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List of Acronyms and Abbreviations

aisbl	Association internationale sans but lucratif (legal form of the PRACE-RI)
ACENET	Advanced Computing Research in Atlantic Canada
BoD	PRACE Board of Directors
BDA	Big Data
BDEC	Big Data and Extreme Computing
CEF	Coordinating European Facilities
CHPC	Centre for High Performance Computing, South AfricaCoEs Centres of Excellence (in HPC)
CoE	Centre Of Excellence in HPC
CRM	Customer relationship management
DEISA	Distributed European Infrastructure for Supercomputing Applications, former European consortium (2002–11) of national supercomputer centres
DoA	Description of Action (formerly known as DoW)
DSM	Digital Single Market
EC	European Commission
ECI	European Cloud Initiative
EDI	European Data Initiative
EESI	European Exascale Software Initiative
EESI2	Follow-up project of EESI
EGI	European Grid Initiative
ELI-DC	European Laser Institute
ELIXIR	Integrated computing services for European researcher, Hinxton, UK
EMBL	European Molecular Biology Lab, Heidelberg, Germany
ENES	European Network for Earth System modelling
EOSC	European Open Science Cloud
EPOS	European Plate Observing System
ERIC	European Research Infrastructure Consortium
ESA	European Space Agency, Paris, France
ESFRI	European Strategy Forum on Research Infrastructures
ESRF	European Synchrotron Radiation Facility, Grenoble, France
ETP4HPC	European Technology Platform for High Performance Computing
EuroFusion	
EUDAT	European Data project (see https://eudat.eu/what-eudat)
EuroHPC	see http://eurohpc.eu
EXDCI	European Extreme Data & Computing Initiative
FET	Future and Emerging Technologies

FETHPC	Future and Emerging Technologies in HPC
GDP	Gross Domestic Product
GÉANT	Collaboration between National Research and Education Networks to build a multi-gigabit pan-European network. The current EC-funded project as of 2015 is GN4
GP	General Partners aka Non Hosting Members of Tier-0 system
Graphene	FET flagship Graphene
HM	PRACE Hosting Members
HPB	The Human Brain Project
HPC	High Performance Computing; Computing at a high performance level at any given time; often used synonym with Supercomputing
HPDA	High Performance Data Analytic
HP-SEE	High-Performance Computing Infrastructure for South East Europe's
ILL	Institut Laue-Langevin, Grenoble, France
IPCEI	Important Project of Common European Interest (HPC-BDA)
IPs	PRACE Implementation Projects
IPR	Intellectual Property Rights
ITER	International Thermonuclear Experimental Reactor
KPI	Key Performance Indicator
LinkSCEEM	Linking Scientific Computing in Europe and Eastern Mediterranean
MB	Management Board (highest decision making body of the project)
MD	Managing Director
MOOC	Massively Open Online Course
MoU	Memorandum of Understanding
Opex	Operational Expenditure
PATC	PRACE Advanced Training Centres
PRACE	Partnership for Advanced Computing in Europe; Project Acronym
PRACE 1	PRACE agreement for the Initial Period of five years
PRACE 2	The upcoming next phase of the PRACE Research Infrastructure following the initial five year period
RI	Research Infrastructure
RIKEN	Kokuritsu Kenkyū Kaihatsu Hōjin Rikagaku Kenkyūsho, Japan
SHAPE	SME HPC Adoption Programme in Europe
SKA	Square Kilometer Array, large scale radio telescope project
SME	Small and Medium Enterprise
SSC	PRACE Scientific Steering Committee
SWG	PRACE Strategy Working Group
TB	Technical Board (group of Work Package leaders)
Tier-0	Denotes the apex of a conceptual pyramid of HPC systems. In this context the Supercomputing Research Infrastructure would host the Tier-0 systems
Tier-1	National or topical HPC centres
UF	PRACE User Forum
VAT	Value Added Tax
VI-SEEM	Virtual Research Environment (VRE) in Southeast Europe and the Eastern Mediterranean (SEEM)
VISIONAIR	The Vision Advanced Infrastructure for Research, Grenoble, France
WP	Work Package
XSEDE	Extreme Science and Engineering Discovery Environment, NSF-funded virtual organization that integrates and coordinates the sharing of advanced digital services, USA

List of Project Partner Acronyms

BADW-LRZ	Leibniz-Rechenzentrum der Bayerischen Akademie der Wissenschaften, Germany (3rd Party to GCS)
BILKENT	Bilkent University, Turkey (3rd Party to UYBHM)
BSC	Barcelona Supercomputing Center - Centro Nacional de Supercomputacion, Spain
CaSToRC	Computation-based Science and Technology Research Center, Cyprus
CCSAS	Computing Centre of the Slovak Academy of Sciences, Slovakia
CEA	Commissariat à l'Energie Atomique et aux Energies Alternatives, France (3rd Party to GENCI)
CESGA	Fundacion Publica Gallega Centro Tecnológico de Supercomputación de Galicia, Spain, (3rd Party to BSC)
CINECA	CINECA Consorzio Interuniversitario, Italy
CINES	Centre Informatique National de l'Enseignement Supérieur, France (3rd Party to GENCI)
CNRS	Centre National de la Recherche Scientifique, France (3rd Party to GENCI)
CSC	CSC Scientific Computing Ltd., Finland
CSCS	See ETHZ
CSIC	Spanish Council for Scientific Research (3rd Party to BSC)
CYFRONET	Academic Computing Centre CYFRONET AGH, Poland (3rd Party to PNSC)
EPCC	EPCC at The University of Edinburgh, UK
EPSRC	Engineering and Physical Sciences Research Council, funding agency, UK
ETHZurich (CSCS)	Eidgenössische Technische Hochschule Zürich – CSCS, Switzerland
FIS	Faculty of Information Studies, Slovenia (3rd Party to ULFME)
GCS	Gauss Centre for Supercomputing e.V., Germany
GENCI	Grand Equipement National de Calcul Intensif, France
GRNET	Greek Research and Technology Network, Greece
INRIA	Institut National de Recherche en Informatique et Automatique, France (3rd Party to GENCI)
IST	Instituto Superior Técnico, Portugal (3rd Party to UC-LCA)
IT4I	IT4Innovations National supercomputing centre at VŠB-Technical University of Ostrava, Czech Republic
IUCC	INTER UNIVERSITY COMPUTATION CENTRE, Israel
JKU	Institut fuer Graphische und Parallele Datenverarbeitung der Johannes Kepler Universitaet Linz, Austria
JUELICH	Forschungszentrum Juelich GmbH, Germany
KIFU	Governmental Information Technology Development Agency, Hungary
KTH	Royal Institute of Technology, Sweden (3rd Party to SNIC)
LiU	Linkoping University, Sweden (3rd Party to SNIC)
NCSA	NATIONAL CENTRE FOR SUPERCOMPUTING APPLICATIONS, Bulgaria
NTNU	The Norwegian University of Science and Technology, Norway (3rd Party to SIGMA2)

NUI-Galway	National University of Ireland Galway, Ireland
PRACE	Partnership for Advanced Computing in Europe aisbl, Belgium
PSNC	Poznan Supercomputing and Networking Centre, Poland
RISCSW	RISC Software GmbH, Austria
RZG	Max Planck Gesellschaft zur Förderung der Wissenschaften e.V., Germany (3rd Party to GCS)
SIGMA2	UNINETT Sigma2 AS, Norway
SNIC	Swedish National Infrastructure for Computing (within the Swedish Science Council), Sweden
STFC	Science and Technology Facilities Council, UK (3rd Party to EPSRC)
SURFsara	Dutch national high-performance computing and e-Science support center, part of the SURF cooperative, Netherlands
UC-LCA	Universidade de Coimbra, Laboratório de Computação Avançada, Portugal
UCPH	Københavns Universitet, Denmark
UHEM	Istanbul Technical University, Ayazaga Campus, Turkey
UiO	University of Oslo, Norway (3rd Party to SIGMA2)
ULFME	UNIVERZA V LJUBLJANI, Slovenia
UmU	Umea University, Sweden (3rd Party to SNIC)
UnivEvora	Universidade de Évora, Portugal (3rd Party to UC-LCA)
UPC	Universitat Politècnica de Catalunya, Spain (3rd Party to BSC)
UPM/CeSViMa	Madrid Supercomputing and Visualization Center, Spain (3rd Party to BSC)
USTUTT-HLRS	Universitaet Stuttgart – HLRS, Germany (3rd Party to GCS)
WCNS	Politechnika Wroclawska, Poland (3rd Party to PNSC)

Executive Summary

This deliverable updates the analysis of the stakeholder management performed by PRACE-4IP project within the context of the transition from "PRACE 1" to "PRACE 2". PRACE 2, the second phase of the pan-European Research Infrastructure (RI) took over from PRACE agreement for the Initial Period - so-called PRACE 1 - for the 2017 - 2020 period. A first analysis has been documented within a previous deliverable [54] issued in February 2017, but since then major initiatives have moved forward, that will reshape the European HPC ecosystem: the main ones are the European Data Initiative (EDI), the European Open Science Cloud (EOSC) and the EuroHPC initiative. This deliverable will complete previous analysis in light of the changes these new initiatives could have on our relationship with our stakeholders.

This work follows analyses of stakeholder management, performed within PRACE Preparatory Phase project (PRACE-PP) in 2008 [15],[16], and the update within PRACE-3IP project in 2014 [18]. Whereas previous deliverables were focused on identification of core stakeholders of the project and on the legal aspect of relationship with other entities, this one is focused on the evolution of the HPC ecosystem. This could be summarised as a global race to Exascale (potentially available at the beginning of next decade). And everybody around the world is accelerating pace on that race (at least for USA, China and Japan, that decided to afford the huge cost of tools, considered more strategic than ever). Recent evolutions of the European ecosystem are taking shape as well, with the three pillars of the European Commission (EC) strategy for High Performance Computing (HPC) – infrastructures, technologies, applications. Within the global framework of a Digital Single Market (DSM) strategy for Europe, announced by the EC in April 2016, we explore how the (on-going) EOSC initiatives will impact our way to engage with our stakeholders. The definition of "rules of engagement" to EOSC will define how PRACE services would/could be understood by our users, and offer new ways to engage with emerging communities of HPC users. We also provide early analysis on potential services provided by EDI and on how the different options for a Governance structure of EDI could impact our relations with our stakeholders, especially with GÉANT, in the context of building a world-class converged pan-European HPC, Big-Data, network and Cloud Ecosystem.

Links with various categories of stakeholders are described and commented – other compute infrastructures in Europe or worldwide, different kinds of European projects or initiatives (flagships, other kinds of research infrastructures, H2020 projects etc.); user communities including new or emerging areas; funding agencies and policy makers; SMEs for which PRACE SHAPE programme offered an HPC adoption strong support.

The latest MoUs signed between PRACE RI or PRACE projects and these partners are reminded, a complete list of them is provided in the Annex.

1 Introduction

This deliverable provides an analysis of the stakeholders management analysis performed by PRACE-4IP project, within the context of "PRACE 2", taking into account the evolution of the HPC European ecosystem, with high impact initiatives such as the European Data Initiative (EDI), the European Open Science Cloud (EOSC) and the EuroHPC initiative.

This follows previous analyses of stakeholder management, performed within PRACE Preparatory Phase project (PRACE-PP) in 2008 [15], [16], with a first update within PRACE-3IP project in 2014 [18], and a second one [54] issued in February 2017, within the context of the transition from "PRACE 1" and "PRACE 2" at the early stage of the implementation process of the second period of operations of the PRACE pan-European Research Infrastructure (RI), so-called PRACE 2. PRACE 2 took over from PRACE agreement for the Initial Period, so-called PRACE 1, for the 2017 - 2020 period. Whereas previous deliverables were focused on the early identification of core stakeholders of the project and on the legal aspects of relationships with other entities, this one is focused on the latest evolutions of the HPC ecosystem, with strong European initiatives (EDI, EOSC, and EuroHPC) on a global race to Exascale, with an accelerating pace (at least for USA, China and Japan, with very important amount of funding), and a European ecosystem that is taking shape, with the three pillars of the EC strategy for HPC:

- HPC infrastructures and services, with the Partnership for Advanced Computing in Europe (PRACE);
- HPC technologies via the Future and Emerging Technologies (FETHPC) programme / and with the advisory role of European Technology Platform for High Performance Computing (ETP4HPC), and
- HPC applications via the establishment of Centres of Excellence (CoEs), funded by the e-Infrastructures programme.

The launch of a Digital Single Market (DSM) strategy for Europe, announced by the EC in April 2016, provides a new horizon, with the proposed concept of European Cloud Initiative (ECI) encompassing the notions of an underlying federated pan-European Data Infrastructure (EDI, as a rich infrastructure with computing, data storage, access and processing, and networking capabilities), together with a European Open Science Cloud (EOSC) to organise access and delivery modes for scientists, industrial users, public services and even toward single citizen. In April 2017 an ambitious pan-European initiative called EuroHPC started [59], now signed by 13 countries (Belgium, Bulgaria, Croatia, France, Germany, Greece, Italy, Luxembourg, Netherlands, Portugal, Slovenia, Spain and Switzerland) and the EC, towards the funding of a pan-European HPC infrastructure for science, industry and public services This encompasses the co-funding and exploitation of two pre-Exascale systems in 2020/2021 and 2 Exascale systems in 2022/2023, fostering the use of European technologies.

At the European and International levels PRACE strives to establish a vivid community around HPC services and competencies. Part of this work is to create networks and cooperation with other scientific, research, industrial and HPC-related projects, programmes and organisations. This encompasses work with the US XSEDE initiative (joint PRACE and XSEDE allocation calls, joint organisation of international HPC Summer schools, including Japan RIKEN and Compute Canada), a MoU firmed with CHPC (Centre for High Performance Computing) in South Africa and a coming one with the The Pawsey Supercomputing Centre in Australia, both entities being strongly involved into the SKA (Square Kilometer Array) large scale radio telescope project.

Other examples include transnational cooperation such as with ITER fusion project, or with European regional projects, such as LinkSCEEM within the Southern Europe region; links with other H2020 projects, such as Graphene and Human Brain Project (HBP) flagships, Future and Emerging Technology (FET) flagships. PRACE also engaged within fruitful collaborations with other RIs and e-RIs (such as GÉANT, EUDAT or EGI for instance).

Many projects supported by PRACE have links with large scale instruments or European initiatives, such as ENES, EC-EARTH, ESO, CERN, Van Allen Belt Probes, LASERLAB-EUROPE, and the Herschel telescope. PRACE-4IP project has a specific task for analysing new prototypal innovative services, for instance with large-scale scientific instruments.

PRACE SHAPE (SME HPC Adoption Programme in Europe) programme is of particular importance for the relation of PRACE with the industrial world: it brings together PRACE HPC sites and experts with SMEs using HPC. This pan-European programme supporting HPC adoption by SMEs is a very successful initiative with already strong results reported within this document (chapter 4.7.5).

Other user groups of special interest are the emerging communities in humanities and social sciences (such as paleontology). Such communities bring and need new uses of HPC, often a combination of “classical” numerical modeling with data analytics, Big Data or Artificial Intelligence. These targets require specific care and efforts including training, but will also teach us a lot.

Funding bodies and policy making organisations are key stakeholders, and they are needed to provide sustainable funding and ensure that HPC, as a strategic tool in Europe, is handled appropriately.

To ensure the appropriate connection with these very diverse stakeholders, numerous actions have been put in place, coordinated by the Board of Director (BoD) of PRACE. The PRACE communication team acts both at the level of PRACE RI and PRACE projects, and specific bodies are in charge of providing advice and guidance from our users: a User Forum (UF), a Scientific Steering Committee (SSC) and an Industrial Advisory Committee (IAC).

A list of Memorandums of Understanding (MoUs), signed between PRACE RI or PRACE projects and these partners is provided in annex.

In this document:

- Chapter 2 defines some concepts and elements of theory useful for stakeholder management, linking them to the PRACE ecosystem;
- Chapter 3 gives an overview of local (European) and global (worldwide) HPC landscape, as a general setting of PRACE context; it has been fully updated with regard to the new development of EOSC, EDI and EuroHPC;
- Chapter 4 describe the different links and relationships established by PRACE;
- Chapter 5 provides a short conclusion.

2 Introduction to Stakeholder Management and HPC ecosystem

2.1 Historical background of PRACE

PRACE (Partnership for Advanced Computing in Europe), the pan-European Research Infrastructure (RI) for High Performance Computing (HPC) is established as an international not-for-profit association (aisbl) with 25 member countries: Belgium, Bulgaria, Cyprus, Czech Republic, Denmark, Finland, France, Germany, Greece, Hungary, Ireland, Israel, Italy, Luxembourg, The Netherlands, Norway, Poland, Portugal, Slovakia, Slovenia, Spain, Sweden, Switzerland, Turkey and the United Kingdom. Austria left the consortium. Its mission is to enable high impact scientific discovery and engineering research and development across all disciplines to enhance European competitiveness for the benefit of society. To fulfill this mission, the collaboration and commitment of a wide range of stakeholders is very important. The work to identify them and define the proper interactions has initiated during the Preparatory Phase of 2008 and continued during PRACE-3IP project (see [15][16][18]).

PRACE-4IP project involves participants from HPC Centres from these 25 countries. These partners constitute our internal stakeholders, whereas PRACE academic, industrial and SMEs users constitute our core group of external stakeholders. PRACE seeks to realize this mission by offering them world class computing and data management resources and services through a single and fair pan-European peer review process for open research.

PRACE also seeks to strengthen the European users of HPC in industry through various initiatives. PRACE has a strong interest in improving energy efficiency of computing systems and reducing their environmental impact.

The computer systems and their operations accessible through PRACE are provided by 5 PRACE hosting members (BSC representing Spain, CINECA representing Italy, ETHZ/CSCS representing Switzerland, GCS representing Germany and GENCI representing France).

This work is not performed in isolation, but in a complex and highly competitive global environment, as highlighted by the EC communication “High-Performance Computing: Europe's place in a Global Race” [33], the numerous actors that play a role within this ecosystem are our stakeholders.

2.2 Historical background of Stakeholder Management Theory

Stakeholder Management theory found its root in the work of R. Edward Freeman in the1984 book “Strategic Management: A stakeholder Approach” [27], with a latter synthesis with its 2010 book “Stakeholder Theory: The State of the Art” [28]. In short Stakeholder Management theory is a theory of organisational management and business ethics that was built in opposition to the traditional, more narrowed view of a company, the shareholder view, that defines the primary goal of a company as creating value for shareholder. In contrast, Stakeholder Management theory defines the goal of an organisation as managing its multiple interactions, in a complex environment, with its multiple so-called stakeholders, in order to create value to a wider spectrum of parties, including shareholder among others. Managing well these many stakeholders being a condition for achieving the organisation goals/mission, and by thus producing a sustainable growth of revenue, this is now seen as a positive side effect and not the ultimate and solely target. This is an important change of perspective.

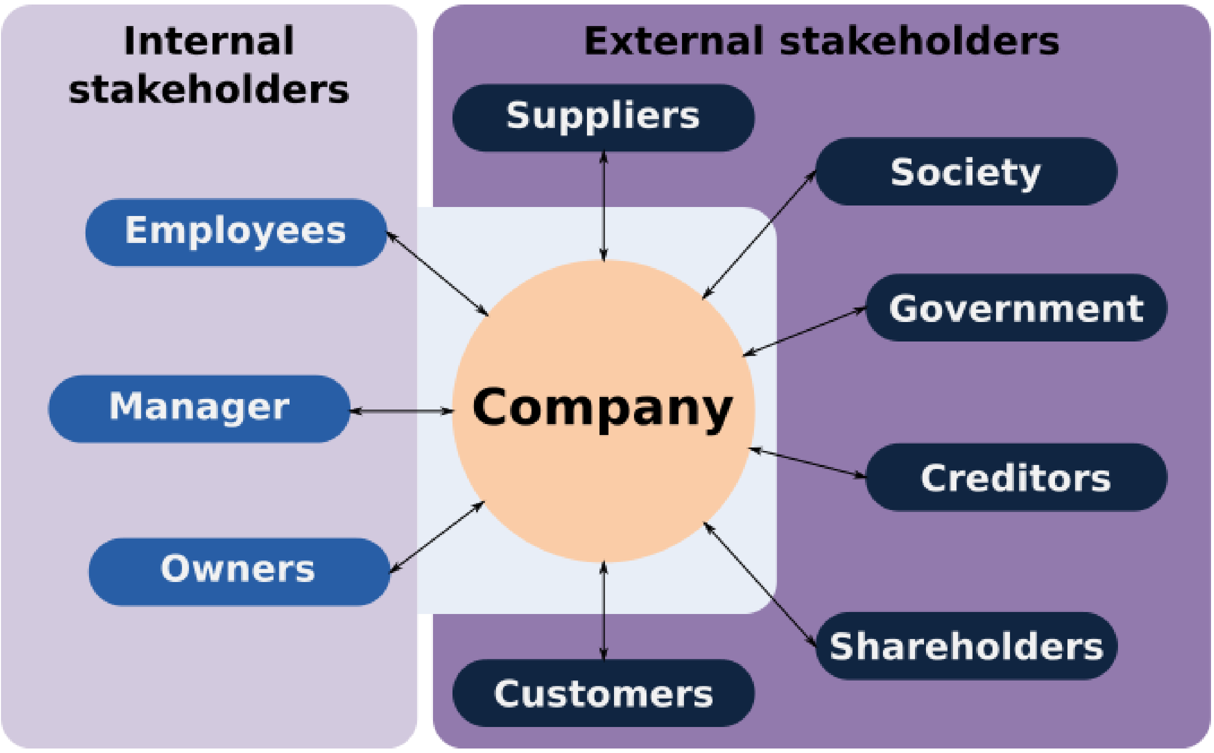

Figure 1: Example of typical internal and external stakeholders (Source: Wikipedia Commons)

From this origin as a tool oriented towards Company management, Stakeholder Management theory has proved its usefulness in a wide larger area, including governmental and other public organisations along with NGOs. The Stakeholder Management theory offers a framework to characterise interaction with a wide spectrum of stakeholders, help stakeholder identification, prioritization of stakeholder, understanding of stakeholder concern and engaging fruitful communication and interaction aiming at a mutual benefit. And when mutual benefit could not be met at the appropriate level with all stakeholders it allows at least a better understanding of legitimate (potentially conflicting) concern.

2.3 Application of Stakeholder Management Theory for PRACE

Application of Stakeholder Management theory for PRACE is manifold. High-Performance Computing is a tool used by a very wide variety of scientific fields, if not (yet) by every one of them, with growing emerging community such as Medicine/Drug industry and Human Sciences, with the increasingly link between HPC, Big-Data, HPDA and Deep-Learning widening the scope of application of HPC. The drawback of this very wide community of users is that our Research Infrastructure is not backed-up by a strong community, whereas more specialised instruments, such as telescope or Large Hadron Collider for instance, have a clear unified community dedicated to promote their infrastructure. On the other hand, HPC tools are key to address many highly important societal issues, from climate change to safer aircraft, cleaner engines, or advancement of medicine and drugs, that are of utmost importance for the (well-informed) citizens, who could "promote" the use of HPC, or at least agree with the public costs it requires, "IF" they are properly informed and understand the link between these tools and their interest. Within our context, the relationship with our stakeholders, who are also members of EOSC (or future members of EOSC and potential users of PRACE), must be compliant with EOSC rules of engagement, who are in the process of being designed. Similarly, the relationship with stakeholders who are potential members of EuroHPC must be shaped in a way that facilitates the evolution of these projects / infrastructures. This could move the boundary between internal and external stakeholder.

3 The HPC Ecosystem

The following chapter will give a broad description of the HPC ecosystem on both European and global level. This will also provide an overview of the various external stakeholders.

3.1 Introductory HPC ecosystem overview

“To out compute is to out compete" is a commonly used punch line and this applies to the European HPC strategy.

Over the last decades, the availability and usability of HPC systems has become one of the determining factors for the progress of science. The accuracy of scientific analyses, the quality of scientific results and the potential of national and international collaborations are more and more dependent on the available computing infrastructure. Thus, the EU has set up a European HPC strategy [34] and established a strong cooperation with the HPC stakeholders. A first new element was a contractual Public-Private Partnership on HPC signed in 2014 (cPPP on HPC [35]) between the EC and the European Technology Platform for HPC (ETP4HPC [29]). This cPPP on HPC contributed to an ambitious R&I funding strategy [35] based on three pillars, together with PRACE launched on 2010, addressing:

- HPC facilities via the Partnership for Advanced Computing in Europe (PRACE [6]), established since October 2012 and put forward with PRACE 2;
- HPC technologies via the Future and Emerging Technologies (FETHPC [38]) programme, endorsing the recommendations of ETP4HPC [56];
- HPC applications via the establishment of Centres of Excellence (CoEs), funded by the e-Infrastructures programme [39].

To support and coordinate the collaboration and interactions of these 3 pillars, ETP4HPC together with PRACE and partners from EESI2 (see [40]) have initiated the European eXtreme Data and Computing Initiative (EXDCI [41]) (see Figure 2). A proposal for the second phase of this project has been submitted, with important updates in the coordination between PRACE, ETP4HPC, CoEs and FETHPC projects (see 6.1 Annex 1 for a complete list).

On 19 April 2016, the European Commission published the “European Cloud Initiative - Building a competitive data and knowledge economy in Europe” [55],

The European Cloud Initiative (ECI) builds on the Digital Single Market (DSM) Strategy, which aims to maximise the growth potential of the European digital economy. It aims to develop a trusted, open environment for the scientific community for storing, sharing and re-using scientific data and results, the **European Open Science Cloud** (EOSC). It aims to deploy the underpinning super-computing capacity, the fast connectivity and the high-capacity cloud solutions they need via a **European Data Infrastructure** (EDI). Focussing initially on the scientific community, the user base will be expanded to the public sector and to industry, creating solutions and technologies beneficial for all areas of the economy and society. In order to achieve this will require a collaborative effort open to all those interested in exploiting the data revolution in Europe as an essential component of global growth.

Within this context, PRACE is participating to the EOSCpilot project, contributing to the work package on the future Governance of EOSC and collaborating with GÉANT, in order to pave the path of the future European Data Infrastructure (EDI).

3.2 Description of the EU HPC Ecosystem

3.2.1 EU HPC landscape 2012-2016

Following February 2012 EC communication recognising the need for an EU-level policy in HPC addressing the entire HPC ecosystem [33], all three pillars making up a global HPC value chain have been organised with the concerned stakeholders, and addressed in Horizon 2020 by specific calls [34]. Each pillar has entities that can endorse structuring roles and be voices for the stakeholders.

The "contractual Public-Private Partnership on HPC" (cPPP on HPC) [35] brings together technology providers and users via the ETP4HPC Association - a voice for HPC technology Pillar - and CoEs for computing applications - voices for HPC applications Pillar. The cPPP organises a framework for the orientations and monitoring of the technology- and application-oriented programmes, and works in close cooperation with PRACE.

Mid-2015 the study "SMART 2014/0021" analysed the progress of the European HPC Strategy towards ensuring European leadership in the supply and use of HPC systems and services by 2020. Good progress was observed, reported and documented [36] acknowledging, in particular, that the main actors - the EC, PRACE and ETP4HPC, have done important efforts for coordinating to advance the European HPC strategy.

To enlarge the scope of current PRACE activities towards EDI goals, and put PRACE in a position of prime contributor to EDI with GÉANT, PRACE is analysing its current core (mandatory) activities (access to Tier-0 provided by all HMs for Open R&D for science & industry, training, code enabling, communication, information, Tier-1 for Tier-0 services provided by PRACE partners & aisbl) and will explore what could be the new extended services (provided by all partners or by some partners), that could allow EDI to work as a one-stop-shop for all EC projects/infra on HPC and data.

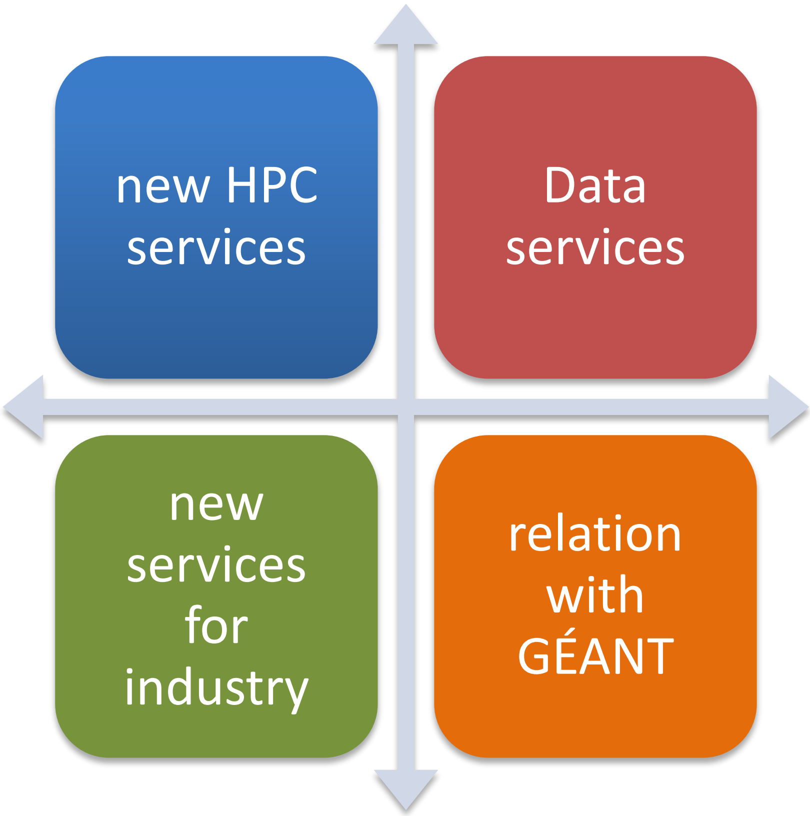

Figure 2: Enlarged scope of current PRACE activities towards EDI goals

3.2.2 A new Ambition for EU HPC: 2016-2107

The launch of a Digital Single Market (DSM) strategy for Europe and the expected new challenges placed by the corresponding new European e-Infrastructures forces all stakeholders to reposition themselves in order to take maximal advantages of this new context, not independently of the mastering of computing technologies and applications. The consequences of that strategy should have major impact on industrial/economical as well as on academic/scientific/technological levels.

A general trend and a framework for analysis is the intertwining of HPC with a growing number of industrial applications and scientific and societal domains. This places HPC as one of the key contributors to the Digital Single Market ((DSM) strategy, which was announced by the EC on April 2016 and actually confirms and widens the scope of the corresponding 2012 EC strategy [37].

In this context the proposed concept of European Cloud Initiative (ECI) includes the notions of an underlying European Data Infrastructure (EDI as a rich infrastructure bridging computing, data storage, access and processing, and networking capabilities), together with a European Open Science Cloud (EOSC) layer to organise access and delivery modes for scientists. The Commission has appointed a High Level Expert Group on the European Open Science Cloud (HLEG EOSC) whose report was released in October 2016. The Report recommends "to close discussions about the 'perceived need' of a science cloud and to take immediate action on the EOSC in close concert with Member States, building on existing capacity and expertise." [42]

Meanwhile and in the same context (November 2015) an initiative led by a few Member States (Luxembourg, France, Italy, Spain) was also announced, so-called IPCEI HPC-BDA, an Important Project of Common European Interest mixing HPC and Big Data objectives [43]. This was understood as an action with strong industrial structuration, from volunteering countries wanting to optimise and align different aspects of a large European HPC and Big Data initiative with the objectives of the DSM. A few months after that, a new pan-European initiative called EuroHPC was launched, partly overlapping the IPEIC objectives, and becoming the priority for the concerned Member States.
In March 2017 the EuroHPC was launched [59] and signed so far by 13 countries (Belgium, Bulgaria, Croatia, France, Germany, Greece, Italy, Luxembourg, Netherlands, Portugal, Slovenia, Spain and Switzerland) and EC, towards the funding of a pan-European HPC infrastructure for science, industry and public services, targeting the joint procurement of 2 pre-Exascale systems in 2020/2021 then 2 Exascale systems in 2022/2023, fostering the use of European technologies.

Based on an unprecedented global funding composed by H2020, FP9 and Coordinating European Facilities (CEF) from the EC and Member States side, and private funding on the other side, EuroHPC will address, utilizing a Joint Undertaking agreement (like the one used for the EuroFusion agreement), the following 4 pillars:

- Infrastructure: acquisition of an infrastructure (using PPI or similar mechanism) and providing and managing access to users;
- Applications and skills: development of HPC applications, support to industry (including SME), training and outreach;
- Research and innovation: funding R&D for technologies and systems developed in Europe;
- Operating the machines: installation, deployment and operation via hosting entities.

3.2.3 Longer term perspective on Quantum computing

On invitation of Mr. Günther Oettinger, Commissioner for Digital Economy and Society and Mr. Henk Kamp, Minister of Economic Affairs in The Netherlands, a "Quantum Manifesto" [57] has been written to formulate a common strategy for Europe to stay at the front of the second Quantum Revolution. This Manifesto calls upon Member States and the European Commission to launch a €1 billion flagship scale initiative in Quantum Technology. It was endorsed by a broad community of industries, research institutes and scientists in Europe.

Formal link was not established so far, but this is of course a field of research that will be scrutinized in the future, especially with the Virtual Institute for Quantum Computation [58].

This institute integrates all groups which have an effort aiming at building a large scale quantum computer, independently of the physical system used for this purpose. The latter will thus include trapped ions and neutral atoms, cavity QED, solid state devices (such as superconducting qubits, possibly in combination with circuit cavity QED, and spin qubits), all-optical devices, as well as impurity spins in solids, single molecular magnets, and all sort of hybridization between these different implementations.

3.3 HPC Global landscape

High Performance Computing is a highly strategic area which has resulted in numerous initiatives in recent years. Examples of these include the National Strategic Computing Initiative (NSCI) firmed by President Barak Obama in 2015, the Japanese Post-K-flagship project, current PRACE, ETP4HPC and CoEs projects, and current EuroHPC initiative in Europe, Tianhe and Sunway HPC clusters in China, and more prospective projects such as the ones related to Quantum Computation.

In this section, we provide an overview of the HPC Ecosystems on other continents. On the fiftieth TOP500 list of the fastest supercomputers in the world (November 2017), China, still defending its n°1 place acquired in 2013 (Sunway TaihuLight at 93 petaflops and Tianhe-2 (Milky Way-2) at 34 petaflops), has overtaking the US in the total number of ranked systems by 202 to 143, as well as in aggregated performance, with 35,4% of the whole Top500, while the US shrank to 29,6% (with "only" 3 systems within the Top10, from number 5 to number 7, the former number 1 five years ago, Titan (DOE), 17 petaflops, Trinity (Los Alamos National Laboratory and Sandia National Laboratories), 14 petaflops, and Cori (NERSC), 14 petaflops).

Far away from these two champions, Japan kept the third place of ranked systems with 35 systems, placing a new number 4 on the Top10 with Gyoukou (Japan's Agency for Marine-Earth Science and Technology), 19 petaflops, along with number 9 and 10, Oakforest-PACS (Joint Center for Advanced High Performance Computing), 13 petaflops and Fujitsu's K computer installed at the RIKEN Advanced Institute for Computational Science (AICS), 10 petaflops, but number one on the High-Performance Conjugate Gradients (HPCG) benchmark.

Then the European partners follow behind, with Germany at the forth place of ranked systems, with 20 systems, France with 18, and the UK with 15. But only the PRACE Swiss system of CSCS Piz Daint rank on the Top10, as number 3 with 19 petaflops.

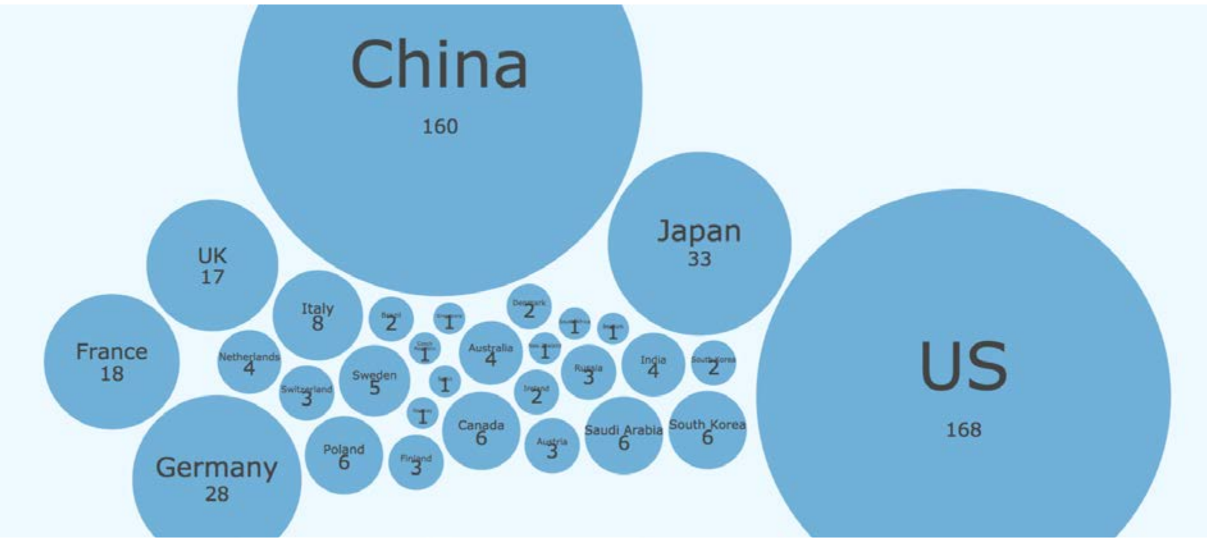

Figure 3: Number of supercomputers per country, June 2017 TOP500 (courtesy of Mahmoud Elbattah)

The above representation of the number of HPC systems within the TOP500 by country (from June 2017, the data from November 2017 arrived too late for a graphic processing, but the overall picture stay the same, except China and US switching first and second place) clearly show “big players”, China and USA, leading the race, followed far away behind by a second lot, Japan, Germany, France and UK, with an order of magnitude between the first two and the 6th one. The combined number of European HPC systems added to only half the numbers of the Chinese or the US ones, and the situation is even worse if we compare the cumulated Flops (see Figure 5 and Figure 6), with only the PRACE Swiss system of CSCS within the Top10, as number 3. From that view, it is very clear that a combined European effort is the only way to compete in this global race, and that strong budget effort will be needed, at national and European levels, to cope with the acceleration of this race toward Exascale. This is one of the goals of EuroHPC.

Figure 4: World Map of Supercomputers, TOP100 June 2017 (courtesy of Mahmoud Elbattah)

A look at the TOP100 location on a map also clearly shows three major regions on HPC: USA, Asia and Europe. This also shows that some efforts towards the other regions of the world could be very useful to help them embrace the HPC technology to produce better sciences. A lot of the MoUs that will be presented later in this document are designed to help improve this situation. The above two images (Fig. 3 & 4) are courtesy of Mahmoud Elbattah, and have been designed within the PRACE Summer of HPC 2017 [14].

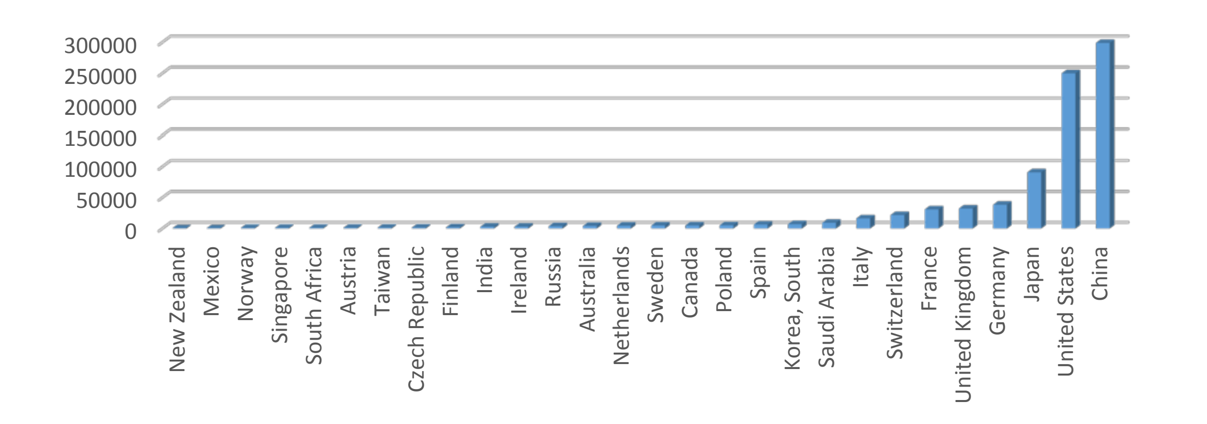

Figure 5: Rmax per country - November 2017 TOP500 List

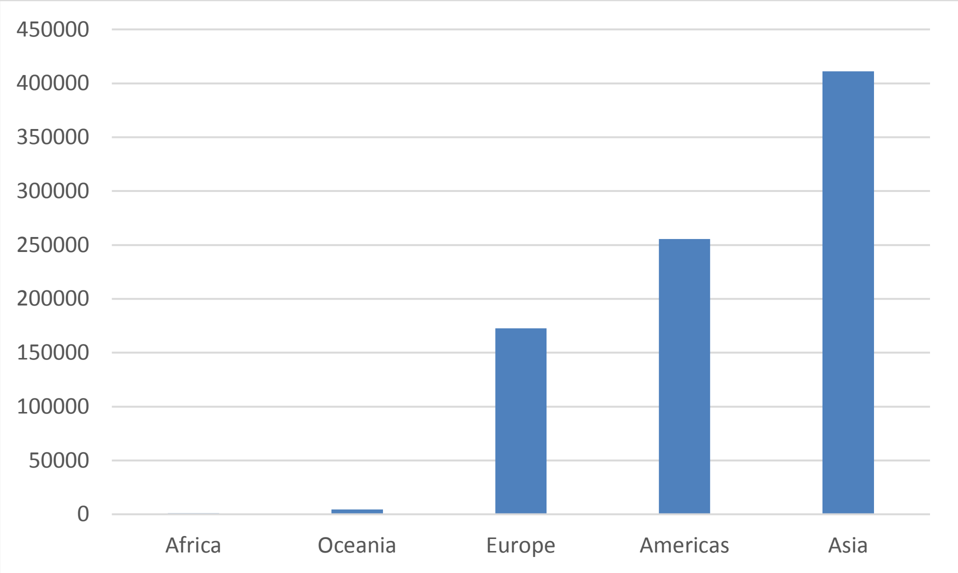

Figure 6: Rmax per world region - November 2017 TOP500 List

3.3.1 Oversea: link with XSEDE USA / RIKEN Japan / Compute Canada

Over the past 60 years, the United States has been a leader in the development and deployment of cutting-edge computing systems. In July 2015 President Obama issued an Executive Order establishing the National Strategic Computing Initiative (NSCI) to ensure the United States continues leading in this field over the coming decades.

The United States dedication to HPC in academia is best exemplified in recent years through its support of the Extreme Science and Engineering Discovery Environment (XSEDE) partnership programmes. Funded $121-million over five years by the National Science Foundation in July 2011, with a further five year $110-million grant, XSEDE 2.0 is now comprised of 19 US based institutions.

XSEDE is a single virtual system of integrated advanced digital resources and services that scientists can use to interactively share computing resources, data, and expertise. Supporting sixteen supercomputers and high-end visualisation and data analysis resources, XSEDE allows scientists and engineers around the world to use these resources and their respective services in an easy and established private and secure environment setting where all resources, services and collaborative support tools can be found for them to be productive.

XSEDE has an extensive outreach programme – engaging students from an undergraduate level either through training, internships, mentoring programmes and their campus champion programmes. Further to this XSEDE has a dedicated "Underrepresented Community Engagement" programme which focuses on engaging a greater number of users of XSEDE services from research groups and fields which have not yet used XSEDE resources.

XSEDE and PRACE have a multi-year history originating back in 2008 when TeraGrid and DEISA leadership began discussing how these two projects could collaborate. As TeraGrid later evolved to XSEDE and as DEISA services were passed on to PRACE, both projects collaborate in various ways such as:

1. Enabling scientists to apply for HPC resources across borders
2. Develop allocation and support categories for international team proposals
3. Allow for joint PRACE and XSEDE allocation calls
    - Requiring both XSEDE -PRACE services to be interoperable with each other
4. Joint organisation of International HPC Summer schools since 2010
    - In 2010 this was organised by DEISA and TeraGrid in Italy;
    - In 2011 this was organised by DEISA, PRACE and TeraGrid in USA;
    - In 2012 this was organised by PRACE an XSEDE in Ireland;
    - Since then this summer school series has continued with the addition of RIKEN (Japan) since 2013 and Compute Canada since 2014.

3.3.2 China

China has great ambitions in the field of HPC and leads the TOP500 list - both in terms of power and installed systems. The sustained effort to develop HPC in China is organised around several initiatives with the clear objective to conquer global leadership capacity of HPC and software development. China faces two main challenges in its HPC aspirations. The first of these is the development of its own processors (due to the US government banning Intel, Nvidia and AMD from selling high end chips to China) and the associated ecosystem (middleware, environment, applications). The second challenge is the formation of home talents in HPC.

Some major Chinese companies and labs in HPC:

1. Sugon (was the #1 market share holder in China HPC market for the past 7 years);
2. Inspur (developed the Sunway BlueLight MPP machine with a "Shenwei" SW-3 1600 processor based on a Chinese 64-bit RISC DEC Alpha architecture);
3. Institute of HPC at Tsinghua University in Beijing;
4. Institute Computer Network Information Centre (CNIC) of the Chinese Academy of Science (CAS) in Beijing.

China is also investing into ARM for some of its processors in its future supercomputers. In 2016, the Phytium Technology Chinese chipmaker introduced its 64 core "Mars" chip with ARMv8 instructions, which could be used for Tianhe-3, under development at the NUDT and the National Supercomputing Centre in Tianjin.

3.3.3 Japan

In 2011, Japan had for some time the world's TOP500 #1 supercomputer, named K. This Fujitsu system was based on SPARC64 VIIIfx CPUs and used its own Torus Fusion (Tofu) interconnect. Fujitsu is working on the Post-K Computer. Fujitsu has been collaborating closely with ARM and contributed to the development of the HPC extensions (called SVE) for ARMv8-A, a cutting-edge ISA optimised for a wide range of HPC. The K computer is being used in a broad range of fields including drug discovery, earthquake/tsunami research, weather forecasting, space science, manufacturing and material development.

The first Exascale Fujitsu system for RIKEN is currently planned for 2020. The expected power consumption is expected to be 3 – 4 times K's (which is some 12.6 MW).

Europe and Japan also cooperate through the ITER project (China, the European Union, India, Japan, Korea, Russia and the United States, engaged in collaboration to build and operate the first device for the commercial production of fusion-based electricity), a set of research activities related to fusion that were decided in 2007 within an international agreement between Europe and Japan. Among this set of activities was the provision and the operation of a state-of-the-art supercomputer located in Japan and used by the European and Japanese researchers. A 2 Pflops ATOS/Bull supercomputer, provided and operated by CEA on the behalf of F4E (Fusion for Energy), with a Japanese contribution related to facility and user support, was in operation in Japan from January 2012 to December 2016. This system was very successful, with a very high availability and usage (typically between 90 and 95% all around the year), making possible the production of close to 600 peer-reviewed papers in major scientific journals.

In July 2016 SoftBank, a Japanese financial holding, surprised the technology world with the acquisition of the British chip designer ARM Holdings for £23.4 billion ($31.4 billion), the biggest ever purchase of a European technology company.

3.3.4 Canada

The main HPC organisations in Canada are ACENET, Calcul Québec, Compute Ontario and WestGrid. Compute Canada is the project which integrates the HPC resources of these four organisations in a similar way to the way PRACE integrates Tier-0 resources. Working together, their joint vision is to make Canada a world-leader in the use of advanced computing for research, discovery and innovation through effectively, efficiently and sustainably deploying a state-of-the-art advanced research computing network supported by world-class expertise which can be used by Canadian researchers and their collaborators in all academic and industrial sectors. The structure of Compute Canada is similar to that of PRACE, with a similar governance and shares similar goals too. Compute Canada has an extensive training programme and has been a partner in the International HPC Summer school series since 2014.

3.3.5 Southeast Europe Region

A number of projects have looked into creating a regional HPC infrastructure. This include:

- HP-SEE: High-Performance Computing Infrastructure for South East Europe's Research Communities project. The aim of this project is to link HPC facilities in South East Europe in a common infrastructure to open up a wide range of new user communities to such resources, fostering international collaboration.
- LinkSCEEM: Linking Scientific Computing in Europe and the Eastern Mediterranean. The aim of this project is to establish a HPC ecosystem in the Eastern Mediterranean region by interlinking and coordinating regional compute, storage and visualisation resources to form an integrated e-Infrastructure. The project objective is to enable scientific research in the region by engaging and supporting research communities with an initial emphasis in fields of climate research, digital cultural heritage and synchrotron radiation applications. Having delivered training events and a Preparatory/Production call this project was a good first step towards introducing and establishing HPC in the region. LinkSCEEM collaborated with PRACE through the joint hosting of training events and the International Conference on Scientific Computing in Cyprus in 2013.

- VI-SEEM is a three-year project funded under Horizon 2020 programme that aims at creating a unique Virtual Research Environment in Southeast Europe and the Eastern Mediterranean, in order to facilitate regional interdisciplinary collaboration, with special focus on the scientific communities of life sciences, climatology and digital cultural heritage. It will significantly leverage and strengthen the research capacities of user communities, thus improving research productivity and competitiveness at the pan-European level. Joining, sharing and exploiting the resources across the SEEM region in a common platform will ensure continuity and expansion of the available resources and services that will further propel excellence across the region.

3.3.6 Others - Asia and Australia

Aside from well-established supercomputing powerhouses like Japan and emerging new players like China, Asian countries like Singapore and South Korea have also recognised the transformational power of supercomputers and invested accordingly.

The National Supercomputing Centre Singapore was established as a national facility of petascale standard to support high performance scientific and engineering computing needs in Singapore. It supports a 1 petaflop system, a 10 Petabyte data service coupled with dark fibre network to support the Singapore Advanced Research and Education Network.

South Korean currently has 5 systems in the TOP500, from #57 (2,9 petaflpos) to 346 (0,74 petaflops) positions. The South Korean government announced in April 2016 that they will invest 86.2 million USD each year for 10 years to assist in R&D in the field, and their plans to develop a Korean-type supercomputer with a processing speed of at least 30 petaflop by 2025.

In Australia, NIC provides world-class services to Australian researchers, industry and government and was the first Southern hemisphere site to host a petaflop supercomputer. It provides HPC computing and high performance data services to national science agencies, along with 35 Australian universities, five Australian Research Council Centres of Excellence, eight NCRIS capabilities, three medical research institutes, and three industry partners. A joint MoU on training, best practises in peer review, industrial involvement is in preparation between PRACE and the Pawsey Institute, one of the Australian national centre, involved in the SKA (Square Array Kilometre) radio telescope.

3.3.7 South America

HPCLatAm gathers a young but growing community of scientist and practitioners of the HPC in Latin America. Through a series of conferences and workshops a steadily growing HPC community is perceived in the region. The main goal of HPCLatAm is to provide a regional forum fostering the growth of the HPC community in Latin America through the exchange and dissemination of new ideas, techniques, and research in HPC.

3.3.8 Russia

Russia is interested in duplicating the achievements of the USA in technology and HPC is included in their aspirations, with the government announcing in 2011 a plan to focus on constructing larger supercomputers by 2020.

Russia has a number of academic supercomputing centres. The Supercomputing centre of the Lomonosov Moscow State University is one of the world-leading petascale centres with strong fundamental science and a serious focus on Supercomputing Education. Despite this, PRACE has yet to approach any supercomputing centres in Russia for any potential collaboration opportunities and this is something that could be explored in the future.

4 Links established with Stakeholders in the HPC Ecosystem

4.1 Providers of HPC services

One of the main achievements of PRACE has been to provide access to high-end Tier-0 resources to computational scientists, mostly in Europe but worldwide as well.

The PRACE RI currently provides access to the following such systems through PRACE project access:

1. Curie a Bull Bullx cluster based in GENCI@CEA, France;
2. Hazel Hen a Cray XC40 System based in GCS@HLRS, Germany;
3. Juqueen an IBM BlueGene/Q system based in GCS@JSC, Germany;
4. Marconi Lenovo System based in CINECA, Italy;
5. MareNostrum a Lenovo SD530 System based in BSC, Spain;
6. Piz Daint a Cray XC40/50 System based in CSCS, Switzerland;
7. SuperMUC IBM iDataplex/Lenovo NextScale System at GCS@LRZ, Germany.

Further to Project Access and these systems, PRACE through its optional programme provides access to Tier-1 national systems through DECI access. Given the high number of resources there is a wide variety of supercomputing architectures available for computational scientists, such as CRAY, BlueGene, clusters, including accelerators (GPUs or Xeon-Phi).

Besides these systems, there is also a great number of other Tier-2 national systems available throughout Europe for computational scientists to use on a national level. Such systems are usually the first computational scientists get access to, upon which they can learn essential programming skills as well as to develop their research projects. Such systems thus act as a first step for users in their initial use of HPC before they can proceed to using possibly larger and more powerful international Tier-1 and Tier-0 resources.

4.2 Link with Centres of Excellence (CoEs)

CoEs are described in section 4.7.7. They represent the spearhead of EU-supported high performance applications and are a structuring part of the HPC use side of the ecosystem [50]. PRACE has thus developed early links with these important stakeholders, mainly via PRACE-4IP project. PRACE aims to support the role of CoEs through various work package and activities. In this section, we identify the major planned activities involving CoEs.

4.2.1 PRACE On-Demand Events with Centres of Excellence

Through the Training work package (WP4), PRACE has be organising a series of on demand events in collaboration with CoEs. These events are advertised on the PRACE Events website [9]. Five such events are planned and these are with the following Centres of Excellence and PRACE Partners:

PRACE-NOMAD Remote Visualization workshop with Leibniz Rechenzentrum

- Center of Excellence for Global Systems Science (COEGSS) with HLRS/PSNC;
- An e-Infrastructure for software, training and consultancy in simulation and modelling (ECAM) and Energy oriented CoE for computer applications (EoCoE) with MdS;
- PRACE / EoCoE workshop on Atos-Bull Xeon-Phi PCP pilot with MdS, Cines Genci;
- E-CAM Workshop on Particle-Based Models and HPC with CSC;
- Performance Optimisation and Productivity (POP) with VSB-TUP/IT4I;
- The Novel Materials Discovery Laboratory (NoMaD) with JKU/RISK Software;
- Materials design at the eXascale (MaX) with ETHZ/CSCS and CINECA;
- PRACE-NOMAD Remote Visualization workshop with Leibniz Rechenzentrum.

4.2.2 Programming Tools, Languages, Libraries & Algorithms for Exascale

PRACE also liaises with CoEs as well as other application owners to identify application requirements with regards to best practices for prototype planning and evaluation - investigating the programming tools, languages, libraries and algorithms needed for future Exascale systems. Existing links with European Exascale projects are leveraged, and links with the emerging applications CoEs developed, so as to understand their requirements.
The goal of this activity is to produce an inventory of tools, languages and libraries needed for Exascale. The maturity of these tools and techniques will then be evaluated using real applications, both from PRACE and from the CoEs. A key goal of this task will be to provide cross disciplinary support for the CoEs, although the outputs will also be useful within PRACE and for other European HPC users. Depending on these requirements, PRACE will help CoEs with any challenges they may face should CoEs lack skills and resources to achieve this (Benchmarks, BPGs, White Papers, CodeVault, libraries). For this task, PRACE has also reserved 0.5% of available time on its systems solely dedicated for the CoEs.

4.3 Link through Operational services for the HPC Ecosystem

PRACE-4IP WP6 “Operational services for the HPC Ecosystem” has three main objectives:

1. Operate and monitor common operational services for the use of the European HPC IR;
2. Analyse new prototypal innovative services;
3. Link with others e-Infrastructures and CoEs (see section 4.7.7 for details);

To achieve these objectives, the partners have issued different interactions with stakeholders:

In point 1) a strong iteration has been put in place with the European Tier-0 centres and the Tier-1 centres involved in “Tier-1 for Tier-0” activity.

In point 2) the contacts with stakeholders have mainly involved the scientific communities, testing with them possible new prototypal services, and establishing links with large-scale scientific instruments.

The provision of repositories for European open source scientific libraries and applications, will promote an adoption of these services by scientific communities and CoEs.

In point 3) is important to underline the cooperation with the e-Infrastructures and the CoEs.

Many MoU have been signed between PRACE and these partners, allowing a specific collaboration with these stakeholders. The full list of MoU is provided in Annex 3, and the more recent ones, with CHPC (South Africa) and between PRACE-RIST-XSEDE is presented in detail within section 4.9.4.

Furthermore, PRACE is an active partner in the WISE series of workshops: “Wise Information Security for collaborating E-infrastructures” cooperating with EGI, GEANT, PRACE, HBP, XSEDE and other e-Infrastructure.

PRACE co organised the DI4R (Digital Infrastructures for Research) conference, Brussels 30 November – 1 December 2017, providing contributions on federated service managements, joint service catalogue, and SME engagements with e-Infrastructures.

PRACE-4IP has also been invited at the e-IRG Workshop under Slovakian EU Presidency (Bratislava 15-16 November 2016) giving a presentation on Federate service management.

4.4 Hardware / Software vendors – technology suppliers

ETP4HPC, created in 2012, is now the voice for/ of vendors and technology suppliers who are active in Europe. As of December 2017, ETP4HPC has 86 members, comprising 15 industrial HPC companies, 30 HPC SMEs, and 39 Research organisations with strong HPC hardware and/or software R&D.

EXDCI project offers extra support and amplification of this link with the vendors with the wider ecosystem.

PRACE has developed relationships with vendors since 2008, now periodically maintained via HPC technology watch activities. PRACE supported HPC prototyping efforts in different phases of its implantation phase projects, and more recently led a PCP (Pre-Commercial Procurement, PRACE-3IP project) on energy efficiency in HPC systems. Three European companies have delivered pilot systems for the final phase of this PCP.

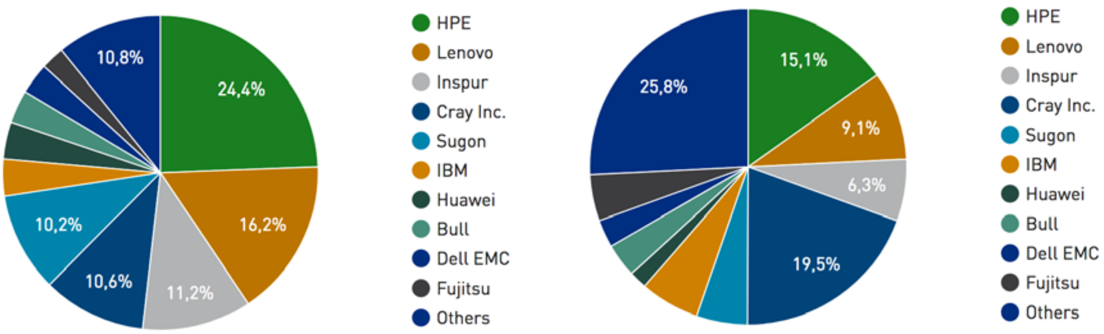

Figure 7: TOP500 split, by Vendors system share and by performance share from November 2017

4.5 Funding bodies

Developing a sustainable funding model is critical to any long-term project and even more - for the large-scale ones.

The PRACE project partners receive EC funding under the PRACE Preparatory and Implementation Phase Projects (PRACE-1IP, 2010-2012, RI-261557, PRACE-2IP, 2011-2013, RI-283493, PRACE-3IP, 2012-2017, RI-312763, PRACE-4IP, 2015-2017, 653838) for a total of €82 million complemented by the consortium budget of over €60 million; and now PRACE5-IP under Grant Agreement Number: EINFRA-730913.

PRACE already analysed possible funding models during its first implementation phase. The deliverable D.2.3.2 [17] of PRACE-1IP analysed the funding models of similar research infrastructures.

There are different methodologies that can be taken as a reference among them the following:

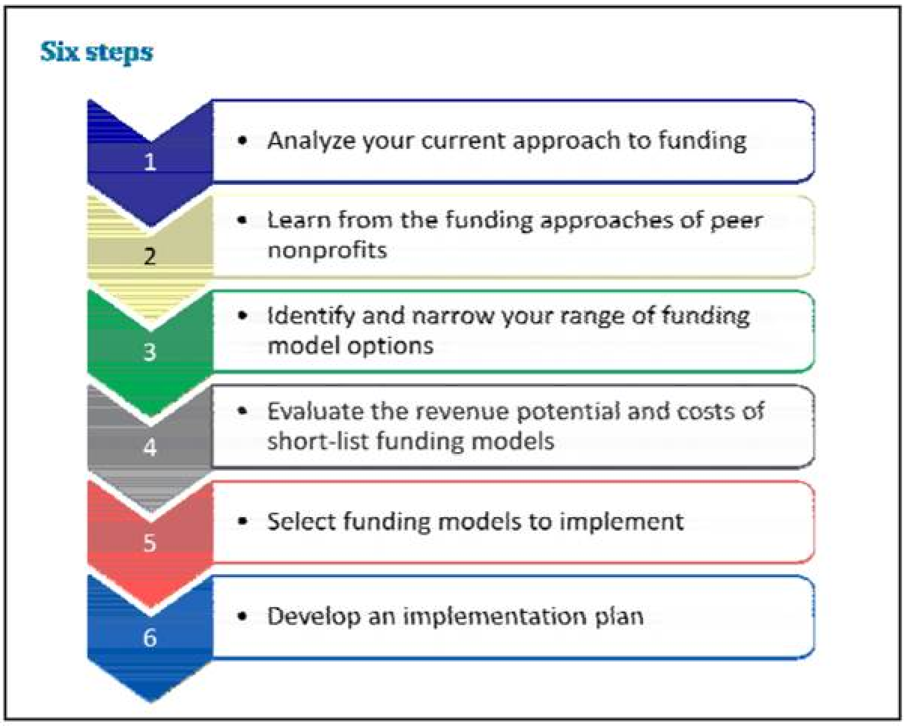

Figure 8: Six steps for identifying and developing the right funding model for organisations [44]

In that deliverable some funding principles were agreed:

- Acceptability to the AISBL;
- Legality;
- Sustainability;
- Meeting the mission of PRACE;
- Fairness to partners within PRACE;
- Transparency;
- Meeting user needs;
- Flexibility;
- Ability to bring to a close.

The initial funding model was confronted with these principles in order to check its suitability and correct it as much as possible with subsequent funding models like PRACE 2.

PRACE has presented in the deliverable D2.2 of PRACE-4IP [21] the new funding model, the so called PRACE 2, aiming a cost model affordable for all partners. The main novelty is a shared participation of Hosting Members and the non-Hosting Members to the cost of High Level Support Team. Aside from the contributions of PRACE Members, external funding is sought for complementing the internal funding model.

HPC is a strategic resource for Europe's future, reflected in the adoption of the EU HPC Strategy in February 2012 [33]. A strong cooperation with the HPC stakeholders is key for the success of this strategy, but also for the successful continuation of PRACE as a key infrastructure project in the field of HPC and its applications in science and industry. Managing proper relation to policy-making and funding bodies on European and national level is a cornerstone on this road. The Work Programme with its deliverables and Milestone structure and schedule provides a sound and transparent basis for preparation of objective executive summaries to justify advantages and advances PRACE membership grants to the participating parties. In doing this, the level, character and role of these bodies in the decision-making process have to be recognise (from European / national level to emerging players).

4.5.1 EU funding

The core EU funding includes:

- Horizon 2020, the EU Research and Innovation programme [45]

The Framework Programme for Research and Innovation (2014-2020) Horizon 2020 is the financial instrument implementing the Innovation Union, a Europe 2020 flagship initiative aimed at securing Europe's global competitiveness. This work was financially supported by H2020 through under Grant Agreement No. 653838 of the DG CNECT.

- European Structural and Investment (ESI) Funds [46]

Over half of EU funding is channelled through five European structural and investment funds (ESIF). They are jointly managed by the European Commission and the EU countries.

- Other sources of funding

There are other accessory funding types like grants, loans or guarantees, in particular from EIB Group (InnovFIN under Horizon 2020) as well as from the Investment Plan for Europe (EFSI). Guides are available on synergies between the different schemes. Coordinating European Facilities (CEF) project could also be applied for HPC.

4.5.2 National funding for PRACE Members

A survey [47] carried out across European countries on the national funding for Research Infrastructures shows that funding instruments vary across countries and are linked to strategic research infrastructures. One of the major funding sources to apply for updating or even building HPC and data infrastructures are national roadmaps of research infrastructures which were defined on similar way like ESFRI roadmap and the last one from December 2016. The opportunities we can see here are dedicated calls on structural funds programmes reserved only for RIs established in former calls, e.g. the Polish and Czech RI lists include HPC systems which are related to PRACE activities and Tier-1 level.

4.6 Policy making organisations

For PRACE, it is a priority seeking participation to the possible extent in the HPC policy making process, its development and applications at European level, in order to secure both direct and indirect external funding. Regarding policy-making institutions, it is important to highlighting the connection between strategic priorities and funding decisions, both at the European and national level. In addition, a proper alignment between national and European priorities is of outmost importance.

The policy makers stand for the society objectives, so these have to be – and are – reflected in PRACE strategic goals and in the very concept of the successor programme PRACE 2. The funding bodies have the responsibility for implementing the consensual strategies, with a focus on the short-term results, however in the context of the general strategic planning.

A good example of this is the ESFRI [48] (European Strategy Forum on Research Infrastructures). The ESFRI's delegates are nominated by research ministers of the EU Member and Associated Countries and include a European Commission representative. The ESFRI has a key role in policy-making on research infrastructures in the EU and contributes to the development of strategic roadmaps. The work of ESFRI allows Member States to align their national roadmaps with the European ones, allocating budget to specific research infrastructures of European interest.

Another important stakeholder is the e-IRG (e-Infrastructure Reflection Group) [43]. e-IRG is a strategic body to facilitate integration in the area of European e-Infrastructures and connected services, within and between member states, at the European level and globally. The mission of e-IRG is to support both coherent, innovative and strategic European e-Infrastructure policy making and the development of convergent and sustainable e-Infrastructure services. In this respect, e-IRG produces strategic and policy reports, analyses and gives recommendations. In 2016, an ESFRI Working Group on investment strategies in e-Infrastructures (incl. e-IRG representatives) was created, where one of the first topics presented was the PRACE 2 programme.

A flexible and very rich in information tool are the Key Performance Indicators (KPIs). The KPIs might be of particular value in the communications with the national authorities, providing a dynamic picture in the proper environmental and historical context. PRACE will focus on developing of tailored KPIs to answer the questions, concerns and demands on these various levels of decision-making processes and bodies [8].

4.7 Users communities - Scientific - Industrial - SMEs

The detailed organisation of the PRACE RI could be found on the PRACE website [13]. It includes bodies in charge of the governance of the organisation, Council, Board of Council and Bord of Directors (BoD), and bodies in charge of providing advice and guidance from our users, through a User Forum (UF), Scientific Steering Committee (SSC), Access Committee (AC) and Industrial Advisory Committee (IAC). Some members of these bodies join into a Strategy Working Group to address specific issues when needed.

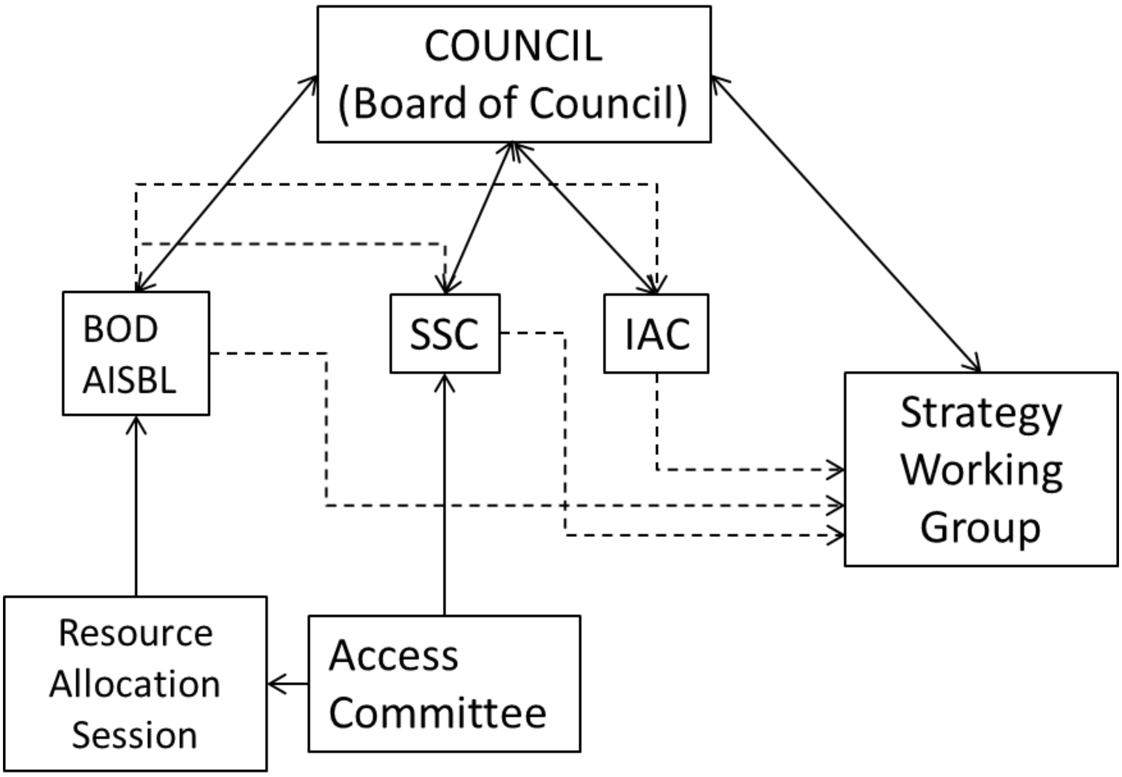

Figure 9: Organigram of PRACE

4.7.1 PRACE User Forum (UF)

The PRACE User Forum (UF) is a body independent from the PRACE aisbl Association (thus not represented within the organigram of PRACE). However, there are close links and interactions with the Association through the BoD. The role of the PRACE UF is to provide a communication channel between the user community and the resource providers, as well as to sustain an open exchange forum between users. As reported in an earlier document (see 3IP-D2.2 [18]), there are a number of national and pan-European initiatives that have been set up to encourage industry and especially SMEs to engage into HPC (see section4.7.5).

4.7.2 PRACE Scientific Steering Committee (SSC)

The Scientific Steering Committee (SSC) is composed of European leading researchers that are responsible for advice and guidance on all matters of a scientific and technical nature which may influence the scientific work carried out by the use of the Association's resources. The SSC has an odd number of members up to a maximum of 21, of which one is appointed Chairman. The members of the Scientific Steering Committee are appointed by the PRACE Council. SSC Members serve a two-year term renewable twice consecutively.

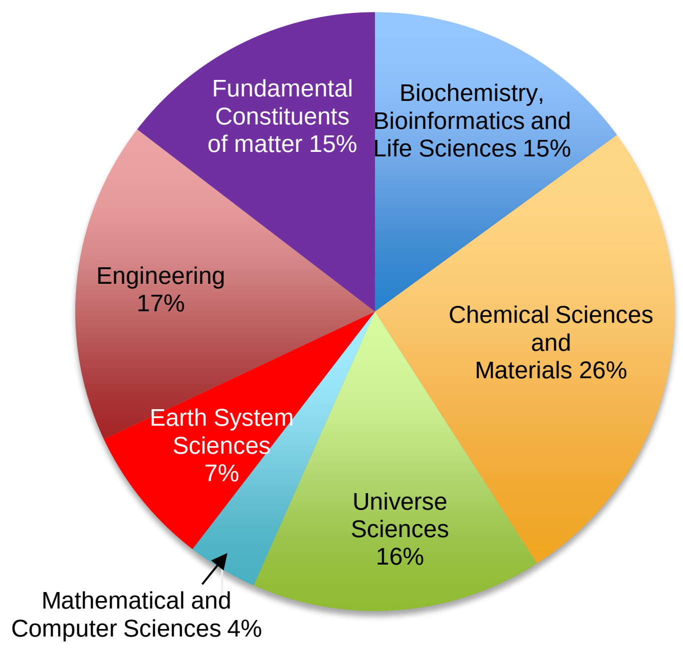

Figure 10: PRACE Distribution of resources (by Call 14, % of total core hours awarded)

4.7.3 PRACE Industrial Advisory Committee (IAC)

The Industrial Advisory Committee (IAC) is composed of European industry representatives (both from multi-nationals and SMEs) representing 11 industrial sectors: Aeronautics/Aerospace, Automotive/Transport, Energy, Engineering/Manufacturing, Oil & Gas, Renewable Energy, Telecommunications/Electronics, ISV, HPC Vendors, Life Sciences, and Finances. They provide PRACE with advice on HPC usage for the benefit of European competitiveness and economic growth. The IAC reserves an observer seat for the Chair of ETP4HPC. A Chair and Vice-Chair are chosen by the committee, who, like all members, are appointed for two years renewable once.

4.7.4 PRACE Access Committee (AC)

The Access Committee (AC) gives advice to the Board of Directors concerning the allocation of resources of the RI. The AC, proposed by the SSC, is composed of researchers experienced in areas of science, engineering and supercomputing. AC is appointed by the Council and shall comprise an odd number of members with a minimum of five, among which a Chairman and a Vice-Chairman is appointed. AC members serve a two years term renewable once.

4.7.5 PRACE Collaboration with SMEs: SHAPE Programme

SHAPE (SME HPC Adoption Programme in Europe) is a pan-European programme within PRACE aiming to equip European SMEs with the awareness and expertise necessary to take advantage of the innovation possibilities opened by HPC, increasing their competitiveness. The mission of this programme is to help European SMEs to demonstrate a tangible Return on Investment (ROI) by assessing and adopting solutions supported by HPC, thus facilitating innovation and/or increased operational efficiency in their businesses [11].

SHAPE was launched in 2013, following consideration of the needs of SMEs and input from various national level SME engagement programmes, that was reviewed as a success (wining HPCwire Readers' Choice Award for the best HPC Collaboration between Government & Industry at Supercomputing 2014).

The PRACE-3IP deliverable D5.3.3 [19] performed a follow-up of the pilot project with SMEs judging the ROI they had gained. The outcomes were largely very positive: some hired staff to continue their HPC work started under SHAPE; many manage to run their software much more quickly and much more cheaply; and many have been able to offer enhanced and new services to customers, thus increasing their competency and market offerings. In addition, there was a commitment to continue working with HPC in the future from all of the SMEs.

SMEs awarded a SHAPE support, are matched with a PRACE partner for technical expertise, and can apply for PRACE machine time. The SMEs are expected to undertake some promotion of this collaboration, and to produce a white paper, available via the PRACE website [12]. SHAPE continue under PRACE-5IP, its process is under constant review, with feedback from both PRACE partners and the SMEs to try and streamline the process for all parties concerned.

SHAPE results in short:

- First 5 calls: 39 projects funded from 9 different countries;
- 6th call closed on Friday 1st December 2017;
- Different fields, including computational fluids dynamics, steel casting, medicine, genomics, environment and renewable energies, artificial intelligence, etc.

Participation in the Programme has been monitored to evaluate possible benefits, ROI and business impact obtained by the SMEs:

- SHAPE is of real value to the SMEs;
- Many positive outcomes for the businesses involved in the activity;
- Tangible measures of the ROI in many of the projects:
  - new staff people hired;
  - contracts have been won;
  - costs have been reduced;
  - HPC Access;
  - in house HPC systems installed.
- Optimism that improvement in service will lead to an increase in customer numbers;
- Adopting HPC: Companies R&D will be accelerated along with reduced costs;
- Commitment to continue working with HPC: in-house or via PRACE resources.

4.7.6 Example of the Climate Science community

Represented by ENES, the climate community is collaborating and participating in all three funding pillars of the EU. Together with the weather community, the Centre of Excellence in Simulation of Weather and Climate in Europe (ESiWACE) was initiated and started in September 2015; the HPC Task force of ENES is exploring the feasibility to apply for dedicated access on PRACE for high-end experiments within the international CMIP6 experiments; and synergies are elaborated with the FET HPC project ESCAPE (Energy-efficient Scalable Algorithms for Weather Prediction at Exascale), initiated by the weather community.

4.7.7 Centres of Excellence - CoEs

In 2015 eight Centres of Excellence (CoEs) for computing applications were selected following a H2020 e-Infrastructures call [50], meant to help strengthen Europe's existing leadership in HPC (high-performance computing) applications and cover important areas. A ninth Centre of Excellence, CompBioMed, has joined the initial group of eight selected in 2015. The CoEs and their topics are:

- EoCoE - Energy oriented Centre of Excellence for computer applications;
- BioExcel - Centre of Excellence for Biomolecular Research;
- NoMaD - The Novel Materials Discovery Laboratory;
- MaX - Materials design at the eXascale;
- ESiWACE - Excellence in SImulation of Weather and Climate in Europe;
- E-CAM - E-infrastructure for software, training and consultancy in simulation & modelling;
- POP - Performance Optimisation and Productivity;
- COEGSS - Centre of Excellence for Global Systems Science;
- CompBioMed - started in 2016 - Computational Biomedicine.

Since 2016 CoEs have seats in the governance body (Partnership Board) of the HPC cPPP.

4.8 Link with other H2020 HPC projects: FETHPC & Flagships

4.8.1 H2020-funded FETHPC projects

PRACE-4IP Deliverables D5.1 “Market and Technology Watch Report Year 1” ([22] April 2016) and D5.2 “Market and Technology Watch Report Year 2. Final summary of results” ([23] April 2017) contain a thorough description of EU projects (Horizon 2020, but also FP7, as well as Eureka ITEA2 and ITEA3) in the area of HPC, including Exascale objectives.

All 21 R&D projects stemming from FETHPC are up and running, (plus two Coordination and Support Actions, EXDCI and Eurolab4HPC, for ecosystem development and extra prospective) [51], they are presented in [31]. Two new ‘co-design’ projects funded in 2016 have been added to the FETHPC portfolio.

Some documentation on the progress and potential of these projects can be found at [29][41]. ETP4HPC and EXDCI have produced Handbooks at the occasion of BoF sessions at SuperComputing (2015, 2016 and 2017 [56]), with up-to-date details of the European HPC Technology Projects within the European HPC Eco-system (see [32]).

4.8.2 Extreme Data and Computing Initiative - EXDCI

EXDCI (Coordination and Support Action funded under FETHPC) objective is to coordinate the development and implementation of a common strategy for the European HPC Ecosystem.

PRACE (acting as coordinator), and ETP4HPC joined their expertise in this 30 months project, starting from September 2015. EXDCI aims to support the road-mapping, strategy-making and performance-monitoring activities of the ecosystem [41].
EXDCI is putting together PRACE, ETP4HPC, FETHPC and CoE projects and all the other stakeholders via joint technical activities (incl. road mapping with synchronized updates of the ETP4HPC' Strategic Research Agenda and the PRACE' Scientific Case, training studies) and major events such as the European HPC Summit Week, organised for the first time in May 2016 in Prague, and with its 3rd edition in 2018 taking place in Ljubljana, Slovenia. A specific action towards an international liaison with US DoE, Japan and China allowed the organisation of multiple BDEC (Big Data and Extreme Computing) workshops, leading to a joint position paper called "Pathways to Convergence" [53]. ETP4HPC and EXDCI are also developing specific and active links with Big Data cPPP (BDVA association) and HiPEAC, especially regarding road mapping cross-referencing or synchronisation. EXDCI is thus a strong tool for EU HPC ecosystem development and strengthening.
In particular, within this context, ETP4HPC issues and maintains a Strategic Research Agenda (SRA) as a mechanism to provide contextual guidance to European Researchers and Businesses and also to guide EU priorities for research in the Horizon 2020 HPC programme. This SRA delineates a roadmap for the achievement of European exascale capabilities focusing on the following areas: HPC System Architecture and Components, Energy and Resiliency, Programming Environment, System Software and Management, Big Data and HPC Usage Models, Balance Compute, I/O and Storage Performance, Mathematics and algorithms for extreme scale HPC systems and Extreme-Scale Demonstrators.

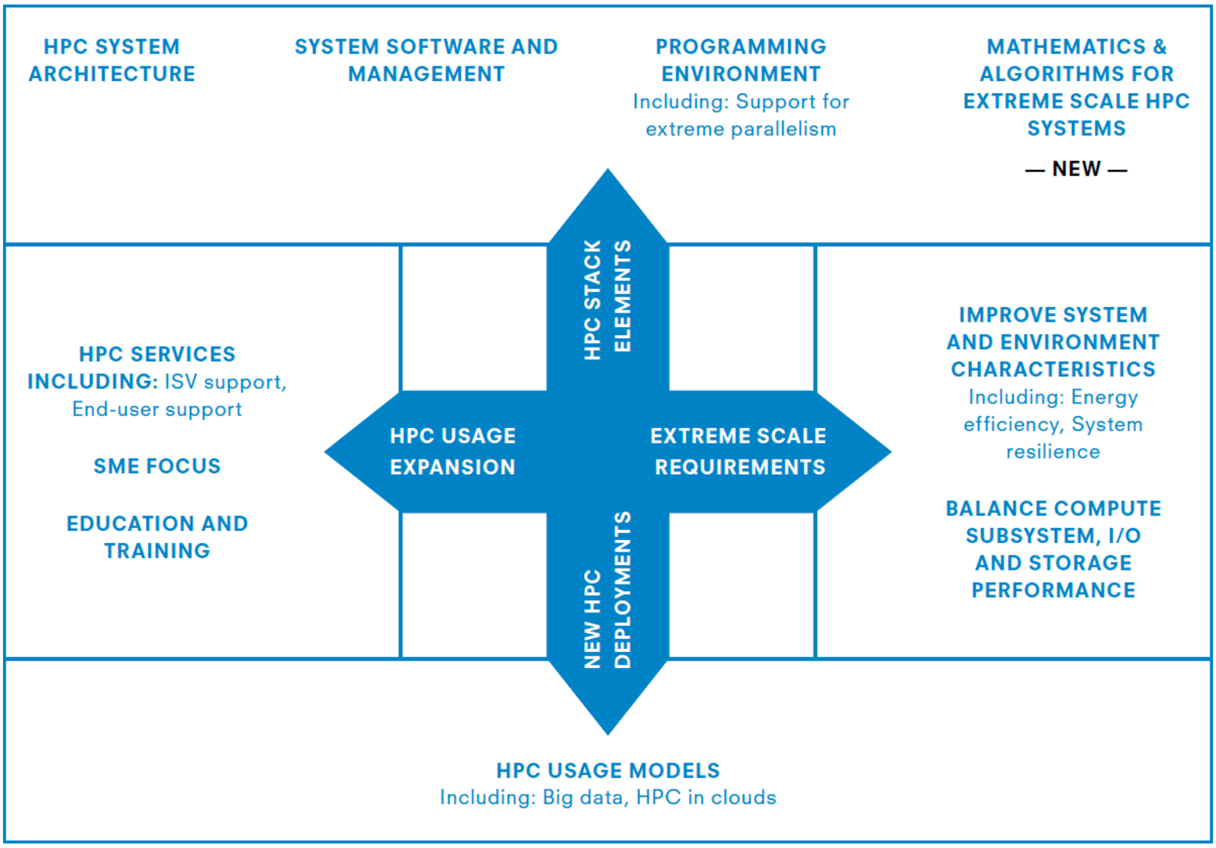

Figure 11: The four dimensions of the EXDCI/ETP4HPC SRA

4.8.3 EuroLab-4-HPC

EuroLab-4-HPC (Coordination and Support Action) funded under FETHPC is another two-year Horizon 2020 Coordination and Support Action focussing on a longer-term HPC research agenda, plus focus on education, innovation and business stimulation. FETHPC projects (RIAs and CSAs) all together form a community were growing interactions and mutual awareness of activities are observed. Details on the current FETHPC projects can be found in chapter 6.1 Annex 1: The new European HPC research landscape.

4.8.4 Graphene and Human Brain Project (HBP) Flagships

Graphene and Human Brain Project (HBP) projects are Future and Emerging Technology (FET) Flagship, founded by the European Commission. With a budget of 1 billion EUR, the Graphene Flagship represent a new form of joint, coordinated research on an unprecedented scale, forming Europe's biggest ever research initiative. The Graphene Flagship is tasked with bringing together academic and industrial researchers to take graphene from the realm of academic laboratories into European society in 10 years, thus generating economic growth, new jobs and new opportunities.

The Human Brain Project (HBP) is a major international scientific research project, involving over 100 academic and corporate entities in more than 20 countries. Funded by the European Commission (EC), the ten-year, 1 billion EUR Project was launched in 2013 with the goal "*to build a completely new ICT infrastructure for neuroscience, and for brain-related research in medicine and computing, catalysing a global collaborative effort to understand the human brain and its diseases and ultimately to emulate its computational capabilities.*"

PRACE and FET Flagships had already multiple interactions, with FET projects using PRACE facilities at the following call:

- 13th Call: project linked to the Graphene Flagship programme: SMoG – Simulation driven Morphing of supported led by Dr. V. Tozzini. 20.5 million core hours on Marconi – KNL @CINECA, IT.
- 12th Call: project linked to Graphene Flagship: Charge and Spin Hall Kubo Conductivity by Order N Real Space Methods led by Dr. S. Roche. 19.8 million core hours on MareNostrum @BSC, SP.
- 9th Call: project AESFTl led by M. Calandra of CNRS, partner in the Graphene Flagship Initiative. 9 million core hours on CURIE @GENCI @CEA, FR.
- 8th Call: Prof. S. Roche project Longitudinal and Transverse Electronic Transport in Atomically Doped Graphene from First Principles, 22 million core hours on CURIE @GENCI @CEA, FR. See PRACE Success story: [60].
- 8th Call: project PentaGate-L, Tracing lipid-mediated gating and permeation of pentameric ligand-gated ion channels in atomic detail, by Dr. M. Baaden of CNRS, partner in HBP Flagship. 21 million core hours on CURIE @GENCI @CEA, FR.
- 7th Call: project linked to HBP Flagship: SMOLER, Synaptic Mechanisms underlying Odor LEarning and Recognition led by Dr. M. Migliore. 13 million core hours on Fermi @CINECA, IT.
- 6th Call: project in chemical sciences & materials by Prof. S. Roche, linked to Graphene Flagship, 14.4 million core hours on CURIE @ GENCI@CEA, FR.

Many projects supported by PRACE have links with large scale instruments or European Initiatives, such as ENES, EC-EARTH, ESO, CERN, Van Allen Belt Probes, LASERLAB-EUROPE, the Herschel telescope, and the Human Brain Project.

4.8.5 SESAME-NET

The aim of SESAME-Net was to create an open and inclusive European network of Competence Centres and Organisations joining forces in order to raise SMEs' awareness on HPC and demonstrate its features and benefits. SESAME Net became an entry point to HPC for SMEs even for SMEs from countries that did not have such centres.

The project started in June 2015 and run until May 2017. The project compiled a large number of Best-practice guides that target both HPC Competence Centres and SMEs. The project has also produced a series of success stories presenting successful adoption of HPC in the industrial context. SESAME-Net Project has setup an online discussion forum between HPC centres and SMEs to enhance their interaction, and built a pan-European database of potential industrial HPC users. This material is available on the project web site [24].

Members of the SESAME-Net Project Consortium have participated at the PRACE IAC events that took place during PRACEdays 2017 in Barcelona. Soon after, T. Ilijaš, Project Coordinator of SESAME-Net Project and Head of the SESAME Network, was elected as a board member of the PRACE IAC in charge of Engineering/Manufacturing/SMEs. His duties include the transfer of best practices from SESAME Network to PRACE, including the HPC4SME Assessment Tool, whose objective is to offer SMEs the possibility to evaluate their own potential of using HPC. SESAME Network consists of companies and academic institutions from 13 European countries.

4.8.6 Pre-Commercial Procurement (PCP)

Pre-Commercial Procurement (PCP) is a model of procurement that is being promoted by the European Commission (EC) and is gaining usage in many European Union member states. In particular High Performance Computing (HPC) has been identified as an area in which basic R&D coupled with PCP can drive European innovation. In response to the Call FP7-INFRASTRUCTURES-2012-1 some partners of the PRACE-3IP formed an international consortium called the Group of Procurers (GoP), in order to perform a PCP on "Whole System Design for Energy Efficient HPC":

- CINECA (Italy);
- CSC (Finland);
- EPCC (UK);
- JUELICH (Germany);
- GENCI (France);
- PRACE AISBL as observer.

The goal of the PCP started by PRACE is to procure innovative R&D services that result in highly energy efficient HPC system components that are integrated into supercomputers. To allow for a fair comparison of the solutions proposed by different competitors, the project defined four benchmark applications. These applications were selected such that they reflect the needs of several relevant scientific user communities in Europe. For all of them both, time-to-solution as well as energy-to-solution were determined at the beginning of the project on state-of-the-art systems. In its final phase, PCP pilot systems were deployed within PRACE centres, allowing the demonstration of the improvements that the French company Bull, the Italian company E4, and the British company Maxeler were able to achieve.

This project was a new way to engage relationship with technology providers. Not co-design, as it was a competitive process, but deeper relationship and interaction than for a regular procurements. Furthermore, this process included an Open Dialogue Event, that took place in September 2012, that allowed PRACE to present its need to all major players. Moreover, it allowed to require that the overall R&D should be performed in Europe (80% in our case).

4.8.7 Public Procurement for Innovative Solutions (PPI)

The first coordinated acquisition at European level of world-class innovative HPC solutions has been launched [25], with a Public Procurement of Innovative solutions (PPI) aiming to catalyse the efforts to vitalise the European HPC ecosystem with a better coordination of supply and demand in a European acquisition market for HPC. This joint initiative could create benefits in multiple respects:

- More supercomputing resources will be efficiently exploitable for science and engineering applications in Europe within PRACE or future EuroHPC;
- R&D on HPC architectures and technologies in Europe will be strengthened as suitable incentives will be provided by this joint procurement process;
- The coordinated approach will give a greater weight and allow having more impact on design of the solutions according to the needs of scientists and engineers in Europe.

4.9 Summary of PRACE activities

In this section we give an overview of the main activities carried out by PRACE throughout the years and its implementation phase (IP) projects (statistics from February 2017), reminder and summary of computing resources granted; of training efforts, of dissemination actions.

4.9.1 Summary of Training activity

Since 2008 PRACE has offered a diverse training programme, including seasonal schools, workshops, scientific and industrial seminars. Additionally, the PRACE Training Portal [10], provides access to video tutorials and an extensive range of training materials. In 2017, two new educational opportunities were introduced: Massive Open Online Courses (MOOCs) and the CodeVault, a core repository for training codes open to everyone worldwide.

4.9.2 Summary of Access to Resources provided

One of the main objectives of PRACE throughout the years has been to provide Tier-0 access to researchers through a peer review system. By Call 15th for Proposals for PRACE Project Access, the following resources have been allocated throughout the years:

Call	# awarded projects	Total amount of Awarded Core Hours
EAC	10	324.328.480
1st Call	9	362.758.784
2nd Call	17	397.800.000
3rd Call	24	721.621.862
4th Call	43	1.129.084.877
5th Call	57	1.509.100.361
6th Call	57	1.273.060.000
7th Call	35	1.085.437.568
8th Call	44	1.191.203.286
9th Call	43	1.176.981.443
10th Call	48	1.083.399.847
11th Call	18	600.209.738
12th Call	25	638.243.942
13th Call	30	808.799.970
14th Call	62	2.074.536.666
15th Call	46	1.683.905.000
Grand Total	**568**	**16.060.471.824**

Table 1: Awarded projects up to 15th Call

4.9.3 Summary of Dissemination activity

PRACE has been very active throughout the years in the Communication and Outreach WP3 task. PRACE has been present at 44 events which include conferences, symposiums and seminars. PRACE has organised 5 PRACE Industrial Seminars, which were successfully merged into the PRACE Scientific and Industrial Conference (PRACEdays) in 2014. In 2016, the EXDCI project started with the organisation of the European HPC Summit Week, of which PRACEdays became the central event, with a second edition that took place from 16 May to 18 May 2017 in Barcelona, Spain. The fascinating conference included keynotes about European and international HPC strategy, scientific achievements, and industrial applications of HPC. The Barcelona Supercomputing Center (BSC) provided as local host an enjoyable environment and an excellent organisation.

PRACEdays17 was part of the European HPC Summit Week which offered a large number of interesting workshops from different actors in the HPC eco-system. The entire EHPCSW 2017 welcomed more than 350 attendees and 270 of them participated in PRACEdays17: a significant growth rate in attendance. The plenary sessions at PRACEdays17 provided the audience a wide range of keynote presentations: from the European Commission on the European Data Infrastructure (EDI) to an international speaker from China on Innovation of Intelligent Manufacturing Driven by Cloud HPC. Several parallel sessions covered a diversity of HPC related topics from leading speakers from science and industry. The third day offered the attendees an interesting panel discussion on "Support to HPC code: The gap between scientific code development and exascale technology. The software challenges for extreme scale computing faced by the Community" moderated by Irma Martinez.

PRACEdays17 closed with the traditional PRACE Award Session:

- Best Student Poster Award for M. Vögele (Max Planck Institute of Biophysics) for" *Finite size effects on the dynamics in simulations of lipid membranes*"
- Best Poster Award to F. Nathan Oliveira (BSC) for "*Nonlinear electromagnetic stabilization of ITG microturbulence by ICRF-driven fast ions in ASDEX Upgrade*"
- Best Industrial Presentation Award to Fabien Pierrat (Acobiom) for "*The MaRS (Matrix of RNA-Seq) Project*"
- Best Scientific Presentation Award to Alberto Giacomello (Sapienza University of Rome) for "*Robust bioinspired surfaces for underwater operation*"
- PRACE Ada Lovelace Award for HPC to Frauke Gräter (HITS)

Figure 12: Award Session at PRACEdays17 with S.Bogaerts, F. Oliveira, F.Gräter, A.Gregersen, M. Vögele, A.Giacomello, E.Lindahl

Figure 13: Group photo of EHPCSW17 participants

PRACE is present at science fairs and museums around Europe, to introduce the general public to PRACE, with particular emphasis on schoolkids. The workings of a supercomputer are made insightful and fun with video games, posters, and Fact Sheets. Additionally, PRACE has successfully carried out 5 Summer of HPC programmes since 2012, and produces a large amount of communication material, such as: PRACE Digest (7), PRACE Annual Report (5), Women in HPC Magazine, PRACE Fact Sheets (8). Other publications include: PRACE Scientific Case for HPC in Europe 2012-2020; and a Special Report on HPC for All. PRACE is present on social media such as LinkedIn, Twitter, Google+, YouTube, and Facebook.

Other major events for 2017 were the booth at ISC17 and SC17 and at the Digital Infrastructures for Research (DI4R) conference. At ISC17 PRACE signed a MoU with CHPC, South Africa (see section 4.9.4), and we welcomed more than 300 ISC visitors, with a dedicated booth space for the EXDCI project. At SC17 Tom Tabor, CEO of Tabor Communications, publisher of HPCwire presented personally the distinguished HPCwire readers and editor choice award in the category “Outstanding Leadership in HPC” to Prof. Dr. Anwar Osseyran, Chair of the PRACE Council, member of the Executive Board of SURF and CEO of SURFsara. In addition PRACE was also honoured to receive a shared HPCwire Editors’ Choice award in the category “Top HPC Enabled Scientific Achievement award”. At the second edition of the DI4R in Brussels, Europe’s leading e-infrastructures, EGI, EUDAT, GÉANT, OpenAIRE, PRACE and RDA Europe, invited all researchers, developers and service providers for two days of brainstorming and discussions under the theme “Connecting the building blocks for Open Science”. For the first time PRACE participates in the Organisation and Programme Committees of this innovative conference. DI4R 2017 have displayed the policies, processes, best practices, data and services that – leveraging today’s national, regional, European and international initiatives – are the building blocks of the European Open Science Cloud (EOSC) and European Data Infrastructure EDI). The conference has demonstrated how open science, higher education, and innovators can benefit from these building blocks, and contributed to advance integration and cooperation between initiatives.

4.9.4 Summary of PRACE Memorandum of Understanding (MoU)s

PRACE receives requests for collaborations from various organisations around the world, e.g. in Europe EGI-CSIRT (sharing information on security incidents and specific vulnerability risks), GÉANT (Network services) or EUDAT (data services and security), and abroad with RIST (Japan), XSEDE (USA), China, Singapore, South America and the Pawsey Supercomputing Center (Australia).

Recent requests have been received from RIST (Japan) and XSEDE (USA) to produce a successor to the existing RIST MoU (signed by PRACE aisbl in 2014). A meeting was held at SC16 with RIST (Japan) and XSEDE (USA), at which A. Kennedy (Chair of BoD in 2016) and F. Berberich (member of BoD) represented PRACE. An approach was also received from the CHPC (South Africa). Due to the increased importance of international collaborations and the many requests PRACE received, the BoD will work on an International Strategy in order to define clear rules and priorities in the collaboration with international partners. A list of MoUs is provided in 6.3 - Annex 3: PRACE partnerships. The outcome of the PRACE-RIST-XSEDE meeting was the creation of a three party MoU. On 4 April 2017, the Research Organization for Information Science and Technology (RIST) (President: Masahiro Seki), the Partnership for Advanced Computing in Europe (PRACE) (Managing Director: Serge Bogaerts) and the Extreme Science and Engineering Discovery Environment (XSEDE) (Principal Investigator: John Towns) concluded the MoU on information exchange concerning promotion of use of advanced research computing. The MoU between RIST, PRACE and XSEDE will strengthen and deepen their co-operation at the international level and reinforce the advanced research computing ecosystem. As it is extremely beneficial for the three parties to exchange information in the area of promotion of shared use of advanced research computing resources and services, an MoU with following elements has been agreed upon:

1. *Exchange of information:* Mutual exchange of experiences and knowledge in user selection and user support etc. is helpful for the three parties in order to execute their projects more effectively and efficiently.
2. *Interaction amongst the staff of the parties in pursuing any identified collaboration opportunities:* Due to the complex and international nature of science, engineering and analytics challenge problems that require highly advanced computing solutions, collaborative support between RIST, PRACE and XSEDE will enhance the productivity of globally distributed research teams.
3. *Holding technical meetings:* Technical meetings will be held to support cross organisational information exchange and collaboration.

On 17 May 2017, a ceremony was held during PRACEdays17 (16-18 May, Barcelona, Spain). The representatives of each party gave presentations in celebration of the signature of this MoU.

In the framework of this MoU a joint PRACE-XSEDE-RIST call is planned. The call will address support actions for interoperability for PRACE, XSEDE and RIST with test allocations and in a 2nd step joint allocations for production for PRACE and XSEDE. The call is scheduled for the 2nd quarter in 2018.

Figure 14: RIST-XSEDE-PRACE MoU signature

An approach was also received from the Centre for High Performance Computing, South Africa (CHPC). On 20 June 2017, PRACE and the CHPC signed a MoU during the International Supercomputing Conference 2017. The purpose of this MoU is to implement a fruitful exchange of information in the fields of computational science and engineering. In addition, the aim is to identify collaboration and partnership opportunities as a strategic objective. To achieve these objectives, a set of tasks will be identified and supervised by coordinators designated by the CHPC and PRACE. The follow-up of the implementation of this MoU will also be the subject of technical meetings between the two parties.

Figure 15: CHPC (South Africa) – PRACE MoU signature

Due to the increased importance of international collaborations and the many requests PRACE received, the BoD will work on an International Strategy in order to define clear rules and priorities in the collaboration with international partners. A list of MoUs is provided in 6.3 - Annex 3: PRACE partnerships

5 Conclusion

In conclusion, the whole society is probably the ultimate stakeholder that should benefit, directly or indirectly, from our work. Over the past two decades, HPC has developed into a key scientific tool, alongside theory-based and experimental research methods. PRACE ensures that all European research and development institutions have access to high-performance computing systems and services, enabling them to tackle the diverse range of challenges facing humanity. Computer simulations speed up the process of acquiring knowledge tremendously, by shortening or even completely substituting complex, time consuming laboratory experiments. This global trend requires significant amount of effort by PRACE, in order to continue assisting the traditional HPC community (represented by CoEs), while opening its doors to new user communities from Artificial Intelligence and Big-Data and their fast-evolving technologies. And all these should be realized under the prism of the way to Exascale (ETP4HPC) and in the context of EOSC / EDI within the DSM.

The EU HPC ecosystem has been moving significantly forward since PRACE's creation in 2010, with important EC communications and the launch of successive new initiatives and programmes under and along Horizon 2020. This constitutes a successful strategy, but a lot remains to be done. The European HPC ecosystem remains a complex but vivid one, in the midst of a rapidly evolving and competitive worldwide landscape. PRACE 2 is a step further in this direction, and will continue to evolve in the context of the EuroHPC initiative. PRACE and partners (all ecosystem stakeholders) must keep a close eye on worldwide HPC developments, and leverage solid tools and methods to stay in the race, reacting dynamically – leveraging actions and methods such as those explained in this report. PRACE can and must contribute to positively influence EU policy for better and stronger public and private investments in HPC, joining forces with other strong voices, but also reaching the general public and making HPC both well-understood and fancy.

6 Annexes

6.1 Annex 1: The new European HPC research landscape

The new European HPC research landscape is comprised of 9 Centres of Excellence, 2 Coordination and Support Actions and 19 Research and Innovation Actions (over various fields), all of which are supported by PRACE and ETP4HPC.

Horizon 2020 had a call for proposals titled “Towards exascale high performance computing”. The aim of the call was to attract projects that can achieve world-class extreme scale computing capabilities in platforms, technologies and applications.

Starting in autumn 2015, 21 projects were selected – 2 Coordination and Support projects (EXDCI and Eurolab-4-HPC) and 19 Research and Innovation Projects. Then two more ‘co-design’ projects were funded from the FETHPC 2016 call. The projects are briefly described below.

<u>Coordination and Support Projects</u>

EXDCI

PRACE, ETP4HPC and EESI come together within EXDCI to coordinate the strategy of the European HPC Ecosystem in order to deliver its objectives. In particular, EXDCI will harmonize the road-mapping and performance monitoring activities of the ecosystem to produce tools for coherent strategy-making and its implementation by:

- Producing and aligning roadmaps for HPC Technology and HPC Applications;
- Measuring the implementation of the European HPC strategy;
- Building and maintaining relations with other international HPC activities and regions;
- Supporting the generation of young talent as a crucial element of the development of European HPC.

EuroLab-4-HPC

The EuroLab-4-HPC project goal is to build connected and sustainable leadership in high-performance computing systems by bringing together the different and leading performance orientated communities in Europe, working across all layers of the system stack and at the same time, fuelling new industries in HPC.

<u>Research and Innovation Projects</u>

ALLScale - An Exascale Programming, Multi-objective Optimisation and Resilience Management Environment Based on Nested Recursive Parallelism

The AllScale environment, the focus of this project, will provide a novel, sophisticated approach enabling the decoupling of the specification of parallelism from the associated management activities during program execution. Its foundation is a parallel programming model based on nested recursive parallelism, opening up the potential for a variety of compiler and runtime system based techniques adding to the capabilities of resulting applications.

AllScale will boost the development productivity, portability, and runtime, energy, and resource efficiency of parallel applications targeting small to extreme scale parallel systems by leveraging the inherent advantages of nested recursive parallelism and will be validated with applications from fluid dynamics, environmental hazard and space weather simulations provided by SME, industry and scientific partners.

ANTAREX - AutoTuning and Adaptivity appRoach for Energy efficient eXascale HPC systems

The main goal of the ANTAREX project is to provide a breakthrough approach to express application self-adaptivity at design-time and to runtime manage and autotune applications for green and heterogenous HPC systems up to the Exascale level.

ANTAREX will solve the challenging problem where energy-efficient heterogeneous supercomputing architectures need to be coupled with a radically new software stack capable of exploiting the benefits offered by the heterogeneity at all the different levels (supercomputer, job, node) to meet the scalability and energy efficiency required by Exascale supercomputers. ANTAREX will tackle this by proposing a disruptive holistic approach spanning all the decision layers composing the supercomputer software stack and exploiting effectively the full system capabilities (including heterogeneity and energy management).

ComPat - Computing Patterns for High Performance Multiscale Computing

This project we will develop multiscale computing algorithms capable of producing high-fidelity scientific results which are scalable to exascale computing systems. One of the main objectives of the project is to develop generic and reusable High Performance Multiscale Computing algorithms that will address the exascale challenges posed by heterogeneous architectures thus enabling to run multiscale applications with extreme data requirements while achieving scalability, robustness, resiliency, and energy efficiency. The project approach is based on generic multiscale computing patterns which allow the implementation of customized algorithms to optimise load balancing, data handling, fault tolerance and energy consumption under generic exascale application scenarios. An experimental execution environment will be used to measure performance characteristics and develop models that can provide reliable performance predictions for emerging and future exascale architectures. The viability of the approach will be demonstrated by implementing nine grand challenge applications which are exascale-ready.

ECOSCALE - Energy-efficient Heterogeneous COmputing at exaSCALE

ECOSCALE tackles the problem of refining HPC applications and the architecture of future HPC systems through a co-design approach that spans a scalable HPC hardware platform, a middleware layer, a programming and a runtime environment as well as a high-level design environment for mapping applications onto the system. It aims to achieve this by proposing a scalable programming environment and hardware architecture tailored to the characteristics and trends of current and future HPC applications - reducing significantly data traffic, energy consumption and delays.

This will be achieved through a novel heterogeneous energy-efficient hierarchical architecture and a hybrid MPI+OpenCL programming environment and runtime system.

ESCAPE- Energy-efficient SCalable Algorithms for weather Prediction at Exascale

ESCAPE aims for innovative actions which will fundamentally reform Earth-system modelling by developing world-class, extreme-scale computing capabilities for European operational numerical weather prediction (NWP) and future climate models.

This is required as existing software are ill-equipped to adapt to the rapidly evolving hardware or current processor arrangements are not necessarily optimal for weather and climate simulations.

It will aim to achieve this by:

- Defining and encapsulating the fundamental algorithmic building blocks ("Weather & Climate Dwarfs") underlying weather and climate services. This is the pre-requisite for any subsequent co-design, optimization, and adaptation efforts;
- Combining ground-breaking frontier research on algorithm development for use in extreme-scale, high-performance computing applications, minimizing time- and cost-to-solution;
- Synthesizing the complementary skills of all project partners. This includes ECMWF, the world leader in global NWP together with leading European regional forecasting consortia, teaming up with excellent university research and experienced high-performance computing centres, two world-leading hardware companies, and one European start-up SME, providing entirely new knowledge and technology to the field.

ExaFLOW - Enabling Exascale Fluid Dynamics Simulations

Fluid Dynamics (FD) simulations can be used in the analysis of many systems in the natural world. The complexities and nature of fluid flows implies that the resources needed to computationally model such problems is virtually unbounded. FD simulations therefore are a natural driver for exascale computing and have the potential for substantial societal impact.

The main goal of this project is to address algorithmic challenges to enable the use of accurate simulation models in exascale environments. Driven by problems of practical engineering interest the project will focus on important simulation aspects including:

- Error control and adaptive mesh refinement in complex computational domains;
- Resilience and fault tolerance in complex simulations;
- Heterogeneous modelling;
- Evaluation of energy efficiency in solver design;
- Parallel input/output and in-situ compression for extreme data.

The algorithms developed by the project will be prototyped in major open-source simulation packages in a co-design fashion, exploiting software engineering techniques for exascale. Building on the results of previous exascale projects (such as CRESTA and EPiGRAM) the project will exploit advanced and novel parallelism features required for emerging exascale architectures. The results will be validated in a number of pilot applications of concrete practical importance in close collaboration with industrial partners.

ExaHyPe - An Exascale Hyperbolic PDE Engine

Many aspects of our life, but also cutting-edge research questions, hinge on the solution of large systems of partial differential equations expressing conservation laws. Yet, our ability to exploit the predictive power of the models in which they are used is still severely limited by the computational costs of their solution.

This project will develop a new exascale hyperbolic simulation engine based on high-order communication-avoiding Finite-Volume/Discontinuous-Galerkin schemes and thus yielding high computational efficiency. Utilising structured, spacetree grids that offer dynamic adaptivity in space and time at low memory footprint the project will consequently optimise all compute kernels to minimise energy consumption and exploit inherent fault-tolerance properties of the numerical method.

As a general hyperbolic solver, the exascale engine will drive research in diverse areas and relieve scientists from the burden of developing robust and efficient exascale codes. Its development is driven by precise scientific goals, addressing grand challenges in geo-physics and astrophysics.

ExaNest - European Exascale System Interconnect and Storage

ExaNeSt will develop, evaluate and prototype the physical platform and architectural solution for a unified Communication and Storage Interconnect whilst taking into account the physical rack and environmental structures required to deliver European Exascale Systems.

The consortium brings technology, skills and knowledge across the entire value chain and using direction from the ETP4HPC roadmap will model, simulate and validate through prototype, a system with:

- High throughput, low latency connectivity, suitable for exascale-level compute, their storage and I/O, with congestion mitigation, QoS guarantees, and resilience;
- Support for distributed storage located with the compute elements providing low latency that non-volatile memories require, while reducing energy, complexity and costs;
- Support for task-to-data software locality models to ensure minimum data communication energy overheads and property maintenance in databases;
- Hyper-density system integration scheme that will develop a modular, commercial, European-sourced advanced cooling system for exascale in around 200 racks while maintaining reliability and cost of ownership;
- The platform management scheme for big-data I/O to this resilient, unified distributed storage compute architecture;
- The ability to demonstrate the applicability of the platform for the complete spectrum of Big Data applications.

All aspects will be steered and validated with the first-hand experience of HPC applications and experts, through kernel turning and subsequent data management and application analysis.

ExaNode - European Exascale Processor Memory Node Design

ExaNoDe will investigate, develop and pilot a highly efficient, highly integrated, multi-way, high-performance, heterogeneous compute element aimed towards exascale computing and demonstrated using hardware-emulated interconnect. Utilizing low-power processors and advanced nanotechnologies ExaNoDe will be based on the Unimem memory and system design paradigm thus providing low-latency, high-bandwidth and resilient memory access, scalable to Exabyte levels.

The ExaNoDe compute element aims towards exascale compute goals through:

- Integration of the most advanced low-power processors and accelerators supported by research and innovation in the deployment of associated nanotechnologies and in the mechanical requirements to enable the development of a high-density, high-performance integrated compute element with advanced thermal characteristics and connectivity to the next generation of system interconnect and storage;
- Undertaking essential research to ensure the ExaNoDe compute element provides necessary support of HPC applications including I/O and storage virtualization techniques, operating system, semantically aware runtime capabilities and PGAS, OpenMP and MPI paradigms;
- The development of an instantiation of a hardware emulation of interconnect to enable the evaluation of Unimem for the deployment of multiple compute elements and the evaluation, tuning and analysis of HPC mini-apps.

ExCAPE - Exascale Compound Activity Prediction Engine

The ExCAPE considers scalable machine learning of complex models on extreme data and specifically for predicting compound bioactivity for the pharmaceutical industry.

Small scale approaches to machine learning have already been tried and show great promise to reduce empirical testing costs by acting as a virtual screen to filter out tests unlikely to work. However, it is not yet possible to use all available data to make the best possible models, as algorithms capable of learning the best models do not scale to such sizes and heterogeneity of input data. There are also further challenges including imbalanced data, confidence estimation, data standards model quality and feature diversity.

The ExCAPE project aims to solve these problems by producing state of the art scalable algorithms and implementations suitable for running on future Exascale machines. These approaches will scale programs for complex pharmaceutical workloads to input data sets at industry scale. The programs will be targeted at exascale platforms by using a mix of HPC programming techniques, advanced platform simulation for tuning and suitable accelerators.

EXTRA - Exploiting eXascale Technology with Reconfigurable Architectures

The EXTRA project focuses on the fundamental building blocks for run-time reconfigurable exascale HPC systems and will create a new and flexible exploration platform for developing reconfigurable architectures, design tools and HPC applications with run-time reconfiguration. The idea is to enable the efficient co-design and joint optimization of architecture, tools, applications and reconfiguration technology in preparation for the necessary HPC hardware nodes of the future.

The EXTRA project covers the complete chain from architecture up to the application including:

- More coarse-grain reconfigurable architectures that allow reconfiguration on higher functionality levels and therefore provide much faster reconfiguration than at the bit level;
- The development of just-in time synthesis tools that are optimized for fast and efficient re-synthesis of application phases to new, specialized implementations through reconfiguration;
- The optimization of applications that maximally exploit reconfiguration;
- Suggestions for improvements to reconfigurable technologies to enable the proposed reconfiguration of the architectures.

greenFLASH - Green Flash, energy efficient high performance computing for real-time science

Green Flash is based on a strong interaction between academic and industrial partners and its goal is to design and build a prototype for a Real-Time Controller (RTC) targeting the European Extremely Large Telescope (E-ELT) Adaptive Optics (AO) instrumentation. Technical challenges, emerging from the combination of high data transfer bandwidth, low latency and high throughput requirements need to be tackled and Green Flash, we will propose technical solutions, assess these enabling technologies through prototyping and assemble a full scale demonstrator to be validated with a simulator and tested on sky.

INTERTWInE - Programming Model INTERoperability ToWards Exascale

This project seeks to address the interoperability - both at the specification level and at the implementation level, between different programming APIs which may be used to program highly parallel Exascale systems likely to be composed of a hierarchy of architectural levels.

INTERTWinE will focus on seven key programming APIs - MPI, GASPI, OpenMP, OmpSs, StarPU, QUARK and PaRSEC. Interoperability requirements, and evaluation of implementations will be driven by a set of kernels and applications and the project will implement a co- design cycle, by feeding back advances in API design and implementation into the applications and kernels, thereby driving new requirements and hence further advances.

MANGO - Exploring Manycore Architectures for Next-GeneratiOn HPC systems

MANGO targets to achieve extreme resource efficiency in future QoS-sensitive HPC through ambitious cross-boundary architecture exploration for performance/power/predictability (PPP) based on the definition of new-generation high-performance, power-efficient, heterogeneous architectures with native mechanisms for isolation and quality-of-service, and an innovative two-phase passive cooling system.

MANGO will develop a toolset for PPP and explore holistic pro-active thermal and power management for energy optimization including chip, board and rack cooling levels, creating a hitherto inexistent link between hardware and software effects at all layers.

Ultimately, the combined interplay of the multi-level innovative solutions brought by MANGO will result in a new positioning in the PPP space, ensuring sustainable performance as high as 100 PFLOPS for the realistic levels of power consumption (<15MWatt) delivered to QoS-sensitive applications in large-scale capacity computing scenarios.

MontBlanc-3 - European scalable and power efficient HPC platform based on low-power embedded technology

The Mont-Blanc 3 project follows the Mont-Blanc & Mont-Blanc 2 FP7 projects, and aims to create a new high-end HPC platform that is able to deliver a new level of performance/energy ratio whilst executing real applications - achieving this by integrating work on architecture, simulation and a software ecosystem.

The technical objectives are:

- To design a well-balanced architecture and to deliver the design for an ARM based SoC or SoP (System on Package) capable of providing pre-exascale performance when implemented in the time frame of 2019-2020. The predicted performance target must be measured using real HPC applications;
- To maximise the benefit for HPC applications with new high-performance ARM processors and throughput-oriented compute accelerators designed to work together within the well-balanced architecture;
- To develop the necessary software ecosystem for the future SoC - to ensure this ARM architecture path will be successful in the market.

NextGenIO - Next Generation I/O for Exascale

The overall objective of NEXTGenIO is to design and prototype a new, scalable, high-performance, energy efficient computing platform designed to address the challenge of delivering scalable I/O performance to applications at the Exascale. It will achieve this using highly innovative, non-volatile, dual in-line memory modules (NV-DIMMs) solving a key part of the Exascale challenge and enable HPC and Big Data applications to overcome the limitations of today's HPC I/O subsystems.

The project will deliver immediately exploitable hardware and software results and show how to deliver high performance I/O at the Exascale.

NLAFET - Parallel Numerical Linear Algebra for Future Extreme-Scale Systems

NLAFET will enable a radical improvement in the performance and scalability of a wide range of real-world applications relying on linear algebra software, by developing novel architecture-aware algorithms and software libraries and the supporting runtime capabilities to achieve scalable performance and resilience on heterogeneous architectures. The focus will be on a critical set of fundamental linear algebra operations including direct and iterative solvers for dense and sparse linear systems of equations and eigenvalue problems.

The main research objectives are:

- Development of novel algorithms that expose as much parallelism as possible, exploit heterogeneity, avoid communication bottlenecks, respond to escalating fault rates and help meet emerging power constraints;
- Exploration of advanced scheduling strategies and runtime systems focusing on the extreme scale and strong scalability in multi/many-core and hybrid environments;
- Design and evaluation of novel strategies and software support for both offline and online auto-tuning.

The validation and dissemination of results will be done by integrating new software solutions into challenging scientific applications in materials science, power systems, study of energy solutions and data analysis in astrophysics.

READEX - Runtime Exploitation of Application Dynamism for Energy-efficient eXascale computing

The READEX consortium consists of European experts from academia, HPC resource providers and industry and will develop a tools-aided methodology to exploit the dynamic behaviour of applications to achieve improved energy-efficiency and performance of applications. The developed tool-suite and the READEX Programming Paradigm will be efficient and scalable to support current and future extreme scale systems and together achieve an improvement in energy-efficiency of up to 22.5%.

SAGE - Percipient StorAGe for Exascale Data Centric Computing

The SAGE project will demonstrate the first instance of intelligent data storage, uniting data processing and storage as two sides of the same rich computational model. This will enable sophisticated, intention-aware data processing to be integrated within a storage system infrastructure, combined with the potential for Exabyte scale deployment in future generations of extreme scale HPC systems.

The objectives of the project are to:

- Provide a next-generation multi-tiered object-based data storage system supporting future-generation multi-tier persistent storage media and integral computational capability, within a hierarchy;
- Significantly improve overall scientific output through advancements in systemic data access performance and drastically reduced data movements;
- Provide a roadmap of technologies supporting data access for both Exascale/Exabyte and High Performance Data Analytics;
- Provide programming models, access methods and support tools validating their usability, including ‘Big-Data’ access and analysis methods;
- Co-Design and validate on a smaller representative system with earth sciences, meteorology, clean energy, and physics communities;
- Project suitability for extreme scaling through simulation based on evaluation results.

FETHPC-2016 DEEP-EST

The DEEP-EST ("DEEP - Extreme Scale Technologies") project will create a first incarnation of the Modular Supercomputer Architecture (MSA) and demonstrate its benefits. In the spirit of the DEEP and DEEP-ER projects, the MSA integrates compute modules with different performance characteristics into a single heterogeneous system. Each module is a parallel, clustered system of potentially large size. A federated network connects the module-specific interconnects. MSA brings substantial benefits for heterogeneous applications/workflows: each part can be run on an exactly matching system, improving time to solution and energy use. This is ideal for supercomputer centres running heterogeneous application mixes (higher throughput and energy efficiency). It also offers valuable flexibility to the compute providers, allowing the set of modules and their respective size to be tailored to actual usage.

The DEEP-EST prototype will include three modules: general purpose Cluster Module and Extreme Scale Booster supporting the full range of HPC applications, and Data Analytics Module specifically designed for high-performance data analytics (HPDA) workloads. Proven programming models and APIs from HPC (combining MPI and OmpSs) and HPDA will be extended and combined with a significantly enhanced resource management and scheduling system to enable straightforward use of the new architecture and achieve highest system utilisation and performance. Scalability projections will be given up to the Exascale performance class. The DEEP-EST prototype will be defined in close co-design between applications, system software and system component architects. Its implementation will employ European integration, network and software technologies. Six ambitious and highly relevant European applications from HPC and HPDA domains will drive the co-design, serving to evaluate the DEEP EST prototype and demonstrate the benefits of its innovative Modular Supercomputer Architecture.

FETHPC-2016 EUROEXA

To achieve the demands of extreme scale and the delivery of exascale, we embrace the computing platform as a whole, not just component optimization or fault resilience. EuroEXA brings a holistic foundation from multiple European HPC projects and partners together with the industrial SME focus of MAX for FPGA data-flow; ICE for infrastructure; ALLIN for HPC tooling and ZPT to collapse the memory bottleneck; to co-design a ground-breaking platform capable of scaling peak performance to 400 PFLOP in a peak system power envelope of 30MW; over four times the performance at four times the energy efficiency of today's HPC platforms. Further, we target a PUE parity rating of 1.0 through use of renewables and immersion-based cooling.

We co-design a balanced architecture for both compute- and data-intensive applications using a cost-efficient, modular-integration approach enabled by novel inter-die links and the tape-out of a resulting EuroEXA processing unit with integration of FPGA for data-flow acceleration. We provide a homogenised software platform offering heterogeneous acceleration with scalable shared memory access and create a unique hybrid geographically-addressed, switching and topology interconnect within the rack while enabling the adoption of low-cost Ethernet switches offering low-Latency and high-switching bandwidth.

Working together with a rich mix of key HPC applications from across climate/weather, physics/energy and life-science/bioinformatics domains we will demonstrate the results of the project through the deployment of an integrated and operational petaflop level prototype hosted at STFC. Supported by run-to-completion platform-wide resilience mechanisms, components will manage local failures, while communicating with higher levels of the stack. Monitored and controlled by advanced runtime capabilities, EuroEXA will demonstrate its co-design solution supporting both existing pre-exascale and project-developed exascale applications.

6.2 Annex 2: PRACE bodies (SSC, AC, IAC)

Name	Field	Organisation, Country
Marina Bécoulet	Plasma Physics / Fusion	CEA, France
Carlo Massimo Casciola	Engineering / CFD	University of Rome, Italy
Luke Drury	Universe Sciences	Dublin Institute for Advanced Studies, Ireland
Claudia Filippi	Electronic structure/multiscale modelling	University of Twente, Faculty of Science and Technology, The Netherlands
Frauke Gräter	Biophysics	Heidelberg Institute for Theoretical Studies (HITS)
Laura Grigori	Numerical Mathematics / HPC	INRIA/University Pierre and Marie Curie, France
Dimitri Komatitsch	Computational Earth Sciences	LMA CNRS-MRS, France
Petros Koumoutsakos	Computational Science and Engineering	ETH Zürich, Switzerland
Erik Lindahl (Chair as of 2 March 2017, for 1 yea)	Life Sciences	KTH Royal Institute of Technology, Sweden
Núria López	Computational Chemistry	Institute Catalan of Chemistry Research, Spain
Antonio Navarra	Environmental Sciences	CMCC, Italy
Ignacio Pagonabarraga Mora	Computational Physics	University of Barcelona, Spain
Mike Payne	Computational Physics	University of Cambridge/EPSRC Centre, United Kingdom
Matej Praprotnik	Chemistry / Multiscale Modeling	National Institute of Chemistry / University of Ljubljana, Faculty of Mathematics and Physics, Slovenia
Sinéad Ryan (Vice Chair as of 17 October 2017, until 2 March 2018)	Particle Physics / Mathematics	University Dublin, Trinity College Dublin, School of Mathematics, Ireland
Per Stenström	Computer Science / HPC	University of Technology, Göteborg, Sweden
Julia Yeomans	Physics: Soft and Biological Matter	University of Oxford, Rudolf Peierls Centre for Theoretical Physics, United Kingdom
Claudio Zannoni	Physical Chemistry of Materials	University of Bologna, Italy

Table 2: Scientific Steering Committee (SSC) Membership, 22 November 2017

Name	Field	Country
Edouard Audit	Astrophysics	France
Marc Baaden	Biology / Chemistry	France
Luca Biferale	Turbulence / Engineering	Italy
George Biros	Computational Engineering	USA
Pascale Braconnot	Earth / Climate	France
Giovanni Ciccotti	Structure of Matter / Biological Systems / Molecular Dynamics	Italy
Rafael Delgado	Condensed Matter / Chemistry / Materials	Spain
Wilco Hazeleger	Climate	Netherlands
Simone Hochgreb	Engineering I	United Kingdom
Petros Koumoutsakos (Chair)	Computation Sciences and Engineering	Switzerland
Fernando Martin	Chemistry / Bio	Spain
Luciano Rezzolla	Astrophysics	Germany
Carme Rovira Virgili	Chemistry / Bio	Spain
Dietrich Wolf	Computational / Statistical Physics	Germany

Table 3: Access Committee (AC) Membership, 17 Marsh 2017

Name	Organisation	Field	Country
Dieter Jahn (Vice-Chair, from 18/09/2017 for 2 years)	BASF	Materials/Chemistry	Germany
Gibert Enric	Pharmacelera	Life Sciences / Pharma	Spain
Henk Coenen	NXP	Telecom / Electronics	Netherlands
Lee Margetts (Chair, from 18/09/2017 for 2 years)	NAFEMS	ISV	United Kingdom
Marc Morere	Airbus	Aeronautics / Aerospace	France
Martin Winter	CEFIC	Materials / Chemistry	Germany
Tomi Ilijas	Arctur	Engineering / Manufacturing / SMEs	Slovenia
Alain Martin	EDF	Energy	France
Jean-Pierre Panziera (Observer)	ETP4HPC	HPC Vendors	France

Table 4: Industrial Advisory Committee (IAC) Membership, 22 November 2017

6.3 Annex 3: PRACE partnerships

PRACE has a Memorandum of Understanding (MoU) with:

Extreme Science and Engineering Discovery Environment

GÉANT – European e-infrastructure and services for research and education

EGI – The European Grid Initiative

EUDAT – the collaborative Pan-European infrastructure

EMI – European Middleware Initiative

IGE – Initiative for Globus in Europe

Research Organisation for Information Science and Technology

The Human Brain Project

Centre for High Performance Computing

PRACE is a partner of the following projects:

EESI2 – European Exascale Software Initiative

EXDCI European Extreme Data & Computing Initiative

EOSCpilot The European Open Science Cloud for Research Pilot Project

ELItrans project

eInfraCentral

PRACE is a consortium member of:
EEF – European e-Infrastructure Forum

PRACE is represented in an external board of:

EGI – European Grid Infrastructure

e·nventory – The European e·Infrastructures Observatory

EUGridPMA
PRACE is a Relying Party.

GÉANT

ETP4HPC – European technology Paltform for High Performance Computing

PRACE has collaborated in other ways with:

XSEDE
PRACE and XSEDE jointly organised the 2010, 2011 and 2012 "EU-US Summer Schools on HPC Challenges in Computational Sciences", and published a joint call for Expressions of Interest (EoI) for Joint Access by International Teams.

RIKEN
In 2013 the RIKEN Advanced Institute for Computational Science (AICS) joined up with PRACE and XSEDE to organise the fourth "International Summer School on HPC Challenges on Computational Sciences" (formerly called the EU-US Summer School series).

compute canada – calcul canada
In 2014 Compute Canada – Calcul Canada joined the organisation of the "International Summer School on HPC Challenges on Computational Sciences", becoming the fourth international organiser together with PRACE, XSEDE, and RIKEN.

LinkSCEEM-2
PRACE supported the organisation of CSC 2013 in Cyprus with LinkSCEEM-2

e-IRG
PRACE is a stakeholder in the provision of an ICT based RI

CoPoRI