Infrastructure Pillar. This second pillar is in charge of the development of the European HPC supercomputing and data infrastructure, aiming at reaching supercomputing exascale capacity by 2022/2024.

Since its inception, the EuroHPC Joint Undertaking has launched efforts for the procurement of three “pre-exascale” and five “petascale” machines which are being hosted in Finland, Italy, and Spain (pre-exascale), and in Bulgaria, Czech Republic, Luxembourg, Portugal and Slovenia (petascale)<sup>5</sup>.

EuroHPC is a prime reference initiative for EOSC Future, belonging to the stakeholder group “EOSC Facilitators and Intermediaries”, and identified as one the key groups that indirectly influence EOSC developments. It is thus a group that the project should align and collaborate with to ensure technical advancements, stimulate uptake and support competence development (EOSC Future, 2021, p.4) within the broader European research landscape.

##### 3.1.1 Areas of collaboration and alignment

The Governing board of EuroHPC JU has recently published its work plan for year 2022 (EuroHPC Joint Undertaking, 2021) which includes several topics that are relevant to EOSC and could provide the basis for future engagement activities. These regard technical developments but also opportunities connected to education, training, user support, and around international cooperation, for a common understanding and vision of science, research data and scientific computing.

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<sup>1</sup> European Technology Platform for High Performance Computing (ETP<sub>4</sub>HPC) <http://www.etp4hpc.eu/>

<sup>2</sup> Discover EuroHPC JU <https://eurohpc-ju.europa.eu/discover-eurohpc-ju>

<sup>3</sup> Big Data Value Association (BDVA) <https://www.bdva.eu/> - soon to become DAIRO

<sup>4</sup> European Quantum Industry Consortium (QuIC) <http://www.euroquic.org/>

<sup>5</sup> In some cases, the hosting entities are underpinned by an agreement between several member states, such as in the Finnish case where the system will be jointly owned and operated by a consortium of nine countries including Finland, Belgium, Czech Republic, Denmark, Estonia, Norway, Poland, Sweden, and Switzerland, the Italian consortium including Slovenia and the Spanish consortium including Croatia, Portugal and Turkey.

On the technical side, the work of EuroHPC around the federation of supercomputing and data resources in Europe is of high relevance for EOSC and EOSC Future. While the specific details are still under discussion, the objective of this topic is to develop and operate a platform for federating HPC, quantum computing and data resources, providing union-wide, cloud-based secure services for a wide range of public and private users across Europe. This effort is expected to build on previous work undertaken by the FENIX RI<sup>6</sup>. Therefore, EOSC Future sees the latter as a conduit to facilitate coordination in terms of technical choices and federation efforts between the two larger ecosystems.

The EuroHPC calls related to education, training and user support represent a further opportunity for collaboration. Again, while the details are still to be finalised, the services which will be developed by these calls are very relevant for EOSC and some form of collaboration could be envisaged with consortia which will be involved in designing those services.

Through the dedicated international activities work and funding calls, the EuroHPC JU aims to boost the engagement of key European stakeholders who can contribute to strengthen the HPC environment and help support the engagement of researchers and private users who would both contribute to developing novel algorithms as well as test the applications and codes in diverse academic and industrial cases. Participation of EOSC stakeholders to these joint initiatives should be widely encouraged and actively pursued as these can constitute valuable intermediaries between the two ecosystems.

## 3.2 PRACE

The mission of PRACE (Partnership for Advanced Computing in Europe)<sup>7</sup> is to enable high-impact scientific discovery and engineering research and development across all disciplines to enhance European competitiveness for the benefit of society. PRACE seeks to realise this mission by offering world class computing and data management resources and services through a well-established peer review process. Currently PRACE manages the only Europe-wide HPC programme, distributing around 5 billion core computing hours annually to scientifically and technically excellent European and international open research projects. This volume of resources is much larger than what any individual country can provide or use and can only be achieved by pooling several national resources into this large HPC programme.

### 3.2.1 Areas of collaboration and alignment

The main objective of PRACE is to enable large-scale research projects beyond what national capacities can provide, both in terms of scope and duration. To this end, the access mechanisms include a thorough peer-review process to evaluate the scientific and technical excellence of such projects. One side result of this, is that PRACE principal access mechanisms have a rather long acceptance process (3 to 6 months), which makes them less amenable for direct integration into the EOSC catalogue.

Nevertheless, PRACE has a wide catalogue of HPC-related services that can be integrated and used by EOSC end users. This includes HPC benchmark and development access, the training programme and the support programme. The common characteristic of these services is that the access is provided immediately or after a brief technical review, they are open to both public and private sector, and the only major requirement is to follow the open access research principle. This makes such services amenable for onboarding in the EOSC Platform with little, minor technical adaptations and constitute a first stepping stone to pilot onboarding and listing of HPC resources in the EOSC marketplace.

Specifically in the case of the benchmark and development mechanisms, applications undergo a simple technical assessment to confirm that requests fulfil their scope, and resources are commonly allocated in less than one week. Even if the volume of resources assigned to these mechanisms is relatively low, typically below 5% of the total HPC capacity of PRACE, their importance is high for the user community as they serve key enabling purposes, as follows:

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<sup>6</sup> FENIX RI <https://www.fenix-ri.eu/>

<sup>7</sup> PRACE <https://prace-ri.eu/>

1. the objective of benchmark access is to test the application codes that will be later used in large-scale HPC projects; in this way, potential users can demonstrate that their large-scale project is technically feasible and that it will make an efficient use of the high-value HPC resources requested. As a consequence, this is a prerequisite before applying to large-scale calls; and
2. development access provides time and resources to perform code evaluation and optimization on real HPC systems, in order to test and confirm their efficiency before engaging into a large-scale project. Moreover, the results from development projects are also useful for the rest of the community, which can later benefit from the optimizations undertaken.

Because of their scope and nature, these two HPC access mechanisms are amenable for onboarding in the EOSC Platform for the benefit of PRACE and EOSC community, but also the whole European HPC community, since this increased visibility will be followed by an increased usage, technical publications and extended base of large-scale HPC codes available. Further integration should rely on the efforts that PRACE hosting sites are conducting through the FENIX initiative<sup>8</sup>, related to federation and interoperability.

Furthermore, PRACE also organises the EuroHPC Summit Week, the annual event for science, industry and policy makers in HPC. Building on the past experience of PRACE days, this event includes keynotes and workshops aimed at promoting coordination of the different European actors. This event provides a good platform to further discuss potential synergies between EOSC future and the EuroHPC ecosystem.

### 3.3 FENIX

The FENIX infrastructure is based on the agreement of different European Tier-0 HPC centres to align their offering of compute and storage services. In addition to the traditional extreme-scale computing and data services, FENIX provides a set of cloud services as well as services needed for federation. Six European supercomputing centres, namely BSC (Spain), CEA (France), CINECA (Italy), CSC (Finland), CSCS (Switzerland) and JSC (Germany) are currently part of the Fenix Infrastructure<sup>9</sup>.

The initial version of the infrastructure is being realised through the ICEI (Interactive Computing E-Infrastructure) project, which is part of the European Human Brain Project (HBP), and also has developed a resource allocation mechanism to provide resources to HBP users and European researchers at large and drive the expansion of the e-infrastructure to other communities that provide additional resources.

Since 2018, the project has been delivering operational cloud and high-performance computing, storage and networking services to over 100 projects, over 150 active users to the neuroscience communities and beyond via specific PRACE-ICEI calls (in collaboration with PRACE) and several thousands of users of cloud hosted platforms for the neuroscience communities. It is also used for providing urgent access to COVID-19 related research projects through the PRACE Fast Track<sup>10</sup>. Moreover, the project has an active outreach and engagement effort through the Fenix Users Forum<sup>11</sup> and offers both virtual and hands-on training events.

#### 3.3.1 Areas of collaboration and alignment

EOSC Future provides a framework and channel for FENIX to further work with research communities, especially the ESFRI clusters, and follow the needs of current and developing scientific and engineering areas. These communities are seen on the longer term as key drivers for the evolution of its e-infrastructure services portfolio. The two initiatives are both addressing issues around harmonisation and federation of both compute and data services in order to provide scientific communities with optimal sharing and scaling possibilities, while also supporting interdisciplinarity and long-term sustainability. Because FENIX is expected to play a role in designing and supporting the upcoming supercomputing federation, EOSC Future should prioritise this stakeholder in its engagement strategy.

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<sup>8</sup> FENIX Research Infrastructure <https://fenix-ri.eu/>

<sup>9</sup> About FENIX <https://fenix-ri.eu/about-fenix>

<sup>10</sup> PRACE Support To Mitigate Impact Of COVID-19 Pandemic, <https://prace-ri.eu/prace-support-to-mitigate-impact-of-covid-19-pandemic>

<sup>11</sup> FENIX User Forum <https://fenix-ri.eu/infrastructure/fenix-user-forum>

### 3.4 Related projects

The HPC landscape is continuously expanding as developments in the area are supported through multiple public and private mechanisms and funding schemes. Below we highlight, DICE and EGI-ACE, two of the key INFRAEOSC-07-2020 projects that work on establishing connections between the data and the HPC environments by particularly focusing on resource allocation. These are complemented by another project, Phidias, which contributes to the development of applications in the HPC Continuum and provides a prime example of bridging data-driven scientific community, FAIRification and HPC opportunities. A similar example is provided in the case of the EOSC regional projects (INFRAEOSC-5b), specifically EOSC Nordic and its NICEST2 use case working to enhance performance and optimize Earth System Model workflows on future computing resources like EuroHPC and LUMI.

#### 3.4.1 DICE - Data Infrastructure Capacity for EOSC<sup>12</sup>

DICE is one of the projects funded by the INFRAEOSC-07-2020 call. The project aims to provide EOSC with state-of-the-art data management services together with the associated storage resources. Besides the provisioning of the services already in production, the consortium aims to enhance data management service provisioning by integrating/updating services in order to provide solutions to cover the whole research data lifecycle.

##### 3.4.1.1 Areas of collaboration and alignment

In this realm, a dedicated activity is being carried on, to integrate data services with computing platforms to enable analysis, data replication, and data publication for high performance computing (HPC) and cloud computing environments. This will help the users to get their research data from computation to publishing much easier and thereby help in getting wider access to research data. This activity is planned by using the B2DROP<sup>13</sup> service as a tool to maintain "recipes" for analysis, B2SAFE<sup>14</sup> as a tool to safely store results of simulations/analyses, and B2SHARE<sup>15</sup> as a tool to share and publish datasets. The technical integration is now ongoing following the plans reported in the corresponding project deliverable (Mallmann et al., 2021).

This activity is performed jointly by the EUDAT (specifically Jülich) and CSCS teams and the results will act as a blueprint for data management solutions for European HPC systems (like the EuroHPC ones) based on services made available through the EOSC Platform. This will improve data management practices within computing environments beyond basic storage and archives for bit preservation. The results will be shared with the EOSC Future team to support the technical interoperability work as part of the EOSC Future INFRAEOSC-07-2020 Collaboration Agreement<sup>16</sup>.

#### 3.4.2 EGI-ACE - Advanced Computing for EOSC<sup>17</sup>

EGI-ACE (a project also funded by the INFRAEOSC-07-2020 call) has a mission to empower researchers from all disciplines to collaborate in data- and compute-intensive research through free-at-point-of-use services. The "EOSC Compute Platform", delivered by the EGI-ACE project, is a system of federated compute and storage facilities, complemented by diverse access, data management and compute platform services. The EOSC Compute Platform is designed to support a wide range of scientific data processing and analysis use cases, including the hosting of scientific services and data spaces.

##### 3.4.2.1 Areas of collaboration and alignment

The infrastructure layer of the EOSC Compute Platform initially builds on compute cloud, container and High Throughput Compute facilities. During EGI-ACE this layer will be extended with some HPC systems, and the

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<sup>12</sup> DICE <https://www.dice-eosc.eu>

<sup>13</sup> EUDAT B2DROP services <https://b2drop.eudat.eu>

<sup>14</sup> EUDAT B2SAFE services <https://b2safe.eudat.eu>

<sup>15</sup> EUDAT B2SHARE services <https://b2share.eudat.eu>

<sup>16</sup> New services coming up to EOSC-Core <https://eosc-portal.eu/news/new-services-coming-eosc-core>

<sup>17</sup> EGI-ACE <https://www.egi.eu/projects/egi-ace/>

access to federated HPC resources will be demonstrated by Open Science workflows that span across all EOSC Compute platform continuum.

The HPC integration work in EGI-ACE is focused on the following technical areas:

1. Federated user access management on HPC systems.
2. Availability and reliability monitoring of federated HPC sites.
3. Integrated usage accounting across HPC, cloud and HTC sites.
4. Access to distributed, federated data from HPC systems.
5. Portable container-based applications for cloud compute, HTC and HPC systems.

These areas are investigated by four HPC centres, CESGA (ES), ICT-BAS (BG), LIP/INCD (PT), and TUBITAK (TR), all members of the EuroCC project.

The findings will be configured on these sites and will be validated through four scientific workflows:

- Climate research use case from ENES (CMCC, Italy);
- High Energy Physics simulations for the High Luminosity run of the Large Hadron Collider (CERN);
- Cross platform fusion workflows (UK Atomic Energy Authority);
- Photon and neutron science use case from the ELI-NP Research Infrastructure (IFIN-HH, Romania).

The work will deliver an architecture blueprint for HPC providers about how to provision HPC resources with the EOSC platform federated access management, monitoring, accounting, data and application access mechanisms. The blueprint will be a deliverable due in June 2022. EGI-ACE will engage with external HPC providers after that to boost the uptake, and ultimately increase the presence and accessibility of HPC systems via the EOSC Compute Platform, and the EOSC Portal.

### 3.4.3 PHIDIAS - Prototype of HPC/Data Infrastructure for On-demand Services<sup>18</sup>

PHIDIAS is an EU-funded project financed by the Innovation and Networks Executive Agency (INEA) under the European Union's Connecting Europe Facility (CEF). The project addresses the development and concrete realisation of a set of HPC based interdisciplinary services and tools to exploit large satellite datasets of public European interest. PHIDIAS aims at creating access services to increase the HPC and data capacities of the European Data Infrastructure in the context of the CEF on open data.

#### 3.4.3.1 Areas of collaboration and alignment

In addition to the disciplinary focus on building a prototype for Earth's scientific data and high-performance computing services, PHIDIAS also looks at optimising and industrialising the management of workflows for extensive reusability, ensuring open access to standardised HPC services, improving FAIRification processes and open access, developing new data-processing models coupled with HPC capabilities and deploy data-processing methods as a service for the scientific community.

There is a shared interest for workflow automation, FAIRification processes and optimisation of data-processing methods. The prototype catalogue being developed by PHIDIAS will be connected with the EOSC platform, enriching its catalogue with HPC related services and datasets.

#### 3.4.4 EOSC-Nordic<sup>19</sup>

The EOSC-Nordic EC-funded project focuses on Open Science and data and services FAIRification activities in the Nordic countries, in support of the broader adoption of EOSC in the region.

NICEST<sub>2</sub>, one of the demonstrator projects in EOSC-Nordic also called "FAIR Climate data and software for the Nordics" is piloting building blocks of possible EOSC-Nordic services and how to make climate data, services

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<sup>18</sup> Phidias <https://www.phidias-hpc.eu>

<sup>19</sup> EOSC-Nordic <https://www.eosc-nordic.eu>

and scientific methods more FAIR and efficiently running on powerful HPC systems like the LUMI supercomputer.<sup>20</sup> In the longer term this will help enhance the performance and optimise Earth System Model workflows on future computing resources provided through EuroHPC in a way that is interoperable with the EOSC web of FAIR data and services.

### 3.5 Other: HPC Excellence and Competence Centres and data community networks

#### 3.5.1 HPC Centres of Excellence (CoEs)

Currently 15 European Centres of Excellence (CoEs) for High Performance Computing (HPC) applications<sup>21</sup> have been selected following the calls under the European Research Infrastructures. These aim to promote the use of upcoming exascale and extreme performance computing capabilities and to support scaling up existing parallel codes towards exascale performance.

The CoEs have a specific role in addressing the skills gap in computational science in the targeted domains like engineering, environmental science, renewable energy, materials modelling and design, molecular and atomic modelling, especially via specialised training designed for increased adoption of advanced HPC in industry and academia. CoEs bring together the European world-class knowledge and expertise in applying established mechanisms, user driven development, performance tools and programming models for HPC, optimization of HPC applications performance and co-design activities for real systems based on leading edge technologies.

##### 3.5.1.1 Areas of collaboration and alignment

The HPC Centres of Excellence hold a key role in the EuroHPC work plans as effective mechanisms to ensure advanced computing solutions are tailored to specific disciplinary challenges on the one hand, while supporting a gradual move of scientific applications and code to the pre-exascale and hopefully exascale, on the other.

Centres of excellence enable these challenging transitions by addressing architectural issues, code scalability, management of complex workflows and large dataset sets in collaboration with established research communities they share with the other stakeholders and initiatives like the EOSC.

The CoEs have offered alternative forms of collaboration and can be leveraged as nodes or point of contact between the EuroHPC and the EOSC. They facilitate the uptake and exploitation of high-performance computing within the specialised communities, supporting the tailored approaches and skill development best suited to them.

Two examples of CoEs looking at strategic areas of application such as climate modelling and personalised medicine and how they interact with the EOSC, are detailed below.

#### 3.5.2 Centre of Excellence in Simulation of Weather and Climate in Europe (Phase 2) - ESIWACE<sub>2</sub><sup>22</sup>

ESiWACE<sub>2</sub> organises and enhances Europe's excellence in weather and climate modelling to enable leading European weather and climate models to leverage the performance of pre-exascale systems with regard to both compute and data capacity as soon as possible. ESIWACE<sub>2</sub> also prepares the weather and climate community to be able to make use of exascale systems when they become available. For model developers, it offers a number of services: special software packages, public HPC services and training programs that support the weather and climate community.

With respect to EOSC, the provision of data generated on EuroHPC systems and downstream analysis could gain importance. The European climate modelling community, also organized in the IS-ENES consortium (Infrastructure for the European Network for Earth System Modelling), relies on services such as the globally operated ESGF (Earth System Grid Federation), and increasingly on cloud-based approaches. IS-ENES already gained initial experience in the context of EOSC Future by providing access to data generated in climate

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<sup>20</sup> HPCwire, LUMI Supercomputer Aids in Nordic Climate Modelling  
<https://www.hpcwire.com/off-the-wire/lumi-supercomputer-aids-in-nordic-climate-modeling/>

<sup>21</sup> The Centres of Excellence <https://www.hpccoe.eu/eu-hpc-centres-of-excellence2/>

<sup>22</sup> Centre of Excellence in Simulation of Weather and Climate in Europe (Phase 2) <https://www.esiwace.eu/>

research through the ENES Climate Analytics Service (ECAS) and will further develop this work within the ESIWACE2 project duration and beyond.

### 3.5.3 Centre of Excellence in Computational Biomedicine - CompBioMed<sup>23</sup>

CompBioMed is a European Commission H2020 funded Centre of Excellence focused on the use and development of computational methods for biomedical applications. CompBioMed seeks to exploit the third pillar of science in order to render predictive models of health and disease more relevant to clinical practice by providing a personalised aspect to treatment. It facilitates the uptake and exploitation of high-performance computing within the biomedical modelling community, in order to bring benefits to many areas. These span from education and training of the next generation of computational biomedicine researchers, through new access mechanisms best suited to the community, to the impact of the methods on healthcare delivery within industry and the clinical context, especially in advancing personalised and precision medicine. The data managed and produced is of immediate use to clinicians and researchers in these areas, and in the intermediate term to industrial researchers and drug/medical device manufacturers and ultimately to patients.

In the Cardiovascular research pillar in CompBioMed, researchers create high fidelity simulations of the human cardiac conduction system along with the full biventricular description of the cardiac muscle. This is a multi-disciplinary collaborative work that aims to reproduce human anatomy as closely as possible. The main application being used is “Alya”, developed at the Barcelona Supercomputing Centre, which performs cardiac electro-mechanics simulations from tissue to organ level which focus on a FEM-based electro-mechanical coupling solver, optimised for HPC infrastructures. Alya is available for use to researchers in various HPC centres in Europe such as MareNostrum at BSC (Spain), SuperMUC at LRZ (Germany), and Snellius at SURF (The Netherlands).

The typical workflow using the Alya applications covers data creation and transfer (the raw data is collected at a lab and stored locally on tapes. A copy of the data is transferred to BSC), data pre-processing (at BSC, researchers pre-process the data which includes manual and automated steps for image stitching, segmentation and meshing), data replication (the pre-processed data needs to be replicated from BSC to other HPC centres such as SURF. The replicated data will then be used to run simulations on the supercomputers in these sites), data processing and analysis (running simulations and analyse output data), data publication (output data is published repository and made discoverable for reuse).

CompBioMed is collaborating with EUDAT in the DICE project in optimising the dataflow between the HPC centres to facilitate the large data transfers in making the replicas, to bring the data close to the computing facilities and to publish and preserve these large datasets.

### 3.5.4 HPC National Competence Centres (NCCs)

Leveraging funding from EuroHPC JU, two initiatives EuroCC and CASTIEL<sup>24</sup> are building a European network of 33 national HPC competence centres aiming to bridge the existing HPC skills gaps while promoting cooperation and the implementation of best practices in national contexts across Europe.

#### 3.5.4.1 Areas of collaboration and alignment

Implemented at national level and connected at pan-European one, this network is achieved through a series of focused activities, support and consultancy for academia, industry and public administration on a high level, such as guidance, knowledge transfer, use cases, and awareness raising.

The NCCs network aims to align scientific, public and private national stakeholders in HPC, data analytics and data driven-science under national strategies whilst consolidating complementary cross-country collaborations. Considering their focus and activities, there is an understandable overlap between these

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<sup>23</sup> CompBioMed <https://www.compbioimed.eu/>

<sup>24</sup> HPC National Competence Centres (NCCs) <https://www.eurocc-access.eu/> and <https://www.castiel-project.eu>



networks of national stakeholders and those involved in the Open Science, FAIR data networks and platform supporting the activities of the EOSC at national levels.

### 3.5.5 Data Community Networks: Leveraging the Research Data Alliance (RDA)

A partner in the EOSC Future project, the Research Data Alliance (RDA) is a community driven organisation bringing together more than 12300 members from 146 countries<sup>25</sup>. It was launched in 2013 by the European Commission, the United States Government's National Science Foundation and National Institute of Standards and Technology, and the Australian Government's Department of Innovation with the goal of building the social and technical infrastructure to enable open sharing and re-use of data.

RDA has a grass-roots, inclusive approach covering all data lifecycle stages, engaging data producers, users and stewards, addressing data exchange, processing, and storage. It has succeeded in creating the neutral social platform where international research data experts meet to exchange views and to agree on topics including social hurdles on data sharing, education and training challenges, data management plans and certification of data repositories, disciplinary and interdisciplinary interoperability, as well as technological aspects.

#### 3.5.5.1 Areas of collaboration and alignment

RDA provides an easy to access forum to bridge communities. At its 18<sup>th</sup> Plenary, held in November 2021, a session on "Combining data community strengths and HPC opportunities" was organised showcasing European and international examples of scientific or infrastructure initiatives that have succeeded in combining strengths of the data management community and the opportunities fostered by HPC. The focus spanned from defining and testing specific scientific use cases that use HPC, to prototyping HPC based services and tools for the data community to explore or drive competence building. The session aimed to pinpoint some of the technical and social challenges in terms of wider integration and interoperability of data, data infrastructures and HPC but also how this connection can be explored and nurtured in the future.

Follow-up activities for the Research Data Alliance 19<sup>th</sup> Plenary and the International Data Week Conference (June 2022) are foreseen under the umbrella of a Birds of a Feather (BoF) meeting designed to scope interest around challenges and stakeholders working on bringing together the Data and HPC communities.

The set-up of an Interest Group on Bridging Data and HPC could be a natural development of this exercise to be leveraged by EOSC Future to showcase engagement efforts and other alignment activities with EuroHPC, PRACE and other HPC stakeholders.

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<sup>25</sup> RDA in a Nutshell, December 2021 <https://www.rd-alliance.org/about-rda>

## 4 Engagement strategy and plan

EOSC Future aims firstly to facilitate the integration of EuroHPC resources to EOSC, through targeted activities around technical alignment and optimising onboarding processes to help stimulate the use of the high-performance computing capacity using FAIR data and federated infrastructures.

We expect that the EOSC Association will engage with the EuroHPC JU for high-level discussions related to the provisioning of EuroHPC resources through EOSC and governance topics.

Our level of engagement in this project will be primarily at technical level, focusing on how architecture, resource allocation and access management of HPC resources can enrich the EOSC Future offering. Our objective is to pilot the integration of FENIX sites and the EuroHPC installations and resources into the EOSC Future architecture and have some of these resources available through the EOSC Portal by the end of the project. A set of technical proofs of concept and demos, testing reports and recommendations will be key outcomes of these activities.

### 4.1 EOSC Future, FENIX and the Science Clusters

EOSC Future efforts have been focused during the first months of the project on strengthening links with FENIX. Since FENIX is expected to play a major role in the federation of EuroHPC centres and in delivering a pan-European computing infrastructure, it is of utmost importance to align activities and look for synergies. Our approach has been to start from the needs and requirements of the ESFRI science clusters involved in EOSC Future to initiate this collaboration.

#### 4.1.1 Scoping requirements and areas of collaboration

EOSC Future organised a "Joint EOSC/HPC workshop" on 23 April 2021 between representatives of the FENIX RI and representatives of the five ESFRI clusters: ESCAPE (astronomy and particle physics), ENVRI - FAIR (environmental research), PaNOSC (photon and neutron research), EOSC - Life (life sciences) and SSHOC (social sciences and humanities). The workshop aimed at identifying HPC requirements and use cases and invited the science clusters to share their vision and plans on their e-Infrastructure needs as well as how they envisage possible collaboration with the HPC centres (including the challenges they foresaw based on previous experience). The workshop also provided a unique opportunity for FENIX to present their service offer and plans to ESFRIs and analyse whether what is being offered and prepared meet the needs of potential users. The existing collaboration between FENIX and GEANT around AAI was also showcased.

The workshop highlighted a strong interest from most clusters to work with FENIX, and the three following topics were identified as potential areas of collaboration: AAI & federated access, resource allocation & access policies, and data movement & staging to computing environments. Following this initial scoping, it was decided to pursue the discussion on a bilateral level between FENIX and each cluster. Additional meetings were organised with ESCAPE and PANOSC, whose requirements in terms of HPC needs were the most articulated at the time. Discussions with the other clusters are planned to begin in Spring 2022. Concrete collaboration started with ESCAPE in June 2021 and led to a Proof of Concept (PoC), presented at the EOSC Future Mg internal technical review and showcasing how an ESCAPE user can access the FENIX environment and move data from one storage element to another.

#### Main engagement activities and outputs

- Meetings between FENIX and EOSC Future for information exchange on technical developments, further definition of areas of collaboration and plan of activities
- Technical meetings between FENIX and EOSC Clusters coordinated by EOSC Future
- Proof of Concept (PoC) around the topics identified as potential areas of collaboration: AAI & federated access, resource allocation & access policies, and data movement & staging to computing environments

- Demos and/or other documentation of PoCs and other alignment exercises
- Collect information on the amount of resources Science Clusters require and what type (i.e. large block allocation, project based or other), procedures and resource allocation programmes needed

#### 4.2 HPC providers to EOSC - How to make HPC resources part of the EOSC Marketplace

EOSC providers are a key stakeholder category for EOSC Future (EOSC Future, 2021, p.4). The project has dedicated considerable efforts across the various work packages to:

- the coordination between the e-infrastructures to deliver the EOSC-Core,
- engagement with research infrastructures to federate their services and resources into EOSC,
- a variety of public and private sector providers who wish to offer services via EOSC.

HPC providers are a category of service providers that holds considerable potential for EOSC. HPC providers offer both access to HPC computational resources and HPC related specialised services to European researchers and communities and EOSC Future should encourage their onboarding and, in that process, closely consider the specificities of this category of providers.

While cloud services have been more widely onboarded in the EOSC Marketplace with support from projects focusing on cloud providers, the same has not happened for HPC resources. Some of the PRACE access mechanisms and training services have been onboarded in the past in the EOSC Portal but more can be done as part of the EOSC Future activities to increase the engagement of HPC providers.

First of all, an exercise looking at the onboarding procedures and how these apply in the case of HPC resources can provide valuable feedback and contribute in the longer term to optimising the process and facilitate the integration of such resources into the EOSC Portal. CSC, CINECA and BSC, the high-performance computing centres partnering in EOSC Future, also members of FENIX and hosting site for EuroHPC pre-exascale systems, will constitute a first focus group to review the onboarding process from an HPC provider perspective and feedback on the exercise should be shared in support of activities around onboarding under tasks 6.1 and 6.2. In their assessment, partners should also consider other categories of HPC related resources (HPC benchmark and development access, the training and the support programme) that can and should be onboarded to ensure the HPC users have all the conditions to efficiently make use of this type of resources.

Additional analysis work can be run to onboard the current PRACE-ICEI calls as mechanisms offering access to the FENIX resources. These calls, while following the PRACE peer-review process of technical and scientific evaluation) require less time for the allocation of resources and thus can act as a good first step towards the onboarding of future HPC calls for resources.

In the execution of the analyses, the involved partners will cooperate and synergise also with the activities that are ongoing as part of the WP3 Working Group on Compute Continuum<sup>26</sup> which is looking on how to extend the EOSC resource profile for computing resources.

These efforts will produce two sets of recommendations, relevant to EOSC Future on the one hand, for the onboarding process and on how to facilitate the process for HPC providers and on the other hand, to the HPC centres/initiatives on how to better describe their resources in the EOSC Portal. It will be also documented in materials such as HPC focused factsheets as part of the EOSC Provider Toolkit.

Access can also be facilitated by integrating catalogues with HPC listings within the EOSC Future broader catalogue. A starting point can be the PRACE catalogue, and secondly the HPC benchmark and development access, the training programme and the support programme - services where the access is provided immediately or after a brief technical review. Open to both public and private sector, the only major requirement

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<sup>26</sup> EOSC Future WP3 Working Group on Compute Continuum,  
<https://wiki.eoscfuture.eu/display/PUBLIC/Compute+Continuum+Working+Group>

for the use of these services is to follow the open access research principle, making them an ideal first introduction to the use of HPC resources via the EOSC marketplace.

#### Main engagement activities and outputs

- Analyse the current onboarding procedure into the EOSC marketplace and provide recommendations – review exercise performed internally under EOSC Future by BSC, CSC and CINECA under the WP2 strategic alignment efforts
- Liaise to analyse onboarding procedures and potentially onboard calls to facilitate the resources allocation via PRACE-ICEI or other HPC mechanisms that might be identified
- Facilitate listing of PRACE HPC benchmark and development access, the training programme and the support programme in the EOSC Future catalogue
- Document recommendations and outcomes of the analysis work for cross-WP activities (i.e. WP6 activities around onboarding)
- Document recommendations for HPC providers looking to join / provide resources through EOSC e.g. providing information on the benefits of becoming an EOSC provider and guidance on how to best describe HPC services
- Recommendations and guidance to be streamlined to produce HPC focused materials to be included in the EOSC Future Provider Toolkit produced and disseminated by EOSC Future WP10 and the Knowledge Hub developed by EOSC Future WP9

### 4.3 EOSC (Future) value proposition for (Euro)HPC

The EOSC Future thematic pillars were designed to address and divide the complexity of the project into strategic topics which internally facilitate the oversight and coordination of the work and externally allow the EOSC community to understand the EOSC Future mandate and priorities and engage with the project, the work performed and foreseen outputs.

Building an EOSC Future value proposition around key thematic pillars provides a straightforward scalable approach as such a proposition would not be limited to the use in the EOSC context, on the contrary, it is meant to connect research communities and ensure technical alignment beyond the existing research and electronic infrastructures being federated under EOSC.

**Alignment and convergence with the HPC ecosystem is a natural scale-out, and articulating a clear value proposition to the HPC and EuroHPC stakeholders, and HPC providers particularly, will ensure a meaningful engagement and value-add to both the EOSC and HPC sides.**

The value proposition for (Euro)HPC, primarily at technical level, can be articulated around EOSC Future pillars as follows:

**Technical Development and provider onboarding** – The continuous technical developments and the increased integration of additional services and data sources in EOSC constitute a key component of the value proposition for (Euro)HPC.

The EOSC Future assessment of the community adoption and contributions, and interests of the users and providers is a **key source of information and validation for technical development efforts across the EOSC and HPC environments**. Furthermore, the efforts around onboarding, the tailored procedures, emerging business models and service concepts, the integration and interaction between public and commercial services bring forward opportunities for cloud services as well as HPC sectors.

A continuous technical dialogue between EOSC Future and the HPC sector, through focused activities like the FENIX – Science Cluster meetings, will ensure compatibility across architectures and federation efforts.

**Excellent Science and applications** - EOSC Future is committed to implement the necessary mechanisms to better understand researchers' needs and to take the appropriate measures to engage them throughout the design and implementation phases. The close collaboration with research communities and EOSC Future's periodic scenario development, service design and consultation exercises help support new scientific breakthroughs and the development of innovative services to support that.

In its March 2020 Scientific Research Agenda (SRA), the Institutionalised Partnership EuroHPC, the ETP4HPC, highlights EOSC as “**a source of information which helps anticipate upcoming requirements in the area of academic applications**, in particular with respect to **data management** (data logistics, storage, in situ data analysis, interoperability) and **the ease-of-use of HPC infrastructure services** (such as authentication and authorisation mechanisms, portals for accessing computing/ data resources, transfer of data and remote visualisation).” (ETP4HPC, 2021, p.31)

Additionally, the EOSC federation efforts not only support a unified approach and consistency, but they also allow EOSC to play the role of a multiplier to the communities it aggregates. Providers of resources, including HPC providers, will be able to describe and publish their resources through EOSC into multiple locations, in addition to the EOSC Portal, thus reaching more easily specialised or disciplinary communities or opening up new opportunities for multi- and interdisciplinary research.

Other pillars relevant for the (Euro)HPC value proposition:

**Policy & Strategy** related results and stakeholders' engagement are an important asset and mechanism to increase the awareness of EOSC among the broader innovation and research actors' network. These indirect channels help brand **EOSC as an innovation and research system, part of a broader ecosystem**.

In its SRA, the ETP4HPC lists EOSC as one of the key systems connected to the European HPC ecosystem. The **European Digital Continuum** is a blueprint for bringing together a multitude of systems and the **EOSC SRIA acknowledged this convergence of research priorities, visions and use cases and has committed to support its development** “ETP4HPC SRA has been designed to strengthen and develop further the European position with respect to the 'Digital Continuum' during the Horizon Europe programme. EOSC will ensure close collaboration in order to contribute to the Digital Continuum” (European Commission & EOSC Executive Board, 2021, p.36)

Another dimensions of value proposition for the (Euro)HPC in the area of Policy & strategy connects to the role of **EOSC as key driver for Open Science** “Over the past years, numerous policy makers world-wide have articulated a clear and consistent vision of global Open Science as a key factor, which could enable the new paradigm of transparent, data-driven science and accelerate innovation. In Europe, this vision is being realised through an ambitious programme within the EOSC (European Open Science Cloud).” (ETP4HPC, 2021, p.31)

**Skills & Training** are cross-cutting, supporting activities underlying all the areas of value creation. However, the skills and curriculum developed within EOSC Future can eventually be developed into **training and certification approaches to boost impact beyond the EOSC Future mandate and beyond the existing EOSC ecosystem**.

This type value-add also connects to the role of **EOSC as key driver for Open Science in Europe**, of particular relevance to their large shared user-base, as also highlighted in the ETP4HPC SRA: “The goal of the EOSC is to offer 1.7 million European researchers and 70 million professionals in the areas of science, technology, the humanities and social sciences a virtual environment with open and seamless services for storage,

management, analysis and re-use of research data, across borders and scientific disciplines. This will be achieved by federating existing scientific data infrastructures, which is currently dispersed across disciplines and the EU Member States. (ETP4HPC SRA, p.31)

### Main engagement activities and outputs

The primarily technical level of engagement foreseen under EOSC Future is complemented with a set of activities focusing on awareness raising and value definition in order to simulate the onboarding of HPC providers but also increasing visibility so that it will lead to increased uptake and usage of HPC resources on the longer term. Such activities planned over the project upcoming months:

- EOSC Future participation to EuroHPC Summit Week 2022 / PRACEdays22 (March 2022)
- EOSC Future Provider Days session for HPC centres: provider showcases and benefits of EOSC (April 2022)
- EOSC Future "Ask me Anything" session on HPC (June 2022) - targeting both users and providers, leveraging the collaboration with INFRAEOSC 07 projects and the CoEs
- (Euro) HPC spotlights at the EOSC Symposium 2022 (November 2022)
- EOSC HPC Provider Success Story - part of documenting onboarding success stories from the integration of the INFRAEOSC07 projects, the clusters and the WP8 commercial providers (interviews, testimonies) coming from HPC or related resource providers
- Invite input and contributions from HPC actors to the EOSC Future consultations and feedback collection around the EOSC Core releases and EOSC Future Consultation days (the latter in collaboration with the INFRAEOSC 07 projects)

## 5 Implementation and monitoring

To ensure progress in line with the engagement paths underpinning this strategy, a series of milestone activities and outputs have been outlined as illustrated in the timeline below (Figure 5.1).

These activities are organised under WP2 and performed by partners involved under Activity 2.2.3 - *Alignment with Strategic Initiatives* with the support of WP10. Outputs will be streamlined under the umbrella of task 2.2.4 - *Alignment of Core Capabilities and Inclusion Criteria* - looking into aspects related to the EOSC catalogue and supporting the process of connecting and validating resources for EOSC, as well as through the efforts around the onboarding of service providers ranging across several work packages but especially WP6 addressing the requirements, tools and procedures for the onboarding process.

Monitoring will be performed across the threads of activities and specific outputs detailed in the previous section and illustrated in the timeline above. These will be documented in the relative activity reports produced by EOSC Future. The reporting will include assessment measures pertinent to the agreed methodology to document both the alignment activities between EOSC Future, FENIX and the EOSC science clusters (e.g. demos, PoC reports, technical MoUs) and the activities to support to HPC providers onboarding and listing of HPC resources (e.g. Recommendations reports, HPC provider success stories, EOSC provider Tools HPC materials provision).

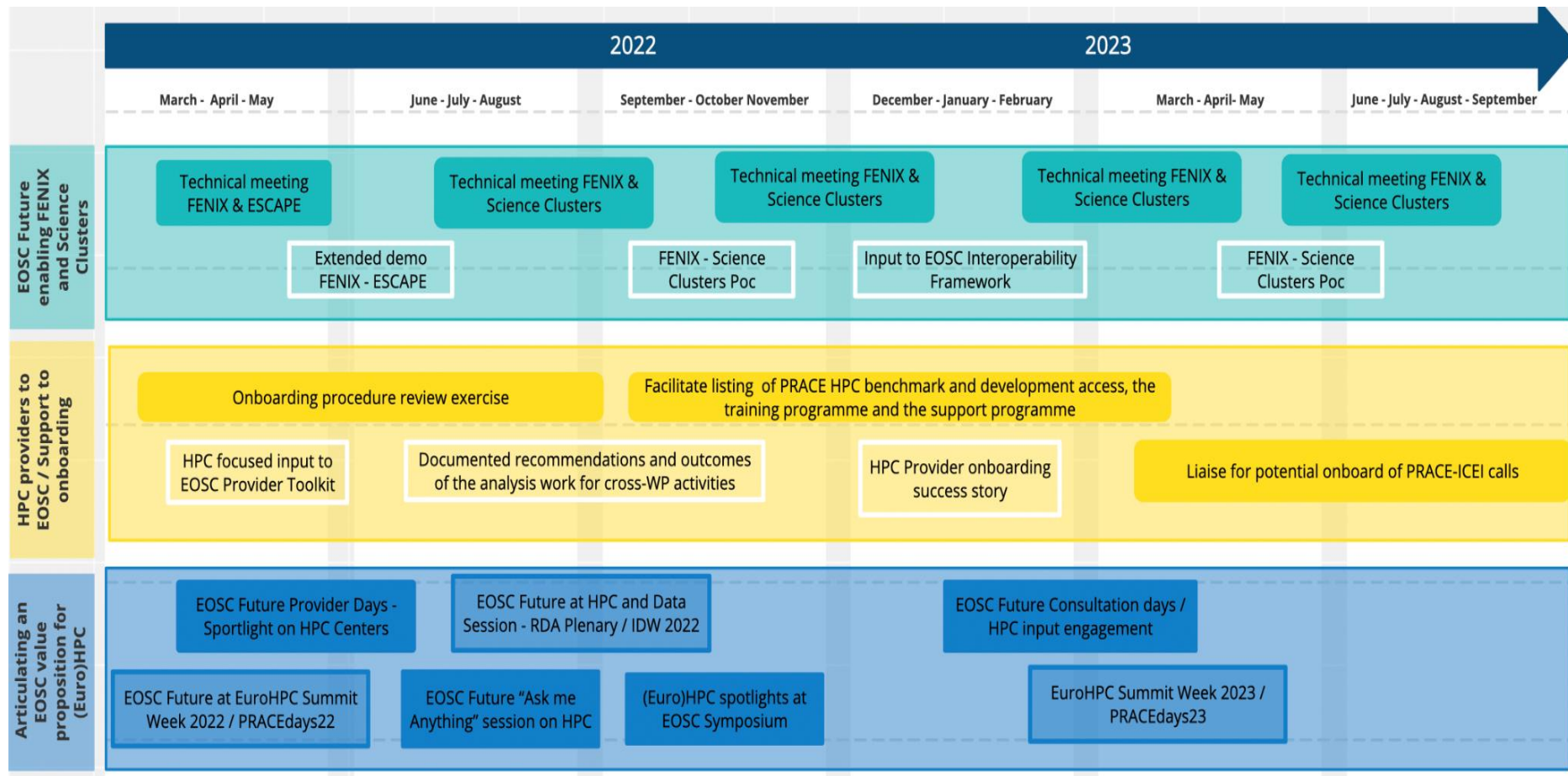


Figure 5.1: EOSC Future (Euro)HPC engagement plan timeline



## 6 Conclusions

The priorities and activities detailed in this deliverable are part of the broader EOSC Future effort to engage with strategic actors and ensure the technical alignment on developments related to EOSC-Core, EOSC-Exchange and other aspects relative to the federation of computing, services and data.

EOSC Future aims to facilitate the integration of EuroHPC resources into the EOSC Platform, increase awareness and stimulate the use of the high-performance computing capacity using FAIR data and federated infrastructures.

The approach detailed in this deliverable focuses mainly making (Euro)HPC resources available through the EOSC Platform (1), coordinating technical choices and aligning the architectures of the federated infrastructures (2) and articulating a value proposition to boost engagement and collaboration (3).

More in detail the deliverable outlines the background work and engagement paths with the key HPC stakeholders particularly EuroHPC, FENIX, PRACE, key related projects and HPC Excellence and Competence Centres.

Considering the diversity of the HPC landscape but also the EOSC Future objectives and resources, the level of engagement foreseen is primarily technical, focusing on architecture, resource allocation and access management streamlined particularly through the collaboration with FENIX. This is complemented with efforts focused on improving EOSC Future onboarding processes including recommendations to be leveraged internally in optimising the onboarding procedures and externally to support providers in making their HPC resources and related services more visible and accessible via the EOSC Marketplace. Nonetheless this will build on and help consolidate the EOSC Future value proposition for EuroHPC and other HPC actors.

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