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**Coordination of the HPC strategy**



**EXDCI**

**European eXtreme Data and Computing Initiative**

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**First holistic vision and recommendations report**

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## List of Acronyms and Abbreviations

*Below is an extensive the List of Acronyms used in previous deliverables. Please add additional ones specific to this deliverable and delete unrelated ones.*

AISBL	Association Internationale Sans But Lucratif (International Non-for-Profit Association)
BDEC	Big Data and Extreme-scale Computing
BDV	Big Data Value
CoE	Centres of Excellence for Computing Applications
cPPP	contractual Public-Private Partnership
CSA	Coordination and Support Action
D	Deliverable
DG	Directorate General
DoW	Description of Work
EC	European Commission
ECMWF	European Centre for Medium-range Weather Forecasts
EESI	European Exascale Software Initiative
ENES	European Network for Earth System modelling
EPOS	European Plate Observing System
EsD	Extreme scale Demonstrators
EU	European Union
FET	Future and Emerging Technologies
FP7	Framework Programme 7
GDP	Growth Domestic Product
H2020	Horizon 2020 – The EC Research and Innovation Programme in Europe
HPC	High Performance Computing
IDC	International Data Corporation
IESP	International Exascale Software Project
INVG	Istituto Nazionale di Geofisica e Vulcanologia (National Institute of Geophysics and Volcanology)
IPCEI	Important Project of Common European Interest
ISV	Independent Software Vendor
IT	Information Technology
KPI	Key-Performance Indicator
M	Month
OS	Operating System
PM	Person Month
Q	Quarter
R&D	Research and Development
R&I	Research and Innovation
RFP	Request for Proposal
ROI	Return On Investment
SHAPE	SME HPC Adoption Programme in Europe

SHS	Social and Historical Sciences
SME	Small and Medium Enterprise
SRA	Strategic Research Agenda
SWOT	Strengths, Weaknesses, Opportunities and Trends
TRL	Technology Readiness Level
US	United States
WG	Working Group
WP	Work Package

## 1 Executive Summary

This document presents a set of transversal recommendations that have been elaborated during the first year of EXDCI. They are complementary to the technical recommendations in the PRACE Scientific Case, the ETP4HPC Strategic Research Agenda (SRA) and other EXDCI Deliverables. These recommendations focus on three aspects of the European ecosystem and form a continuum from fundamental research to exploitation:

1. **Better research instruments:** The improvement of current research instruments, both computing resources and deployment of new technologies, in order to better support applications and researcher discovery processes;
2. **R&D efficiency:** Ensuring that the public and private investment in R&D is carried out in a coherent manner, maximizing the impact of research; and,
3. **Industry competitiveness:** Leveraging R&D excellence and translating its output into industry competitiveness

The recommendations are summarized in the following table:

Recommendations	Expected impact
Encouraging commercial relationships between SMEs and industry through European R&D projects	Industry competitiveness
Concerted approach to HPC training in Europe	
Incentives to increase EU stakeholders participation in international standards initiatives	
IPCEI for advanced HPC research and innovations	R&D efficiency
Paving the way from EsD development towards applications	
Improving capitalization of FETHPC and CoE results	
Operational policies and federation toward convergence	Better research instruments
Big Data and extreme scale international initiative	
Access to advanced technologies	

The short (on purpose) list of recommendations has been proposed by all EXDCI workpackages as the priorities after multiple exchanges with the European HPC ecosystem.

## 2 Introduction

This report proposes a set of recommendations that aims to improve the current European HPC ecosystem. We focus on three aspects of the European ecosystem:

1. **Better research instruments:** The improvement of current research instruments, both computing resources and deployment of new technologies, in order to better support applications and researcher discovery processes;
2. **R&D efficiency:** Ensuring that the public and private investment in R&D is carried out in a coherent manner, maximizing the impact of research; and,
3. **Industry competitiveness:** Leveraging R&D excellence and translating its output into industry competitiveness.

These three aspects form a continuum from fundamental research to academic and commercial exploitation. In EXDCI we have identified a set of decisive areas where new actions can help to achieve the overall goal set by the EU commission President, Jean Claude Juncker: *"Our goal is for Europe to become one of the top 3 world leaders in high-performance computing by 2020."* The proposed recommendations are summarized in Figure 1.

Recommendations	Expected impact
Encouraging commercial relationships between SMEs and industry through European R&D projects	Industry competitiveness
Concerted approach to HPC training in Europe	
Incentives to increase EU stakeholders participation in international standards initiatives	
IPCEI for advanced HPC research and innovation	R&D efficiency
Paving the way from EsD development towards applications	
Improving capitalization of FETHPC and CoE results	
Operational policies and federation toward convergence	Better research instruments
Big Data and extreme scale international initiative	
Access to advanced technologies	

Figure 1: recommendations and expected impacts

These recommendations take into account the major trends of the HPC domain and in particular the advances in data analytics and new disruptive technologies. They are complementary to the technical recommendations that are provided in the PRACE Scientific Case, the ETP4HPC Strategic Research Agenda (SRA) and other EXDCI deliverables.

The remainder of this report provides a description of the discussion process and details the recommendations.



### 3 Holistic Vision Elaboration

The elaboration process has been a collective process involving numerous stakeholders of the international HPC ecosystem. It is illustrated in Figure 2. The EXDCI WPs have collected feedback and information from the global HPC community at large, including from:

1. PRACE members;
2. ETP4HPC members;
3. FET HPC projects and CoE via a questionnaire<sup>1</sup> and EXDCI workshops;
4. International stakeholders via the BDEC initiative<sup>2</sup>;
5. A set of interviews of startups and SMEs.

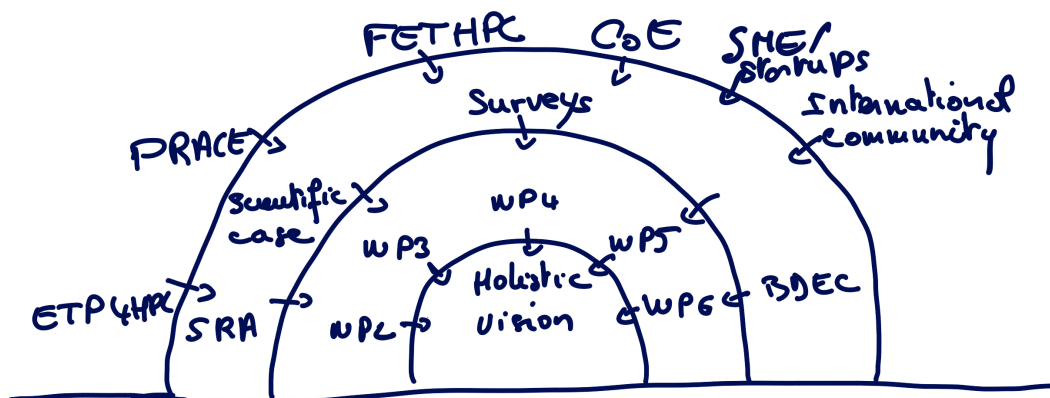


Figure 2: Global HPC stakeholders contributing to the holistic vision

This process has created a set of recommendations that aims at proposing new actions to improve the European HPC ecosystem. We have deliberately kept this set small to enable a focused discussion.

### 4 Operational Policies and Federation toward Convergence

#### *Recommendation issued from EXDCI WP3*

Access to data – generated by large simulations, large instruments and observational systems – is changing the ways in which we think about and address problems in science and societal research, including climate change and environmental hazard and risk analysis. Shared data is catalyzing change in global collaboration and in businesses. A user-driven sustainable data-and-compute e-infrastructure needs to be application-oriented, easily accessible, open and agile so that it can continuously adapt to changes in technology and research practice. Case studies must, therefore, include the relevant science and technology expertise while identifying gaps in missions, resources and capabilities, and also involving appropriate business models to explore how to sustain long-term stewardship.

<sup>1</sup> <https://exdci.eu/activities/questionnaire-coe-fet-hpc>

<sup>2</sup> <http://www.exascale.org/bdec/>

A crucial innovation to be explored are agile strategies that will allow to intimately couple research thinking with technical innovations. These strategies need to be deployed in a multi-organizational context in order to discover solutions and ways forward that closely match domain researchers' requirements, which evolve rapidly as the potential of new capabilities and data is appreciated. Eventually, this will change the focus from HPC production environments and community-specific data services, where middleware standards, security procedures and connectivity are dominating, to research-focused scenarios.

## 4.1 Recommendation

It is recommended that a task force be formed to pioneer the federation of autonomous organizations providing data, computing and data-intensive analysis resources, together with a comprehensive and operational virtual research environment and E-infrastructure devoted to the full path of data use in a research-driven context.

# 5 IPCEI for Advanced Research and Innovations

*Recommendation issued from EXDCI WP2*

An IPCEI meant to enable large HPC projects with strong industrial leadership has been proposed, in answer to the new EC HPC policy (as described in April 2016 communications on the “European Open Science Cloud” initiative, confirmed by the Council of Competitiveness of May 2016, in the more global context of the Digital Single Market and with a strong willingness to accelerate industry and public services digitalization, in addition to putting in place the necessary computing and data services and infrastructures for scientific research).

This IPCEI should allow to overcome some regulation and funding limitations of conventional H2020 instruments – enabling funding for much larger projects; allowing the pooling of different sources of funding from the EC and member states, and overcoming some limitations of state aids and competition rules. H2020-funded FETHPC and CoE projects already increased the industry-research interaction, within the EU HPC cPPP and with a significant support from EXDCI. ETP4HPC is now suggesting including “Extreme Scale Demonstrators” in the 2018-2020 Work Programme, so as to integrate successful H2020 R&D projects outcomes into first-of-a-kind HPC systems including significant European technology. It is recommended that EXDCI considers and actively supports the articulation between the European Open Science Cloud (and its underlying European Data Infrastructure), FETHPC projects incl. Extreme Scale Demonstrators, and this IPCEI. Alignment of timelines and milestones in terms of pre-Exascale and then Exascale systems in this global perspective is a major issue. EXDCI can bring significant added value to this process, via the mobilization of stakeholders, and by leveraging its outcomes in terms of a global vision and recommendations from technologies to applications.

## 5.1 Recommendation

It is recommended that EXDCI considers and actively supports the articulation between the European Open Science Cloud Initiative (and its underlying European Data Infrastructure), FETHPC projects incl. Extreme Scale Demonstrators, and IPCEI.

## 6 Paving the Way from EsD Development towards Applications

*Recommendation issued from EXDCI WP2*

The EsD calls will have a high dependency on the projects started by the H2020-FET-HPC-2014 and H2020-FET-HPC-2016-2017 projects regarding their results and timing. The portfolio of accepted projects in these calls must provide a sound technology basis for building EsDs, and the accepted projects should be actively encouraged to foster cross-project interlock. The structure of the WP16/17 should support cross-project integration, with particular regards to IP visibility and licensing clarity. Lack of coherence between accepted projects, too many disjoint focus areas, and insufficient technology options and readiness might otherwise jeopardise the success of the EsD calls.

It is proposed that EsD calls should be announced within the 2018-2019 work programme. It is proposed that the EsD project calls will have a funding envelope compatible with a spending of €20-40M (30-50% R&D and 50-70% parts costs) per EsD project for phase A (Development, Integration and Testing, involving little or no basic technology research projects) and €3-6M for phase B (Deployment and Use) to cover utilities, operation-manpower and maintenance. Phase A should have a duration of 18-24 months and phase B of 24 months with a validation feedback checkpoint after 9 months. Therefore, total project duration of 32-48 months is envisaged.

The EsD characteristics will need to be further refined, however, they should deliver a high enough TRL to support a stable and effective production environment in their respective Phase B. Their impact on commercial product lines is not expected before 2020. Looking at the hardware characteristics, it is expected that the EsD architectures target scalability of applications up to 200 PFlop/s. This and other hardware characteristics (energy efficiency, I/O bandwidth, resiliency, etc.) will be detailed in the 2017 release of the SRA, also taking into account results from the FETHPC projects and requirements from the CoEs.

The ETP4HPC recommends suitable projects to involve four types of partners for EsD projects: integrators, technology providers, application owners and HPC centers.

### 6.1 Recommendation

It is recommended that development and deployment of ambitious Extreme scale Demonstrator projects should pave the way to advance Europe's competence in research, development and integration of competitive High Performance Systems technology. These projects need new implementation instruments in the area of application & technology co-design and deployment to enable to create solutions for a large variety of complex scientific problems.

## 7 Encouraging Commercial Relationships between SME and Industry through European Projects

*Recommendation issued from EXDCI WP4*

In the frame of WP4 of the EXDCI project, we interviewed European startups and SMEs in order to understand whether there are intrinsic characteristics of the HPC-ecosystem making it particularly difficult for startups to emerge and for SMEs to grow. **One recurrent topic in the 13 interviews that we conducted was about “finding the first client/ the reference client”.**

Such a reference client can be very helpful for the final product development phase and for the product launch itself. They are typically early adopters of the novel technology offered by the startup, accepting sometimes non-finalized products. As such, they help the startup to understand the customer’s needs. In an ideal case, those reference clients contribute to the final development phase of the product with know-how and experience from a user’s point of view. Further, the first client may help the startup to confirm (or to adjust) its pricing strategy and to gain insight into purchasing procedures. And once the product is launched, the product benefits from support via the client’s *renommée*.

In HPC, this reference client has an even higher importance for getting involved in larger HPC systems, i.e. those classified within the Top500<sup>3</sup> list of HPC systems. A typical criteria for being selected for a large system is to have already contributed to a Top500-machine, which leads to a vicious circle: You won’t get accepted for a Top500-machine as long as you have not been selected for a Top500-machine. So finding a reference client is crucial in this set-up.

To find such an early client is generally difficult for startups. However, it seems particularly difficult for HPC startups. The first reason is that in most cases HPC startups offer highly-technological products or services. The group of potential customers that is able to take the role of an expert-adviser is small as to the high technological level (compared for example to a startup in online-sales).

A second reason may be the nature of the HPC market itself: public entities take a considerable part of the market, based on public procurement procedures. As pointed out in D4.2, those procedures request effort, experience, and time - assets a startup is often lacking. Thus, the collaboration with a larger industrial partner is considered useful for tenders.

Within European R&I projects, startups and larger companies get acquainted and collaborate in a less competitive context with complementary skills. European research projects are thus a way to build friendly connections between startups and SMEs on the one hand and larger companies on the other hand. This has also been pointed out by the SME- working group of ETP4HPC. In their 2015 position paper, they advocate for “co-design and co-development partnerships”. We share the belief that the full potential of those friendly connections is not tapped yet and are convinced that they are a solid basis for commercial relations.

## 7.1 Recommendation

Larger companies should be strongly encouraged to extend their collaboration with start-ups and SMEs beyond European R&I actions and to engage in direct business relations.

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<sup>3</sup> <https://www.top500.org>  
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## 8 Big Data and Extreme Scale International Initiative

*Recommendation issued from EXDCI WP6*

The convergence of scientific HPC systems towards Numerical Laboratories (extreme data combined with extreme computing) requires new insights into the manner major international scientific initiatives are organized. In particular, it is expected that the current focus on compute capabilities will shift towards data acquisition (from sensors, instruments, social media, etc.) and data analytics capabilities. Sharing such assets at a global level requires broader integration of international research.

The European Open Science Cloud (EOSC), the European Cloud Initiative (ECI) and the IPCEI (see Section 3) are three pillars of the Digital Single Market strategy of the European Commission. EXDCI can play a role in ensuring that these initiatives maintain coherency with FET-HPC projects and, at the same time, with international roadmapping efforts that are regularly discussed in the BDEC (Big Data and Exascale Computing) forum.

The tendency is now focused on the **convergence** between “big data” and “big compute”. This can only be achieved at a global scale and requires international coordination. Initiatives such as Belmont Forum and Future Earth can provide excellent use cases for convergence and subsequently inform global policy on future investments in e- and data-infrastructures. There are also direct consequences for data policies and for human capacity development.

One example is smart cities that require data analysis, sensor processing, simulation and machine learning, all of this in a context of big data. These data need to be analyzed rapidly and hence coupled with adaptive HPC systems, workflows and technologies. There are a large number of data and data-intensive computing challenges in Earth and Universe sciences. The EU VERCE project has addressed some of these.

### 8.1 Recommendation

The recommendation aims at encouraging the EU to facilitate future international collaborations involving compute-intensive exploitation of scientific data, as advocated by the BDEC consortium. This should be an integrated action, within the EOSC (European Open Science Cloud) initiative, that could associate other major international initiatives in "Data Management and e-Infrastructures", notably those of Belmont Forum and Future Earth.

## 9 Concerted approach to HPC training in Europe

*Recommendation issued from EXDCI WP5*

The EC has stated the aim of attaining European leadership in the supply and use of HPC systems and services by 2020. European research is successfully delivering many technological advances, but no matter how good any new technology may be, supply cannot lead to widespread take-up and effective use unless high-quality training is available and can be easily identified by those who need it.

EXDCI aims to consolidate a synchronized European HPC Community, and one aspect of this is to establish a community of training providers. By bringing the training providers together

into a single community, training gaps can be identified, duplication of effort can be spotted, and resources can potentially be pooled to develop new joint training material and a coherent course timetable, whether for “in person” courses or online teaching.

EXDCI works closely with a disparate community of European technology stakeholders and applications stakeholders, including academic and commercial HPC developers and users, as well as with experts outside of Europe. Many of these stakeholders either provide training and/or have a need for it. EXDCI is therefore well-placed to match those who need training with the experts who can provide it.

As a result of work carried out under EXDCI, we propose to compile a comprehensive and easy-to-find on-line catalogue of existing courses and training material, making this easily accessible by the HPC community at large. A Training Gap Analysis will inform a Training Roadmap for interdisciplinary working. The aim is to bring together training providers and those who need training, from both academic and commercial arenas, covering all layers of the European HPC and Big Data ecosystem, encompassing both hardware and software, including programming models and applications, and covering traditional HPC and emerging fields such as disruptive technologies, data analytics and machine learning, in order to provide complete and comprehensive training opportunities for the whole community.

## 9.1 Recommendation

A concerted approach to HPC training in Europe must be put in place to allow rapid uptake by developers and end-users alike of the new HPC technologies currently being developed through numerous European initiatives. This will allow the European HPC community to keep up-to-date with new technologies and techniques and to become confident in their use, thus helping to secure Europe’s competitive edge in the international arena.

# 10 Improving Capitalization of FETHPC and CoE Results

*Recommendation issued from EXDCI WP4*

FETHPC projects are major producers of novel technologies. Most of these innovative results are taking the form of new software or hardware components. Many of them aim at being proof of concepts, solely for the sake of research, that do not need to survive beyond the projects. Other components may deserve to be pushed further to reach a community of users and/or a market. This is rarely achievable in the timeframe of the projects.

The series of Mont-Blanc projects (<http://www.montblanc-project.eu>) is an interesting example. Started in 2011 the first project established the foundation of the approach. It is only today in 2016 that the results are starting to reach the market via Bull-Atos, who took over the coordination of the third Mont-Blanc project. In this case, continuing effort in a structured manner via FET projects and industrial partnerships has made it possible to potentially generate new commercial revenue. Of course, there is not one unique way to ensure technology development on the long haul until it gets to the users.

For every innovative result the right pathway must be found (new projects, investors, open-source communities, startups...). It is very rare that a new technology reaches the market in an organic and effortless manner. Resources and dedicated people are needed all the way and beyond.

A plan for reaching end users must be established very well in advance of the end of the project. Therefore we recommend that specific best practices and support actions be set up in a systematic way to organize market/community-reaching plan within an early stage of projects. A large variety of stakeholders (private and public) should be involved in these actions.

## 10.1 Recommendation

We recommend that specific best practices and support actions be set up in a systematic way to organize plans for reaching end users and bringing technologies to market within early stage of FETHPC projects.

# 11 Incentives to Increase EU Stakeholders Participation in Standards Initiatives

*Recommendation issued from EXDCI WP4*

International standards de-facto-standards are strongly influencing research experiments, further developments, and industrial products. In the HPC domain they provide long-term visibility for developers, and lay a widely shared and agreed upon basis for further developments. As such, they are a critical basis for large software and hardware products.

In contrast to some application domains such as represented by ETSI or the OpenFOAM initiative (now driven by the ESI group), the European HPC community is not much involved in technological-oriented standards specification efforts. For instance, in OpenMP<sup>4</sup> only ARM is a Permanent Members of the Architecture Review Board (ARB) (13 members), the most influential committee of the association. Europe's representation is stronger at the Auxiliary Members level of the ARB (14 members): BSC, Bristol University, EPCC, and RWTH Aachen University.

In the case of MPI Forum<sup>5</sup>, European stakeholders are also not very involved in the specification of MPI 4.0. Over 17 working groups chairs, only 3 are from European institutions.

Regarding the Big Data community, whose technology is becoming crucial to future HPC applications, the EU stakeholder influence is close to nil. For instance EU stakeholders are not present in the Hadoop Project Management Committee<sup>6</sup>. Overall there is a lack of involvement in technology-oriented initiatives contrary to application-oriented initiatives

This absence has multiple consequences for Europe's position in HPC: First, standards specifications are by construction best suited for the products and technologies represented by the most active members. Not being involved thus means the necessity to adapt to choices and decisions taken by parties following their interests and objectives. Second, not being involved

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<sup>4</sup> <http://openmp.org/wp/about-openmp/>

<sup>5</sup> <http://mpi-forum.org/mpi-40/>

<sup>6</sup> <https://hadoop.apache.org/who.html>

in the specification effort introduces a delay in the acquisition of the corresponding knowledge (it is usually very clear to committee members which direction is being taken year(s) in advance). The effort to catch-up is then important and there is an inherent delay to reach the market.

The low degree of involvements is not due to a lack of competencies in the EU ecosystem. We believe that it is mainly due to a lack of incentive for actions that have long-term effect and require a strong commitment. Indeed, being influential in these bodies implies the need to allocate time and resources for highly skilled experts to attend meetings, as well as for development engineers to perform the necessary experiments to build the technical contributions.

If the current status is to be changed, i.e., to increase participation in standardization bodies, it is mandatory to define efficient incentives.

## 11.1 Recommendation

Incentives for EU stakeholders to participate in international standardization in the extreme scale computing and big data must be increased. New forms of support must be invented to ensure the presence of high-profile scientists and EU industry stakeholders in existing and emerging initiatives.

## 12 Access to Advanced Technologies

*Recommendation issued from EXDCI WP4*

Emerging technologies are strongly influencing software and hardware design. Many research projects are critically depending on early access to these technologies to ensure that they are performed in a timely fashion. Late access is strongly degrading competitiveness of an ecosystem (lack of trained people, software not up-to-date...). Being late on a highly technological market, such as the HPC one, usually means low profits or worse disappearance from the market. For instance, when GPGPU appeared on the market, only single precision floating-point operations were available. Some groups decided to provide double precision by developing software libraries. By the time the library was operational, new GPGPUs with double precision capabilities were on the market, making *de facto* the libraries obsolete. Roadmap knowledge and access to advanced technologies are of paramount importance when planning R&D activities.

Unfortunately, access to advanced technologies is dependent only on the developer/provider wishes and strategy. Most HPC technologies originating in the USA, the EU, especially the academic community, has many difficulties to get access (even under NDA) to new innovations. The result is a research that is based on off-the-shelf products and by essence the leadership is biased towards non-EU researchers. While some topics are insensitive to such considerations, research in HPC is by essence very linked to the most advanced technology.

A given research team is rarely in position to have enough incentive (except of course if the innovation is intended to go the other way) or funding to be provided access to the most advanced technology. Only a heavyweight stakeholder (e.g. PRACE) can have an influence great enough to change the balance of power. Therefore we recommend that the EU



commission creates a body able to facilitate access (technical and legal) to advanced technologies for research groups.

## **12.1 Recommendation**

We recommend that the EU commission ecosystem creates a body able to facilitate access (technical and legal) to advanced technologies for research groups.

## **13 Conclusion**

This report presents a set of recommendations aiming at increasing the European Research instruments, the R&D efficiency as well as the industry competitiveness. They have been created after collecting information from numerous stakeholders of the HPC ecosystem.

This is the first version of this EXDCI deliverable. It is intended to go back the community, in particular the FETHPC projects and the CoEs to complement this version and produce second version of this deliverable.