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References and Applicable Documents

[1] The UK Corporate Governance Code, September 2014 (at s. A.3.1), https://www.frc.org.uk/Our-Work/Publications/Corporate-Governance/UK-Corporate-Governance-Code-2014.pdf

[2] Toward a Stewardship Theory of Management, Academy of Management Review, pp.20-47

[3] http://ec.europa.eu/taxation_customs/taxation/vat/index_en.htm

[4] http://eur-lex.europa.eu/legal-content/EN/TXT/HTML/?uri=CELEX:32006L0112&from=EN

[5] Communication issued in 2012 by Belgian tax authority: Circulaire n° E.T.121.844 (AGFisc N° 1/2012)

[6] https://ec.europa.eu/research/infrastructures/pdf/council_regulation_eric.pdf

[7] http://www.prace-project.eu/

[8] http://www.prace-ri.eu/prace-kpi/

[9] https://events.prace-ri.eu/

[10] www.prace-ri.eu/hpc-access/shape-programme

[11] http://www.prace-ri.eu/white-papers/

[12] http://www.prace-ri.eu/organisation/

[13] https://summerofhpc.prace-ri.eu/

[14] PRACE-PP, D2.5.1 “Analysis of the HPC Ecosystem”

[15] PRACE-PP, D2.5.2 “Report on links with HPC Ecosystem”

[16] PRACE-1IP, D2.3.2 “Funding scenarios for the PRACE infrastructure”

[17] PRACE-3IP, D2.2 “New PRACE Relationships with other Entities”

[18] PRACE-3IP, D5.3.3 “Report on the SHAPE implementation”

[19] PRACE-4IP, D2.1 “First Report on PRACE 2.0 Development”

[20] PRACE 4IP, D5.1 “Market and Technology Watch Report Year 1”

[21] https://sesamenet.eu

[22] https://ec.europa.eu/digital-single-market/en/news/first-milestone-european-hpc-strategy-achieved

[23] http://ec.europa.eu/invest-in-research/pdf/ip_recommendation_en.pdf

[24] 1984 Edward Freeman “Strategic Management: A Stakeholder Approach"

[25] 2010 Edward Freeman, Jeffrey S. Harrison, Andrew C. Wicks “Stakeholder Theory: The State of the Art”

[26] ETP4HPC www.etp4hpc.eu

[27] https://ec.europa.eu/programmes/horizon2020/en/node/824#Article

[28] http://www.etp4hpc.eu/en/euexascale.html

[29] http://www.etp4hpc.eu/en/sc16-bof.html

[30] Com(2012) 45 Communication From The Commission To The European Parliament, The Council, The European Economic And Social Committee And The Committee Of The Regions “High-Performance Computing: Europe's place in a Global Race”

[31] https://ec.europa.eu/programmes/horizon2020/en/h2020-section/high-performance-computing-hpc

[32] https://ec.europa.eu/digital-agenda/en/high-performance-computing-contractual-public-private-partnership-hpc-cppp

[33] https://ec.europa.eu/digital-single-market/en/news/study-high-performance-computing-eu-progress-implementation-european-hpc-strategy-final-report

[34] https://ec.europa.eu/digital-single-market/en/high-performance-computing

[35] http://ec.europa.eu/programmes/horizon2020/en/h2020-section/future-and-emerging-technologies

[36] http://ec.europa.eu/programmes/horizon2020/en/h2020-section/e-infrastructures

[37] http://www.eesi-project.eu/
[38] https://exdci.eu/
[39] https://ec.europa.eu/digital-single-market/en/european-cloud-initiative
[40] http://knowledgebase.e-irg.eu/documents/243153/299805/IPCEI-HPC-BDA.pdf
[41] Finding Your Funding Model: A Practical Approach to Nonprofit Sustainability - By Peter Kim, Gail Perreault, and William Foster – The Bridgespan Group
[42] https://ec.europa.eu/programmes/horizon2020/en/what-horizon-2020
[43] https://ec.europa.eu/info/funding-tenders/european-structural-and-investment-funds_en
[44] http://www.scienceeurope.org/wp-content/uploads/2016/01/SE_Infrastructures_SurveyReport_web_FIN.pdf
[45] http://ec.europa.eu/research/infrastructures/index_en.cfm?pg=esfri
[46] http://ec.europa.eu/research/participants/portal/desktop/en/opportunities/h2020/topics/einfra-21-2017.html
[47] ttps://ec.europa.eu/programmes/horizon2020/en/news/eight-new-centres-excellence-computing-applications
[48] https://ec.europa.eu/programmes/horizon2020/en/news/21-new-h2020-high-performance-computing-projects
[49] http://www.snic.vr.se/international/prace-documents/Digest_final_low_res.pdf
[50] http://www.exascale.org/bdec/

List of Acronyms and Abbreviations

aisbl	Association internationale sans but lucratif (legal form of the PRACE-RI)
ALMA	Atacama Large Millimeter/submillimeter Array
BoD	PRACE Board of Directors
CECAM	Coastal Ecosystem Conservation and Adaptive Management
Capex	Capital Expenditure
CJEU	Court of Justice of the European Union
CoEs	Centres of Excellence
CRM	Customer relationship management
DoA	Description of Action (formerly known as DoW)
DSM	Digital Single Market
EC	European Commission
ECI	European Cloud Initiative
EGI	The European Grid Initiative
ELI-DC	The European Laser Institute
ELIXIR	Integrated computing services for European researcher, Hinxton, UK
EMBL	The European Molecular Biology Lab, Heidelberg, Germany
ENES	The European Network for Earth System modelling
EPOS	The European Plate Observing System
ERF aisbl	Association of European-level Research Infrastructure Facilities, Brussels, Belgium
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
EUDAT	European Data
EVN	European For Very Long BaseLine Interferometry Network
FET	Future and Emerging Technologies

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
ILL	Institut Laue-Langevin, Grenoble, France
IPs	PRACE Implementation Projects
IPR	Intellectual Property Rights
ITER	International Thermonuclear Experimental Reactor
KPI	Key Performance Indicator
LHC	Large Hadron Collider
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
SHAPE	SME HPC Adoption Programme in Europe
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
VISIONAIR	The Vision Advanced Infrastructure for Research, Grenoble, France
WP	Work Package

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
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, Labotatório 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 shows the results of the analysis of the management of stakeholders done by PRACE-4IP project 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, that will take over from PRACE agreement for the Initial Period, so-called PRACE 1, for the 2017 - 2020 period.

This follows previous analyses of stakeholder management, performed within PRACE Preparatory Phase project (PRACE-PP) in 2008 [14][15], and the update of PRACE-3IP project in 2014 [17]. Whereas previous deliverables were focused on the early identification of core stakeholders of the project and on the legal aspect of relationship with other entities, this one is more focused on the latest evolutions of the HPC ecosystem, that could be summarised as a global race to Exascale (potentially available at the beginning of next decade), with an accelerating pace (at least for USA, China and Japan, that decided to afford the huge cost of tools, considered more strategic than ever), and a European ecosystem that is taking shape, with the three pillars of the European Commission (EC) strategy for High Performance Computing (HPC) – infrastructures, technologies, applications. The recent launching of a Digital Single Market (DSM) strategy for Europe, announced by the EC in April 2016, provides a new horizon with an extended and strengthened need and interest for HPC.

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.

PRACE tools and methodologies are explained (CRM, communication, different PRACE bodies that organise and structure stakeholder management); diverse MoUs signed between PRACE RI or PRACE projects and these partners are reminded, and a STEEPLED analysis has been performed to provide a context for evaluating and defining PRACE's role in relation with its external environment.

1 Introduction

This deliverable shows the results of the analysis of the management of stakeholders done by PRACE-4IP project 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, that will take over from PRACE agreement for the Initial Period, so-called PRACE 1, for the 2017 - 2020 period.

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- HPC infrastructures and services via the Partnership for Advanced Computing in Europe (PRACE);
- HPC technologies via the Future and Emerging Technologies (FET) programme, and
- HPC applications via the establishment of Centres of Excellence (CoEs), funded by the e-Infrastructures programme.

The recent launching 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) including the notions of an underlying 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. Meanwhile and in the same context (November 2015) an initiative led by a few Member States (Luxembourg, France, Italy, Spain) has also been announced, so-called IPCEI HPC-BDA, an Important Project of Common European Interest mixing HPC and Big Data objectives.

At the European and international levels PRACE strives to establish an HPC ecosystem. Part of this work is to establish 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); other transnational cooperation such as with ITER fusion project, or with European projects, such as LinkSCEEM (Linking Scientific Computing in Europe and the Eastern Mediterranean) within the Southern Europe region; links with other H2020 projects, such as Graphene and Human Brain Project (HBP), Future and Emerging Technology (FET) Flagships, to name a few. PRACE also engaged within fruitful collaborations with other RIs and e-RIs.

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 relates PRACE sites and experts to 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 4.7.4).

Another group of users of special interest are the emerging communities of users in humanities and social sciences (such as paleontology). Such communities bring and need new usage 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 in Europe is handled at a proper level for such a strategic tool.

A presentation of PRACE communication and Customer Relationship Management tools are also presented, along with our communication and outreach action (more detailed in other specific deliverables).

Last but not least, the whole society is probably the ultimate stakeholder that should benefit, directly or more indirectly from our work.

To ensure the appropriate connection with these very diverse stakeholders, numerous tools have been put in place, with a coordination at the level of 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, and a STEEPLED analysis has been performed to provide a context for evaluating and defining PRACE’s role in relation to its external environment.

In this document:

- Chapter 2 defines some concepts and elements of theory useful for stakeholder management, while reminding fundamentals of HPC EU ecosystem.
- Chapter 3 gives an overview of local (European) and global (worldwide) HPC landscape, as a general setting of PRACE context.
- Chapter 4 gives more details on the different links and relationships established by PRACE.
- Chapter 5 summaries, analyses gaps and gives perspectives.
- Chapter 6 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: Austria, Belgium, Bulgaria, Cyprus, Czech Republic, Denmark, Finland, France, Germany, Greece, Hungary, Ireland, Israel, Italy, The Netherlands, Norway, Poland, Portugal, Slovakia, Slovenia, Spain, Sweden, Switzerland, Turkey and the United Kingdom. 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 fulfil this mission, the collaboration and commitment of a wide range of stakeholders is very important, and work to identify them and to define the proper interaction to engage have been initiated during the Preparatory Phase of 2008 and continued during PRACE-3IP project (see [14][15][17]).

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 members (BSC representing Spain, CINECA representing Italy, CSCS representing Switzerland, GCS representing Germany and GENCI representing France).

This work is not realised 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” [30], 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” [24], with a latter synthesis with its 2010 book “Stakeholder Theory: The State of the Art” [25]. 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.

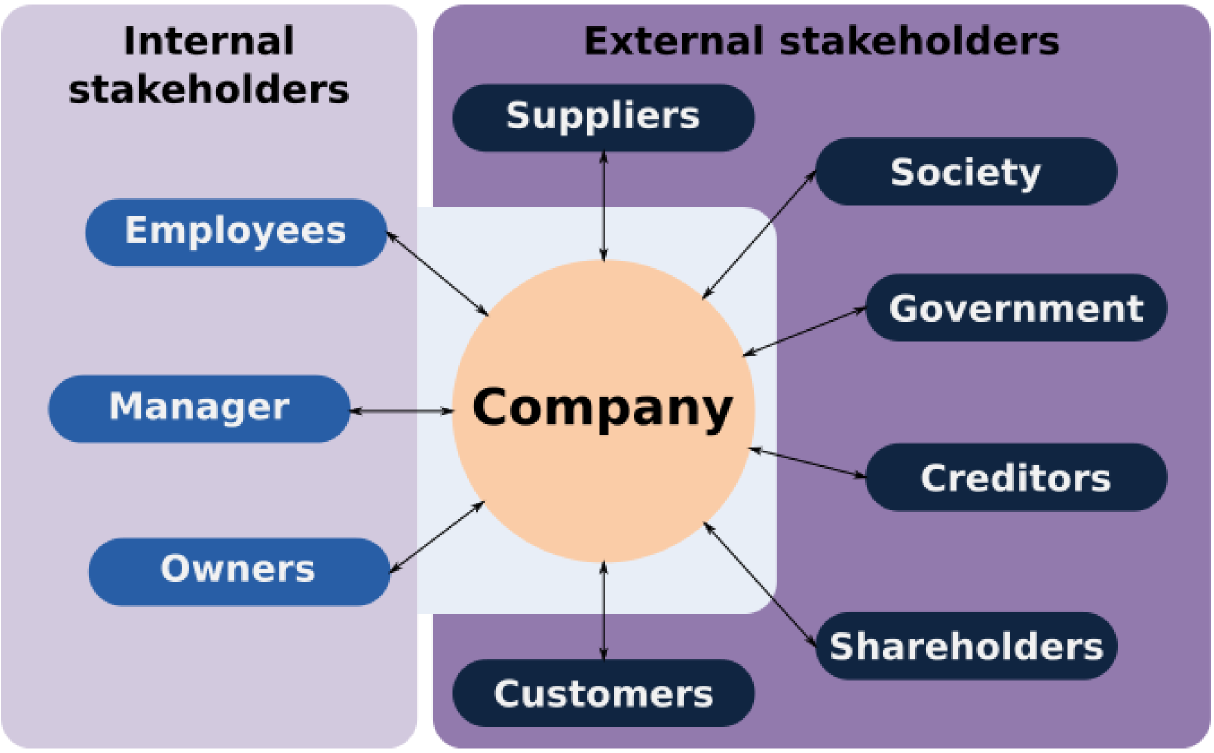

Figure 1: Example of typical stakeholders of a company, divided into internal and external stakeholders. Source: Wikipedia Commons.

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 meet 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 and Big-Data and/or Deep-Learning (High Performance Data Analytic HPDA) widening the scope of application of HPC. But a friend of all is a friend of none, and 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 scientific (or industrial / medical) applications. This analysis is developed in Section 3.6 STEEPLED analysis, and put into Communication and Outreach action as shown in Section 3.5 PRACE for Society.

3 The HPC Ecosystem

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

3.1 Introductory HPC ecosystem overview

“To out compute is to out compete" is a commonly used punchline 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 the analysis, the quality of the results and the potential of national and international collaborations are more and more depending on the available computing infrastructure - not only in climate science, but in science in general. Thus, the EU has set up an European HPC strategy [31] and established a strong cooperation (based on contractual Public-Private Partnership on HPC (cPPP on HPC [32]) with the HPC stakeholders, represented by the European Technology Platform for HPC (ETP4HPC [26]). This cPPP on HPC has developed an ambitious R&I funding strategy [32]based on three pillars, addressing:

- HPC facilities via the Partnership for Advanced Computing in Europe (PRACE [7]), established since October 2012,
- HPC technologies via the Future and Emerging Technologies (FET [35]) programme, and
- HPC applications via the establishment of Centres of Excellence (CoEs), funded by the e-Infrastructures programme [36].

To support and coordinate the collaboration and interactions of these 3 pillars, ETP4HPC together with PRACE and partners from the European Exascale Software Initiative (EESI2 [37]) have initiated the European eXtreme Data and Computing Initiative (EXDCI [38]) (see Figure 2 for an overview of this European landscape).

Figure 2: HPC H2020 landscape

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 [30], 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 in 2014-2015, then 2016-2017 funding periods [31]:

1. Next generation of HPC technologies, middleware and systems towards exascale in FET-HPC calls, following the European Technology Platform for HPC (ETP4HPC) recommendations and roadmap;
2. Supercomputing facilities and services incl. support to PRACE via Implementation Phase Projects;
3. Excellence in HPC application delivery and use via Centres of Excellence for Computing Applications.

Each pillar has entities that can endorse structuring roles and be voices for the stakeholders.

The "contractual Public-Private Partnership on HPC" (HPC cPPP) [32] brings together technology providers and users via the ETP4HPC Association - a voice for HPC technology Pillar - and CoE 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 - the voice for HPC infrastructures.

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 [33] acknowledging, in particular, that the main actors - the EC, PRACE and ETP4HPC, have done important efforts for coordinating to advance the European HPC strategy (as defined in the 2012 Communication "High Performance Computing (HPC): Europe's place in a global race").

3.2.2 A new hope for EU HPC in 2016

The launching 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 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 will have renowned 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 being announced by the EC in April 2016, which actually confirms and widens the scope of 2012 EC strategy [34].

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 recently released (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.” [39]

Meanwhile and in the same context (November 2015) an initiative led by a few Member States (Luxembourg, France, Italy, Spain) has also been announced, so-called IPCEI HPC-BDA, an Important Project of Common European Interest mixing HPC and Big Data objectives [40]. This is 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. The presentation of this intention refers the main objectives of the initiative, namely to bring Europe forward to achieve the following macro-objectives:

1. To ensure an European industrial expertise on key HPC technologies (taking special attention to safety and security);
2. To support and create new usages of HPC by the industry;
3. To guarantee access to world-class HPC facilities for public and private research.

The IPCEI refers three pillars (pillar 1: technology, pillar 2: infrastructure; pillar 3: large-scale pan-European pilots). PRACE is explicitly referred to in the Position paper released by the three countries in November 2015 at the European Data Forum in Luxembourg, as the infrastructure that will provide access to world-class supercomputing facilities and services, the computing and data infrastructure for industry, research technology organisations and academia.

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) established by President Barak Obama in 2015, the Japanese Post-K-flagship project, PRACE and ETP4HPC projects in Europe, Tianhe and Sunway HPC clusters in China, and several similar projects in France. In this section, we provide an overview of the HPC Ecosystems on other continents. In 2016 and 2015, top20 machines represent 40% of top500, but between 2015 and 2016 China moved from 10% to 17,7%, US from 21% to 12,4% and Europe from 3,8% to a mere 2,6%.

In November 2016, systems installed in Europe accounted for only 14% of the computing power in the Top20 (peak or Linpack performance, the figures are the same), for 6 systems. This percentage is even 12% only for systems available for public research (1 system is an industrial and purely private one).

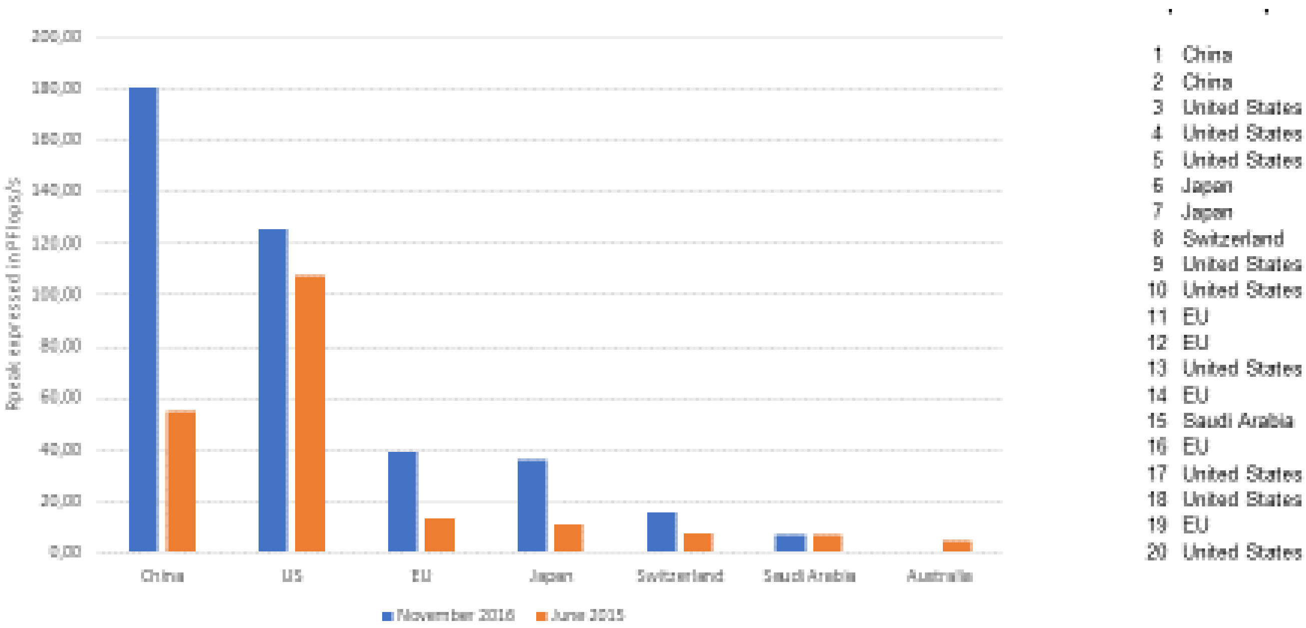

Figure 3: Top20 supercomputer, June 2015 to November 2016 (courtesy of Matteo Valero, BSC)

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, XSEDE is comprised of sixteen US based institutions and the Jülich Supercomputing Centre. XSEDE 2.0 now has received a further five year $110-million grant, includes more partner institutions and aims to expand access of advanced cyberinfrastructure resources to scientists and engineers.

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 onto 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
   - 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 list of the 500 most powerful machines - 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 the Chinese government) and the associated ecosystem (middleware, environment, applications). The second challenge is the formation of home talents in HPC.

Some major companies and labs in HPC:

1. Sugon (was the no.1 market share holder in China HPC market for the past 6 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 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 a plan to acquire 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. It has a governance similar to that of PRACE 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. These include:

- HP-SEE: High-Performance Computing Infrastructure for South East Europe's Research Communities.
  The goal of this project was to link existing and upcoming HPC facilities in South East Europe in a common infrastructure to open up a wide range of new user communities to such resources – thus fostering international collaboration.

- LinkSCEEM: Linking Scientific Computing in Europe and the Eastern Mediterranean.
  The aim of this project was the establishment of 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 main project objective was to enable scientific research in the region by engaging and supporting research communities with an initial emphasis in the fields of climate research, digital cultural heritage and synchrotron radiation applications.
  Having delivered a relatively high number of training events (both general and thematic) and a Preparatory/Production call (which is still ongoing – although under a different name) 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 (SEEM), in order to facilitate regional interdisciplinary collaboration, with special focus on the scientific communities of life sciences, climatology and digital cultural heritage. VI-SEEM will significantly leverage and strengthen the research capacities of user communities, thus improving research productivity and competitiveness on 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 PFlop/s system, a 10 Petabyte data service coupled with dark fibre network to support the Singapore Advanced Research and Education Network.

South Korean currently has a 2.4 PFlop/s system in the Top 500. Despite this, the South Korean government also wants to invest in HPC, announcing 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 PFlop/s 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. During the SC'16 conference in November 2016 in Salt Lake City, discussions happened between PRACE and the Pawsey Institute, one of the Australian national centre, very involved in the SKA (Square Array Kilometre) radio telescope, in order to establish a joint MoU in training, best practices in peer review, industrial involvement.

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. HPCLatAm aims to bring together researchers, developers, and users of HPC to discuss new ideas, experiences, and problems. 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 US 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.

There are two main Russian HPC vendors and these are T-Platforms and RSC. Despite a 2013 US government blacklist, T-Platforms seems to be the more successful of the two companies. T-Platforms leads Russia's Top 50 Supercomputing list and also has international sales of its supercomputers – such as JURECA in Jülich Supercomputing Centre. RSC on the other hand focuses on systems that have energy efficiency at the core and are built with commodity parts to keep the overall price of the system low. Although this has allowed them to sell supercomputers in Russia – mainly due to the more competitive price when compared to US based supercomputers, RSC has struggled with international sales.

Further to this, 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.

3.4 PRACE objectives and perspectives

PRACE aims to provide high-end High Performance Computing (HPC) services to the scientific and industrial communities thereby promoting European competitiveness in science and industry at a global level. These include the provision of world-class computing and data analysis resources through a federated world-class of Tier-0 supercomputing infrastructure whose access is provided through a transparent and fair peer review process based on scientific excellence. Besides this main objective, PRACE has also engaged in training programmes for HPC users, both in science and industry, as well as development and testing of new computer technologies, with emphasis on those aiming at increasing the HPC energy efficiency. The involvement of PRACE with industry is also present in the SHAPE programme, which aims at promoting the usage of HPC by SMEs and in the Open Research access to industry which allowed supporting research projects from more than 50 companies since mid-2012.

During the first phase of the PRACE RI, from 2010 to 2015, the Tier-0 resources were provided by four hosting members (Germany, France, Italy and Spain) based on an initial agreement to supply a predefined amount of resources. These resources were allocated by Hosting Members based on the recommendations of a PRACE-managed peer-review process, relying on a single criterion: excellence in science.

As the so-called agreement of the initial period was about to end, the PRACE Council agreed in September 2015 on the principles of a new integrated programme called PRACE 2 which will allow PRACE aisbl to continue to offer access to European Researchers renewed and competitive HPC and data Tier-0 facilities. This has led to change the model for the next phase of PRACE, called PRACE 2. Based on the principle “who computes, contributes”, this new model is based on a fair contribution of all PRACE partners, Hosting Members providing HPC cycles on their Tier-0 systems and non-Hosting Members contributing to the funding of High Level Support Teams (HLST), which will provide application user support in order to take benefit from upcoming pre Exacale architectures.

A new Hosting Member Switzerland is now providing access to PizDaint, the most powerful HPC system in Europe, based on an hybrid architecture with a peak performance of 15 PFlop/s.

Besides this change, PRACE 2 will continue to be actively engaged in HPC dissemination, industry collaboration, training, and exploration of future supercomputing technologies.

This phase is expected to run from 2017 until 2019, paving the path for PRACE 3 as a persistent pan European HPC Infrastructure, integrated inside the EDI EC vision.

The vision of PRACE is summarised as follows:

1. To provide a world-class HPC infrastructure to European researchers in science and industry comprised at any time of leadership-class pan-European systems, linked with an underpinning network of national and regional systems.

2. Access to PRACE leadership-class systems is awarded to all European researchers on the basis of a fair, equal and transparent peer review process based on scientific excellence and a fair cost sharing principle.
3. Leadership-class systems need to be procured openly in a global market, following clear and transparent principles of user needs, technological leadership, and cost effectiveness.
4. PRACE should be seen as the organisation providing leadership access to compute and data analysis services in science and research in Europe.

3.5 PRACE for Society

This chapter came directly from a set of communications two-page leaflets, the PRACE Fact Sheets, designed to provide a quick overview of PRACE, its operations, its impact and HPC in general. This collection of fact sheets is comprised of:

- What is HPC?
- PRACE in Numbers;
- PRACE in Society (text reproduced below);
- PRACE Summer of HPC;
- PRACE Training & Education;
- PRACE Supports Industry;
- PRACE Success Stories;

Because facts still matter.

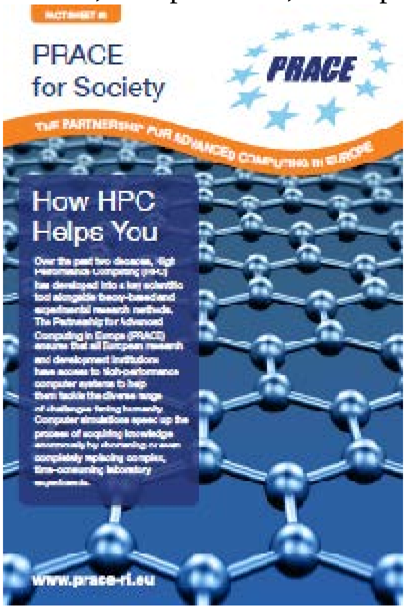

Figure 4: PRACE for Society leaflet

A wide-range of scientific domains and industrial sectors benefit from access to the HPC resources provided by PRACE. Such domains and sectors include climate and earth sciences, energy, construction, materials science, biology, chemistry, automotive, aeronautics, astrophysics, and many more. Below examples from three important domains are highlighted.

3.5.1 PRACE Supports Medicine

Virtually all medical research can benefit from HPC. One of the largest and well-known computer-aided research projects and an EU Flagship initiative, the Human Brain Project (HBP), benefits from the results of research supported by PRACE. Driven by the goal of simulating the human brain right down to the processes which take place at the cellular level, the HBP hopes to gain a better understanding of the brain and the mechanisms that control behaviour and cognition. The aim is to achieve a fundamental understanding of the brain that would help in the treatment of medical conditions such as dementia or Alzheimer's disease. The findings from this research can also be used to stimulate technological advances. For example, the working principle of the human brain could serve as a basis for building computers capable of achieving a similar degree of efficiency – high-performance machines with a low level of power consumption.

Computer simulations carried out within the PRACE projects framework are also used to study heart and cardiovascular diseases, and develop treatments. Heart disease is the leading cause of death worldwide. Based on simulations, researchers formulate new medicines and develop tiny vehicles for delivering them. These transporters consist of nano-molecules from DNA with the ability to deliver medicine directly to the cell when triggered.

3.5.2 PRACE supports natural risks and hazards assessment and mitigation

Extreme weather conditions caused by climate change present new challenges both for researchers investigating adaptation strategies and for insurance companies and government organisations that must deal with the rami cations. Effective adaptation programs rely on substantiated forecasts based on computer simulations. Researchers involved in PRACE projects have created simulations for predicting the development of watercourses that pose potential flood risks and devised technologies that allow insurance providers to more accurately assess risks associated with changing environmental conditions.

3.5.3 PRACE Supports Engineering

Engineering simulations are used to develop safer, faster and more efficient vehicles and aircraft. Automotive and aeronautical engineers use materials science simulations to found new materials that have the potential to improve the efficiency of solar or hydrogen cells, or materials that are extremely lightweight and robust. Graphene – being studied as part of the EU's Graphene Flagship project – is one example of a light but sturdy material, and PRACE infrastructure is being used extensively to support graphene-based nanomaterial research.

3.6 STEEPLED analysis

A STEEPLED analysis provides a context for evaluating and defining PRACE's role in relation to our external environment. STEEPLED stands for Social, Technological, Economic, Educational, Political, Legal, Environmental and Demographic factors. These factors - both positive and negative - define the world in which PRACE operates.

The analysis bellow is a first draft for illustrating the use of this tool, the lists are non-exhaustive, we need to consider for each factor:

- Which are still missing?
- Which of the below are most important now?
- Which are likely to be most important in the near future?
- What factors influence decision on changes?

Factors can overlap and fit into several categories, e.g. policies leading to legislation.

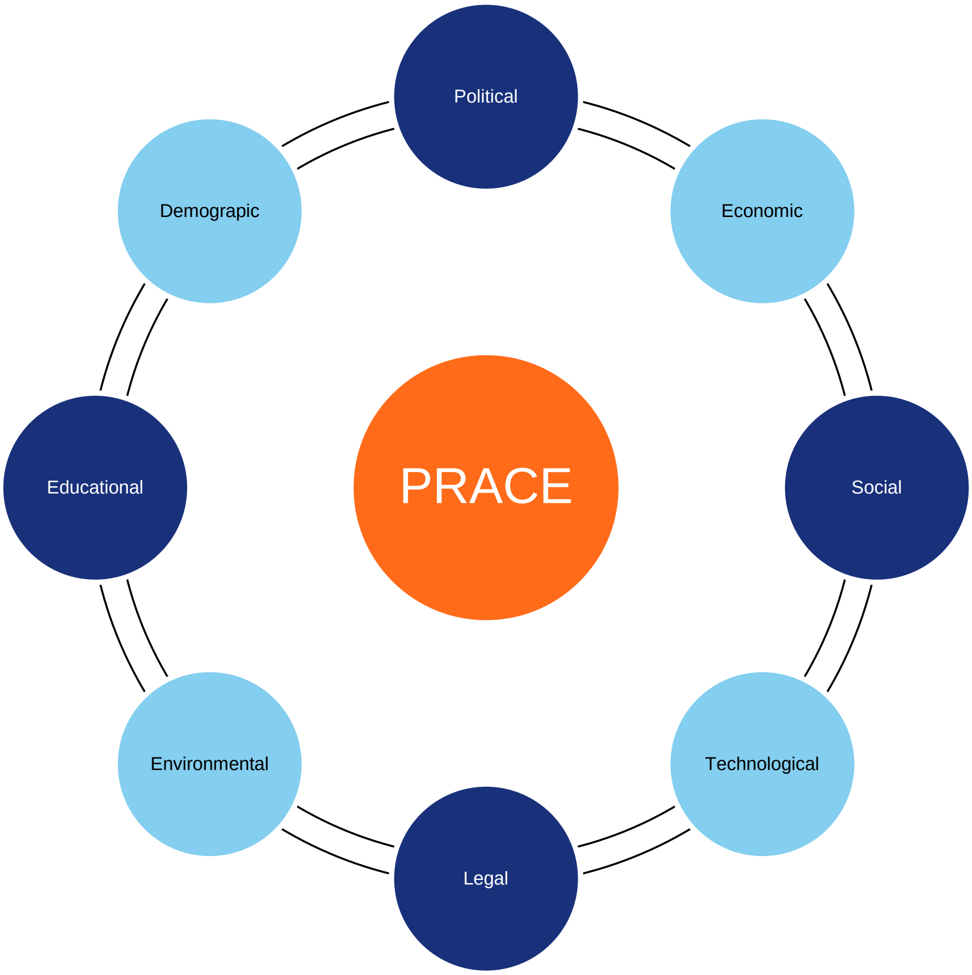

Figure 5: STEEPLED analysis for PRACE

Social: What are the main societal and cultural aspects?

- Section 3.5 gives some examples of applications of HPC of utmost societal importance, which PRACE is supporting;
- There are some difficulties to attract student tower scientific / technological careers;
- Ambivalent love/hate attitude toward science/technology seen as progress or threat;
- The general public is largely unaware of our work and of HPC in general.

Technological: What are current technology imperatives, changes and innovations?

- Industrial R&D is looking at HPC as the next tool for competitive advantage in innovative areas;
- The global race for exascale inspires new technology;
- Short number of technology suppliers for HPC, shorter from Europe, shortest for chips;
- Bridging the gap between scientific domains and computational science;
- Increasing familiarity with HPC;
- Cloud, Grid, BigData can be seen as competitors - alternatives as well as allies - complement.

Economic: What are the important economic factors?

- At international level, we face many major players (USA, China, Japan, Russia) and some new ones (Korea, India…) in a dizzying technological race towards exascale;
- Impact of economic crisis on government budget, including science and research. High-end HPC systems can be under-funded with respect to the EU objectives;
- HPC is identified worldwide as a strong leverage for innovation and growth.

Educational: What are the main educational themes and developments?

- Encouraging science education: training the next generation (computational) scientists;
- Small pool of computational scientists to draw on for our Peer Review Process.

Political: What are the key political drivers of relevance?

- Funding from national and EU governments;
- Maintaining contact with policy makers;
- Changes in governmental policies on R&D;
- Privatisation trends;
- Political climate: Consilium (Council of Ministers representing the Member States' governments) speaking out about HPC and spreading the word about PRACE;
- Horizon 2020.

Legal: Current and impending legislation affecting PRACE:

- National tax-laws prohibiting PRACE to offer certain services without VAT costs;
- New context of the implementation of DSM and EDI at European scale;
- National regulations restricting access to PRACE resources for nationals of certain states.

Environmental: What are the environmental considerations, locally and further afield?

- More extreme climate and environmental occurrences (hurricanes, earthquake) that ask for more precise risk assessment obtainable only with the help of HPC;
- The positive role distributed shared resources play in reducing carbon emissions.

Demographic: Which trends in demographic development are relevant to PRACE?

- Demographic change: the need for research like the “Human Brain Project” or medicine projects becoming ever more needed for an ageing population;
- The need to promote science at large and more specifically computer science to young generations, and to propose adequate formation (and hiring for graduates) to anticipate a shortage of talent, within a “senior” community of computer scientist.

As presented in Section 3.5, PRACE has a strong role to play to tackle some of the most difficult challenges European and worldwide society is facing, such as global environmental threats or medical and social issues of an aging society.

HPC is also seen worldwide as one of the strongest leverage for innovation and growth, the race toward Exascale being strategic for the future competitiveness of their country. This has been well understood by US, China and Japan, who decided to afford the huge cost of this new “race to the moon” competition. This has been also well understood and clearly stated by European institutions and Member State, but with founding issues in the context economic crisis puts a strain on government budget, impacting also budgets for science and research from which the funding of PRACE comes.

This race is run with technologies, at a time where the path to Exascale is not clear and requires assessment of emerging technologies that could tackle Exascale challenges (energy wall, resilience, data management, etc…). Technologies are coming from a short number of HPC suppliers. This is even truer for microprocessor providers, with Intel as a clear American leader and ARM becoming international (under Japanese flag, although most of its R&D is remaining based and operated in Europe).

Beside these social and economic considerations, one can also look at the wider picture of the complex relationship between science and society. Science is being seen by some as the flagship of progress, by others as a potential threat to environment through the technical achievements it allows, or as a threat to job creation with fear of robots and Artificial Intelligence becoming able to do more and more “human” jobs. PRACE as a generic instrument can claim to be at the forefront of the defense of positive societal aspects of computing.

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 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 IBM System X iDataplex based in BSC, Spain;
6. Piz Daint a Cray XC30 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 programme is optional, the number of available systems in each call varies, but in DECI 13 about 15 PRACE members gave access to their resources – with some members giving access to more than one resource. Given the high number of resources there is a wide variety of supercomputing architectures available for computational scientists, such as CRAY's, BlueGene, clusters with and without accelerators (GPUs or Xeon Phis).

Further to these systems there are also a great number of other Tier-2 national systems available throughout Europe for computational scientists to use on a national level.

The importance of such systems should not be underestimated. Such systems are usually the first systems 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 4.7.6. They represent the spearhead of EU-supported high performance applications and are a structuring part of the HPC use side of the ecosystem [47]. 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 current planned activities involving CoEs.

4.2.1 PRACE on Demand Events with Centres of Excellence

Through the Training work package (WP4), PRACE will be organising a series of on demand events in collaboration with CoEs. No firm date as to when these will be delivered has been set, but they will be advertised on the PRACE Events website [9]. Five such events are planned and these are with the following Centres of Excellence and PRACE Partners:

- 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;
- 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 CSCS and CINECA.

4.2.2 Programming Tools, Languages, Libraries & Algorithms for Exascale

PRACE will also liaise with CoEs as well as other application owners to identify application requirements with regards to best practices for prototype planning and evaluation. We will investigate the programming tools, languages, libraries and algorithms needed for future Exascale systems. This task will exploit existing links with European Exascale projects and develop links with the emerging applications CoEs to understand their requirements.
The goal of this task 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;

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.

MoUs have been signed between PRACE projects and:

- EGI-CSIRT team on sharing information on security incidents and specific vulnerability risks for our respective infrastructures;
- GEANT for specific cooperation in the field of Network services;
- EUDAT in the field of data services and security domains;

allowing a specific collaboration with these stakeholders.

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 has been invited to participate to DI4R the Digital Infrastructures for Research meeting, organised by EGI (Krakow 28-30 September 2016), providing contributes 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 2016, ETP4HPC had 80 members, comprising 15 industrial HPC companies, 25 HPC SMEs, and 37 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 are now delivering prototypes for the final phase of this PCP.

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.

PRACE already analysed possible funding models during its first implementation phase. In the Deliverable D.2.3.2 [16] 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:

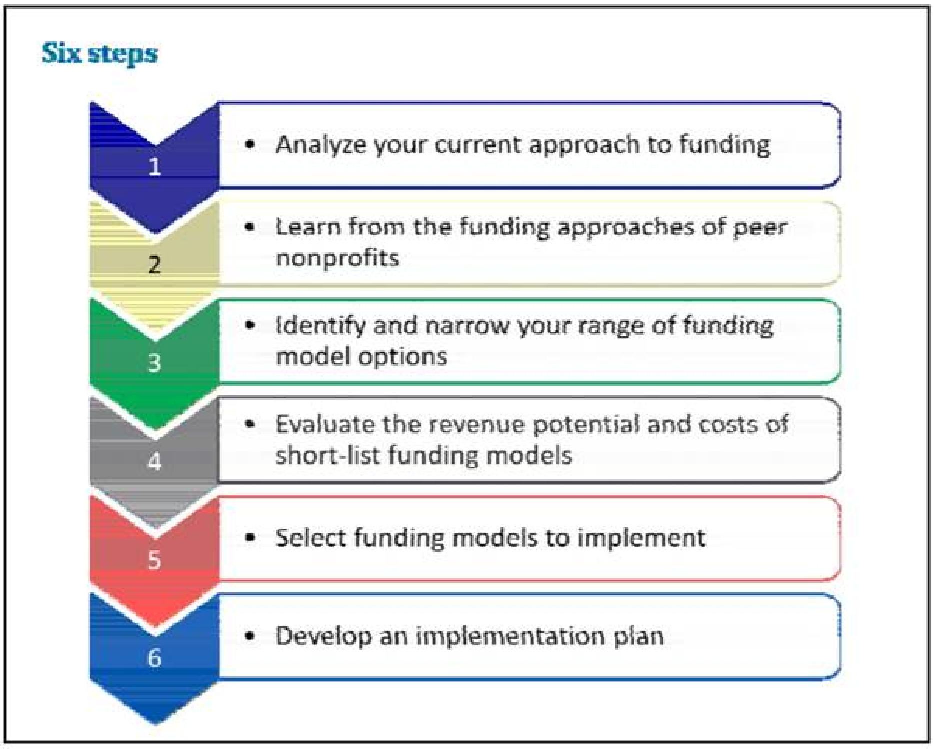

Figure 6: Six steps for identifying and developing the right funding model for organisations [41].

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.

More recently, PRACE has presented in the deliverable D2.1 of PRACE-4IP [19] 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 in the operational costs of the infrastructure, in a distribution based on modulating factors, like GDP.

Aside from the contributions of PRACE Members, external funding is sought for complementing the internal funding model.

High Performance Computing is a strategic resource for Europe's future, reflected in the adoption of the EU HPC Strategy in February 2012 [30]. 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 taken into account (European or national level, HPC Host Countries, countries with large/strong HPC communities, 'junior' partners, emerging players).

4.5.1 EU funding

The core EU funding includes:

- <u>Horizon 2020, the EU Research and Innovation programme [42]</u>

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.

- <u>European Structural and Investment (ESI) Funds [43]</u>

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.

- <u>Other sources of funding</u>

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.

4.5.2 National funding for PRACE Members

A survey [44] 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 March 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.

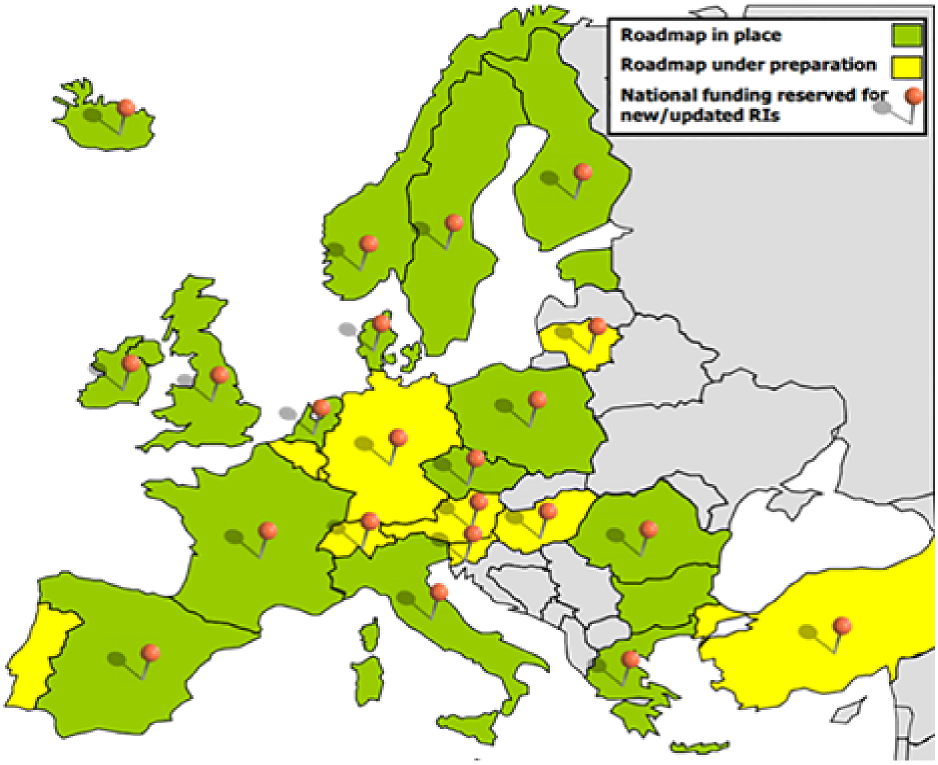

Figure 7: European map of national roadmaps

4.6 Policy making organisations

For PRACE, it is a priority seeking participation to the possible extent in the policy making process in the field of HPC, its development and applications at European level in order to secure both direct and indirect external funding. In regard to policy-making institutions, it is important 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 [45] (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 stakeholder worth to be mentioned is e-IRG (e-Infrastructure Reflection Group) [40]. 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 to the PRACE 2 programme.

A flexible and very rich in information tool are the 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 - SME

The detailed organisation of the PRACE RI could be found at the PRACE website [12].

It includes bodies in charge of providing advice and guidance from our users, through a User Forum (UF), Scientific Steering Committee (SSC) and Industrial Advisory Committee (IAC).

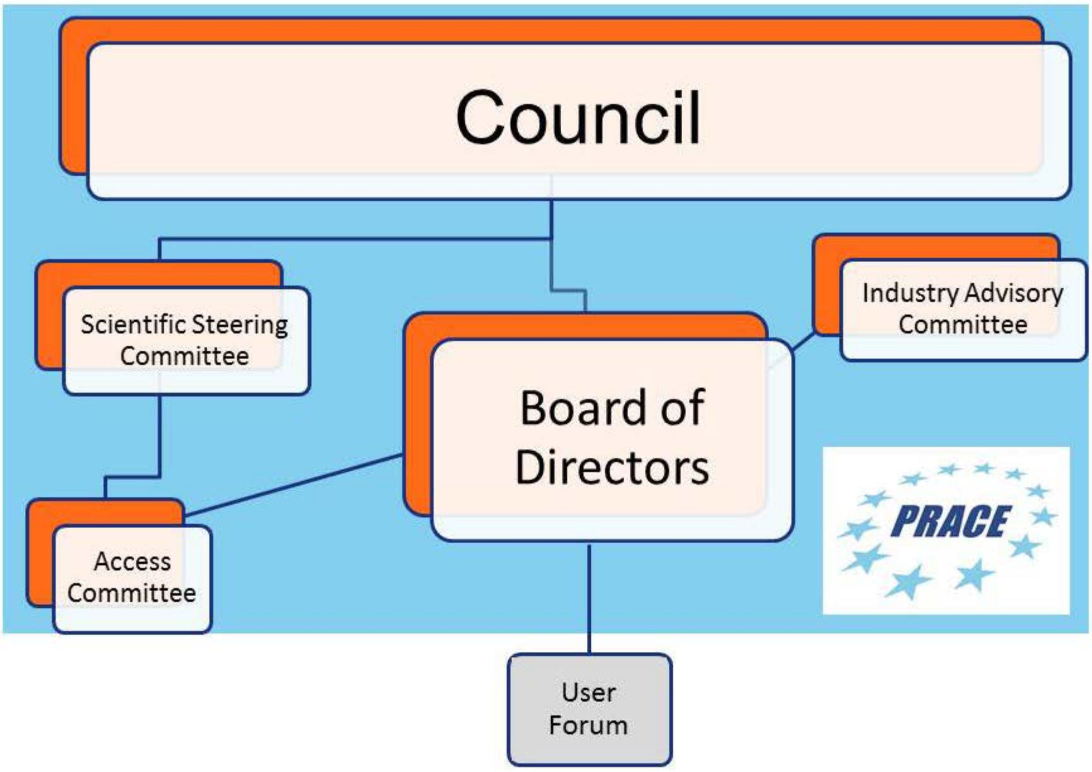

Figure 8: Organigram of PRACE

4.7.1 PRACE User Forum (UF)

The PRACE User Forum (UF) is an independent body from the PRACE aisbl Association. 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 PRACE-3IP-D2.2 [17]), 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. In this regard the ongoing PRACE initiative, the SHAPE programme, will be reported on.

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.

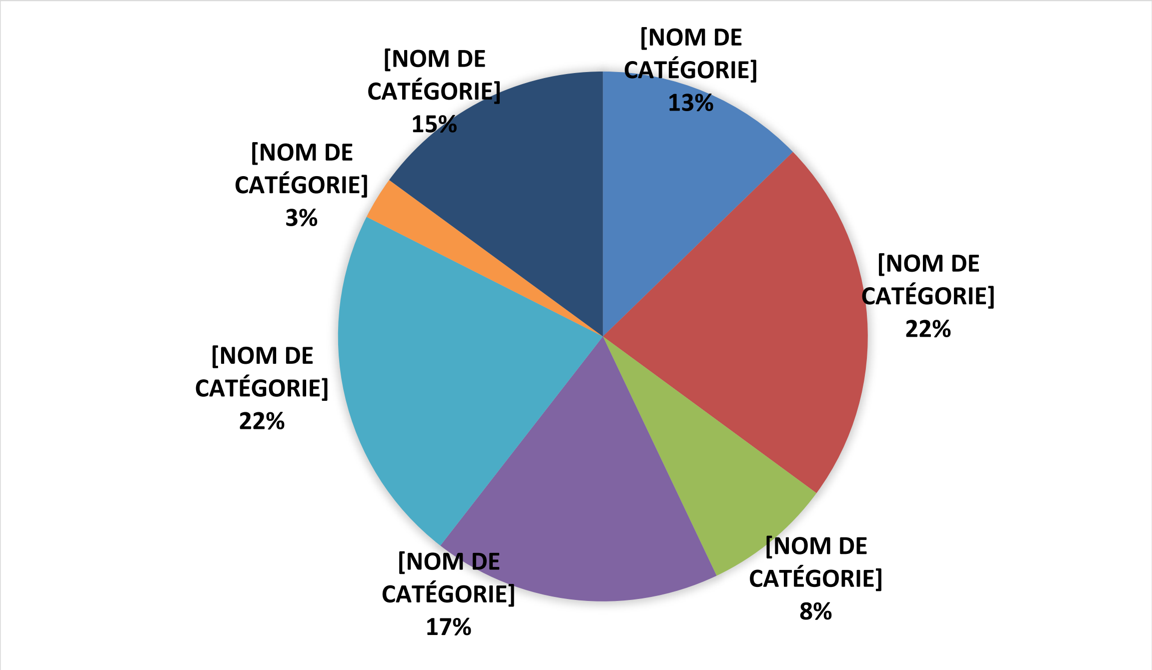

Figure 9: PRACE Distribution of resources by science domains

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 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 [10].

SHAPE was launched in 2013, following consideration of the needs of SMEs and input from various national level SME engagement programmes. The pilot programme concluded and 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 "Report on the SHAPE implementation" [18] performed a follow-up of the original pilot project with SMEs judging the return on investment they had gained from participating in the SHAPE programme. The outcomes were largely very positive: some organisations hiring staff to continue their HPC work started under SHAPE; many can now run their software much more quickly and much more cheaply; and many have, via HPC, been able to offer enhanced and indeed 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, be that in-house, or via further access to PRACE resources. It is planned to have similar follow-up surveys for the latter SHAPE projects.

SMEs awarded a SHAPE support are matched with a PRACE partner for technical expertise, and can apply for PRACE machine time, usually via a Preparatory Access call. The SMEs are expected to undertake some promotion of their collaboration with PRACE (such as via their website, social media, publications), and to produce a white paper once the project has concluded on the technical aspects of the work, publicly available via the PRACE website [11].

Going forward, SHAPE is expected to continue under PRACE-5IP project. The SHAPE process itself is under constant review, with feedback from both PRACE partners and the SMEs taken on board to try and streamline the process for all parties concerned.

SHAPE results in short:

- 3 first calls: 28 projects funded from 9 different countries;
- 4th call closed on 9 September 2016, 4 projects awarded;
- Different fields: hydraulic turbine design, life science, audio technologies, LES turbulence models in race boat sail, airflow simulations, electromagnetic behavior of products, virtual test bench for centrifugal pumps, CFD simulation of innovative hull, 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.

4.7.5 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.

4.7.6 Centres of Excellence - CoEs

In 2015 eight Centres of Excellence (CoEs) for computing applications were selected following a H2020 e-Infrastructures call [47], 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 Deliverable D5.1 “Market and Technology Watch Report Year 1” ([20] April 2016) contains 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 19 R&D projects stemming from FETHPC Call in 2014 are up and running (plus two Coordination and Support Actions, EXDCI and Eurolab4HPC, for ecosystem development and extra prospective) [48], they are presented in [28].

Some documentation on the progress and potential of these projects can be found at [26][38]. ETP4HPC and EXDCI have produced Handbooks at the occasion of BoF sessions at SuperComputing (2015 and again in 2016), with up-to-date detailing with the European HPC Technology Projects within the European HPC Eco-system (**see [29]).**

4.8.2 Extreme Data and Computing Initiative - EXDCI

"Extreme Data and Computing Initiative” 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 as coordinator, and ETP4HPC join their expertise in this 30-month project, starting from September 2015. EXDCI aims to support the road-mapping, strategy-making and performance-monitoring activities of the ecosystem [38]. EXDCI is putting together PRACE, ETP4HPC, FETHPC and CoE projects and all the other stakeholders via joint technical activities (incl. road mapping with synchronised 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 this year in May 2016 in Barcelona. A specific action towards 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" [50]. 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.

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 7.1 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 the space of 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 for Proposals: one project is linked to the Graphene Flagship programme: SMoG – Simulation driven Morphing of supported led by Dr. Valentina Tozzini. The project received 20.5 million core hours on Marconi – KNL @CINECA, Italy.
- 12th Call for Proposals: one project is linked to Graphene Flagship: Charge and Spin Hall Kubo Conductivity by Order N Real Space Methods led by Dr. Stephan Roche. The project received 19.8 million core hours on MareNostrum @BSC, Spain.
- 9th Call for Proposals: project AESFTl led by Matteo Calandra of CNRS, France, is partner in the Graphene Flagship Initiative. The project received 9 million core hours on CURIE @GENCI @CEA, France.
- 8th Call for Proposals: Prof. Stephan Roche of the Catalan Institute of Nanotechnology, Spain, with his project Longitudinal and Transverse Electronic

Transport in Atomically Doped Graphene from First Principles, which received 22 million core hours on CURIE @GENCI @CEA, France, is one of the early adopters of HPC in the Graphene Flagship. See PRACE Success story: www.prace-ri.eu/roche-2014/

- 8th Call for Proposals: project PentaGate-L, Tracing lipid-mediated gating and permeation of pentameric ligand-gated ion channels in atomic detail, led by Dr. Marc Baaden of CNRS and Institut des Biomolécules Max Mousseron, France, is partner in HBP Flagship. The project received 21 million core hours on CURIE @GENCI @CEA, France.
- 7th Call for Proposals: one project is linked to HBP Flagship: SMOLER, Synaptic Mechanisms underlying Odor LEarning and Recognition led by Dr. Michele Migliore. The project received 13 million core hours on Fermi @CINECA, Italy.
- 6th Call for Proposals: a project in chemical sciences & materials by Prof. Stephan Roche of ICREA, Spain is linked to Graphene Flagship and received 14.4 million core hours on CURIE @ GENCI@CEA, France.

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 would like to become an entry point to HPC for SMEs even for SMEs from countries that do not currently have such centres.

The project started in June 2015 and will run until May 2017. So far, the project has 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. The project has also 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. These materials are available on the project web site [21].

Interactions between PRACE and SESAME Net can be set in place via members that are active in both of them or through institutions related to them, but no contact has been initiated so far.

4.8.6 Public Procurement for Innovative Solutions (PPI)

The EC acknowledges the expected launch of the first coordinated acquisition at European level of world-class innovative HPC solutions in a few months [22]. A call for Public Procurement of Innovative solutions (PPI) closed in September 2016, meant 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. A joint procurement is under grant agreement preparation. 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;
- 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 to the PPI Group of Procurer a greater weight and allow having more impact on the design of the solutions according to the needs of scientists and engineers in Europe.

5 Summary, perspectives and further consolidation

5.1 Gap analysis and potential users Emerging Community

High Performance Computing has become an established scientific tool for computational scientists across various sciences. This has complemented their work beyond what just theory and experimentation could and has enabled a different approach to their research which has allowed for new discoveries to be made. The use of HPC in this manner has though mostly been limited to the Natural Sciences such as Physics, Biology and Chemistry as used in the specific research fields of astrophysics, computational biology, computational chemistry, computational fluid dynamics, earth sciences, high energy physics among many others.

In this section we identify other academic disciplines which could possibly use HPC in the future and which PRACE could possibly approach to help them towards making the first steps towards approaching and using HPC in their research.

5.1.1 Humanities and the Arts

Various fields of humanities and the arts can benefit from HPC in various ways.

A PRACE Summer of HPC 2016 project based in BSC demonstrated how this could be done. In this project, computer vision and machine learning were used to identify common castle features from pictures of buildings. In this way a classifier of whether a picture of a building displays a castle or not could be created. HPC was used in the computer vision process to convert high dimensional data into a numeric form an algorithm can use. As many images had to be processed, this processing was done in parallel upon Marenostrum to save time. HPC was also later used in the machine learning process too.

What this project demonstrates is that fields of Humanities such as Archaeology which require the processing of images - which can be a computationally intensive process, can use HPC and the abundance of its many computational nodes to parallelise the processing and thus complete it faster.

Further to this, this project demonstrates how computationally intensive algorithms – such as machine learning, neural networks and statistical classification, are increasingly finding solutions for disciplines beyond computer science into academic disciplines which in the past it would not have been deemed possible for them to find applications. Such algorithms are able to be taught and learn and be used as classifiers, they can be used to identify patterns and similarities in various datasets (which can be a set of images or script) amongst many other abilities.

Given the above, it is easy to envision applications of HPC in other research disciplines such as History (analysis of historic text for common patterns), Linguistics and Languages (analysis to identify similarities in speech and accents), Art (graphic analysis of works of art) among others, music and many others.

Indeed, another PRACE Summer of HPC 2016 project also based in BSC used HPC in the analysis of music to identify similarities in the genres of various artists throughout their careers (such as David Bowie who had a variety of styles in his musical discography).

5.1.2 Cryptography

Cryptography is the science and art of techniques used to conceal messages so these can be transported over a communication medium without the true message value being perceived by an adversary. Different types of Cryptography exist but most of the cryptographic solutions used throughout time are based on computationally hard problems. Examples of Cryptographic algorithms include the Caesar Cipher – used by Julious Caesar to send secret messages to his generals, the Enigma code – used by the Nazis in World War 2, and the Data Encryption Standard – the first publicly available encryption algorithm by NIST.

The practical breaking of Enigma was carried out by Alan Turing who built one of the first "computers" in the process and who later on is credited as the father of Computer Science. It is estimated by historians that Turing's work saved at least two years of World War and thus saved many millions of lives.

The breaking of DES was carried out using computational brute force in the 1990s by a cluster of interconnected household PC's – a commodity made supercomputing cluster.

The Cryptographic research community has not publicly been active in their use of HPC even though cryptographic problems could easily fill all of the world's supercomputers with jobs. It is no secret that government agencies such as the NSA and GCHQ have some of the most powerful supercomputers in their arsenal.

Given that most cryptographic solutions are based on mathematically computationally hard problems (such as factoring very large numbers, elliptic curves and one way functions), supercomputers can easily be used for the cryptanalysis of algorithms (trying to identify weaknesses of algorithms – no matter how small) as this process requires large amounts of computation and analysis of data. Professor Antoine Joux did receive close to 2.1 million hours in the PRACE 4th Regular Call for his project titled "Discrete Logarithms on Elliptic Curves over composite extension fields in characteristic 2" which shows that applications of HPC in cryptography exist. The cryptographic research field is large and this is one community which could be approached by PRACE for applications of HPC towards furthering their research.

5.1.3 Economics

The field of economics can certainly make greater use of HPC, especially in the fields of Financial Economics and Financial econometrics amongst others. In these fields mathematical economic models and statistical models are used upon financial market data for risk analysis, asset pricing and corporate finance. These can possibly be coupled with machine learning algorithms and neural networks for a more guided decision making process. Other fields of economics which may deal with live and quickly interchangeable data could use HPC also. As an example, companies dealing in the stock market - such as hedge funds, use HPC in the acquisition of shares and commodities as well as currency exchange to make huge amounts of profits. PRACE could approach economic academic research groups to see how HPC can help in their research goals.

5.1.4 Palaeontology

Palaeontology is a surprising field in which HPC can be used. In 2009, in the paper titled "Virtual Palaeontology: Gait Reconstruction of Extinct. Vertebrates Using High Performance Computing", the authors used HPC to visually simulate the gait of dinosaurs using palaeontological information obtained from fossils combined with biological knowledge of the anatomy. Since this work of 2009, visualisation tools have become more advanced and easier to use. Thus this field should be more active with HPC and it would be good for PRACE to approach this discipline too. What is key to note in this section is that computationally intensive methods such computer vision, image processing, simulation, visualisation machine learning, computational mathematical models and other such techniques require HPC in general and these techniques are finding more and more applications in academic research fields where in the past they did not. PRACE can foresee such trends and approach research communities accordingly.

5.2 Strengths/Weaknesses/Opportunities/Threats (SWOT) Analysis

A SWOT analysis looks at the organisation itself and how it can use its strengths to take advantage of opportunities, overcome weaknesses and address threats. Please note that a SWOT analysis is not about "*opposites*": i.e. not taking advantage of an opportunity is not considered a threat. It is a risk associated with a decision regarding an opportunity. Assessing risks, inherent to the day-to-day operations of any organisation, is not in the scope of this document.

This SWOT draft focuses on how communication activities will highlight PRACE's strengths.

Translate into tasks	Strengths	Weaknesses
Opportunities	How do we use PRACE's strengths to take advantage of these opportunities?	How do we overcome the weaknesses that prevent PRACE from taking advantage of these opportunities?
Threats	How do we use PRACE's strengths to reduce the likelihood and impact of these threats?	How do we overcome the weaknesses so that threats do not become a reality?

Figure 10: SWOT analysis for PRACE

Strengths

- Strong, established brand;
- Skilled HPC knowledge available (members);
- Unified Peer Review process;
- Collaborative culture.

Weaknesses

- High-level and complex scientific information to be promoted to layperson audiences;
- Shortage of staff and high skilled professional in the European HPC ecosystems;
- Distributed teams make cooperation more complex.

Opportunities

- MoUs signed with other organisations and projects provide opportunities for wider synergies;
- Positive political climate opens doors for PRACE to make its case;
- Exascale and all it could provide to our communities of users.

Threats

- China, Japan, USA will get ahead in the global HPC race if Europe does not invest more in HPC;
- PRACE members have not yet found a unified voice that will influence EU policy making.

This quick SWOT analysis clearly shows the strong strengths of the PRACE brand, now well-renowned within the global HPC community, with positive interaction already in place with many stakeholders, as proved by the many MoUs already signed.

Still, there is a need for a stronger unified voice of PRACE, that could influence EU policy making and promote HPC RI outside our first order community of stakeholders, and keep up with the accelerated pace of supercomputing in other regions.

5.3 Tools and Activities supporting PRACE stakeholder management

The following tools are essential for the support of the stakeholder management:

Generic internal services:

- BSCW - Web-based collaborative workspace system available for PRACE staff which relies on BSCW software. Registration of users is carried out by PRACE PMO.
- DPMDB - DECI Project Management Database is used to administrate DECI projects.
- SVN - Software versioning and a revision control system.
- Wiki - Collaborative workspace and knowledge management for all PRACE staff.

General relationship management:

- Mailing lists - Provided for PRACE project and its users.
- PRACE-RI CRM system - This newly MailerLite hosted service acts as a PRACE contact management database where details of contacts consensually gathered by PRACE are stored and its mass mailing capability is used to distribute PRACE news to these contacts.

Dissemination management:

- PRACE-RI WEB Portal - Running under Wordpress CMS, this web portal publishes all information, documentation and news about PRACE-RI and can be found at [7].
- PRACE Training Portal - Running under TYPO3 CMS, the training portal hosts a collection of materials, tutorials, training videos and events provided by WP4.
- PRACE Events System - Based on the Indico software this site serves as PRACE's event scheduling and organisation web application.
- Summer of HPC website and blog - This page is for the PRACE Summer of HPC programme and blogs made by participating students and can be found at [13].
- Social Media - PRACE has a presence on the following social media: Twitter, LinkedIn a group and a company page), Google+ (via the PRACE business page on Google and the PRACE YouTube Channel), YouTube. Specific channels are used for Training (YouTube) and the Summer of HPC (Facebook).

Project submission and peer review portal:

- PPR Tool - The Project Proposal Revision Tool is used for the submission and the management of the PRACE project proposals applications with regards to the electronic submission of proposals, as well as the follow-up peer review process which includes technical and scientific evaluations and other peer review processes.

5.4 Further Analysis

From the Training Portal of PRACE, Google Analytics data allow us to identify potential future international partnerships, besides countries with which PRACE already cooperates with (EU PRACE Members, USA, Canada, Japan). On the yearly period of November 2015-November 2016 the top 25 from which traffic on the portal was received were:

- India (top 3 traffic from the cities of Bangalore, Chennai, Hyderabad):
  - Supercomputer Education and Research Centre, Bangalore;
  - Chennai and Hyderabad, who also have supercomputing centres.
- Russia (top 3 traffic from the cities of Moscow, Saint Petersburg, Samara):
  - In Moscow there is the Moscow University Supercomputing Center;
  - In St. Petersburg State Polytechnical University operate a 1PFlop/s machine;

  - The Samara State Aerospace University operate a supercomputing center.
- China (top 2 traffic from the cities of Beijing and Guangzhou):
  - Chinese Academy of Sciences in Beijing coordinates academic HPC in China;
  - In Guangzhou the National Supercomputer Center which hosts Tianhe-2, where currently the second fastest supercomputer in the world can be found.
- Brazil (top 3 traffic from the cities of Sao Paulo, Rio de Janeiro, Juiz de Fora):
  - University of Sao Paulo installed a new supercomputer in 2015;
  - Federal University of Rio de Janeiro installed a supercomputer in 2016 (226 TFlop/s).
- South Korea (most traffic from the cities of Seoul and Daejeon):
  - Seoul has many universities and includes the Centre for Manycore Programming at Seoul National University among surely other similar centres;
  - Korea Aerospace Research Institute, Korea Institute of Science and Technology Information, Korea Research Institute of Bioscience and Biotechnology, and Korea Atomic Energy Research Institute are based in Daejon.
- Iran (most traffic from Tehran):
  - The Amirkabir University of Technology in Tehran has a supercomputer.

Similarly, from PRACE website Google Analytics data for the period of November 2015-November 2016, besides countries PRACE already cooperates with (EU PRACE Members, USA, Japan) other countries in the top 25 from which traffic on the portal was received are:

- India (top 3 traffic from the cities of Bengaluru, Pune, Mumbai);
- Brazil (top 3 traffic from the cities of Sao Paulo, Rio de Janeiro, Belo Horizonte);
- Russia (most traffic from Moscow);
- Saudi Arabia (most traffic from Jeddah), King Abdullah University of Science and Technology (2 supercomputers), King Abdul Aziz University (1 supercomputer).

Traffic from these countries and specifically the cities from which they originate – who mostly have large national supercomputing centres, identify countries and centres which have shown an interest in PRACE in one form or another. This could be used by PRACE to identify the known and the unknown supercomputing centres/institutions with which PRACE could possibly collaborate with in some manner for wider International cooperation.

5.5 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.

5.5.1 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. Until 14th Call 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
Grand Total	**460**	**12.302.030.158**

Figure 11: Awarded projects until 14th Call

5.5.2 Summary of Training activity

In terms of Training, the PRACE IP projects have organised 25 Seasonal Schools, more than 350 PRACE Advanced Training Centre (PATC) Events, and 6 International Summer School on HPC Challenges in Computational Sciences (in collaboration with international partners). The Training Portal hosts the training material delivered by over 125 PRACE training events and publicly stores over 1200 documents (1100 pdf files, 120 archive files). Further to this, the Training Work Package (WP4) is preparing two Massive Open Online Courses (MOOCs), one of which has been already made available to the public.

5.5.3 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 2015, the EXDCI project started with the organisation of the European HPC Summit Week, of which PRACEdays became the central event.

The Outreach task of WP3 in the PRACE IP projects presents PRACE at science fairs and museums around Europe (9 science fairs and 3 museums in 2016). This is meant 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 4 Summer of HPC programmes since 2012, where PRACE partners hosted students from Europe and beyond for them to learn and work on a HPC related summer project.

PRACE Communications team (both in WP3 of the IP project and PRACE aisbl) produces a large amount of communication material, such as: PRACE Digest (6), PRACE Annual Report (4), 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+, and YouTube. The PRACE Summer of HPC has its own Facebook page and blog. The PRACE-3IP project saw a pilot campaign called “Dare to Think the Impossible Campaign”. The video game that came out of that is still used at science fairs. PRACE Communications also provides PRACE branded templates and standard slides for presentations, as well as input to members for their local publications, for example: SNIC-PRACE DIGEST No.1 2011-2014 [49].

5.5.4 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), GEANT (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) 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 7.3 - Annex 3: PRACE partnerships.

5.6 Follow-up actions/recommendations

Follow-up / recommendations of this deliverable that provide the results of the analysis of the management of stakeholders done by PRACE-4IP project would be, first, to continue the positive work done so far on stakeholder management by PRACE projects and PRACE Aisbl, and second to deepen some analysis, such as the SWOP or STEEPLED analysis, that have been just drafted so far and could benefit from a dedicated workshop, at the level of some bodies of PRACE, MB, the TB, BoD, or SSC / IAC. Furthermore, it could be interesting to follow the work done on stakeholder management by keeping up to date a matrix such as the one presented below.

Stakeholder category	Stakeholders	Contributions to our organisations capacity for value creation	Strategic Priority/ Focus Area	Tactical Priority/ Focus Area	Engagement Means and Frequency (y, 6, q, m, w, d)
Strategic partners					
Hosting organization					
Funders					
Policy level					
Employees					
Co-investing Collaborators					
Non co-investing Collaborators					
Users					
General public					
International e-Infrastructure communities					
Service providers					

Table 1: Summary of the stakeholder analysis

6 Conclusion

In conclusion, the whole society is probably the ultimate stakeholder that should benefit, directly or more 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 to help them tackle the diverse range of challenges facing humanity. Computer simulations tremendously speed up the process of acquiring knowledge by shortening or even completely replacing complex, time-consuming laboratory experiments.

The EU HPC ecosystem has been tremendously moving forward in the next 10 years, since 2010 with PRACE creation, then in 2012 and 2016 again with EC important communications and the launch of successive new initiatives and programs under and along Horizon 2020 This now makes up a consistent strategy but a lot remains to be done. EU HPC ecosystem remains a complex but vivid one, in the midst of a rapidly evolving worldwide landscape - and a fiercely competitive one. PRACE and partners (all ecosystem stakeholders) must keep a close eye on HPC worldwide developments, and leverage solid tools and methods to stay in the race, reacting dynamically - tools and methods such as those explained in this report. PRACE can and must contribute to positively influencing EU policy for better and stronger public and private investments in HPC, joining forces with other strong voices, but also talking to general public and making HPC both well-understood and fancy.

7 Annexes

7.1 Annex 1: The new European HPC research landscape

The new European HPC research landscape is clearly described by the following figure and is comprised of 8 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. 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.

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

Name	Field	Institution, 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
Laura Grigori	Numerical Mathematics / HPC	INRIA/University Pierre and Marie Curie, France
Dimitri Komatitsch	Computational Earth Sciences	LMA CNRS-MRS, France
Petros Koumoutsakos (Chair)	Computational Science and Engineering	ETH Zürich, Switzerland
Erik Lindahl (Vice-Chair)	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	Particle Physics / Mathematics	University Dublin, Trinity College Dublin, School of Mathematics, Ireland
Christof Schütte	Life Sciences	Free University of Berlin, Germany
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, 20 September 2016

Name	Field	Country
Edouard Audit	Universe	France
Marc Baaden	Biology/Chemistry	France
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
Simone Hochgreb	Engineering I	United Kingdom
Petros Koumoutsakos (Chair)	Computation Sciences and Engineering	Switzerland
Aske Plaat	Data Sciences (Bioinformatics, Social)	The Netherlands
Carme Rovira Virgili	Chemistry/Bio	Spain
Alfonso Valencia	Bioinformatics /Biochemistry/Life sciences	Spain
Hartmut Wittig	Fundamental Physics	Germany
Dietrich Wolf	Computational/Statistical Physics	Germany
Claudio Zannoni	Condensed Matter/Chemistry/Materials	Italy

Table 3: Access Committee (AC) Membership, 19 December 2016

Name	Company	Domain
Anders Rhod Gregersen (Chair)	Vestas	Renewable Energy
Lee Margetts (Vice-Chair)	NAFEMS	ISV
Henk Coenen	NXP	Telecommuncations / Electronics
Marc Morere	Airbus	Aeronautics / Aerospace
Dieter Jahn	BASF	Materials / Chemistry
Enric Gibert	PHARMACELERA	Life Sciences / Pharma
Stéphane Tanguy	EDF	Energy
Christoph Gümbel	Porsche AG	Automotive / Transport
Martin Winter	CEFIC-European Chemical Industry Council	Materials / Chemistry
Jean-Denis Muys	Audionamix	Media / SMEs
Paul Walsh	Nsilico	Life Sciences / Pharma / SMEs
Jean-Francois Lavignon (Observer)	ETP4HPC	HPC Vendors

Table 4: Industrial Advisory Committee (IAC) Membership, 23 June 2016

7.3 Annex 3: PRACE partnerships

PRACE has a Memorandum of Understanding (MoU) with:

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

PRACE is a partner of the following projects:

EESI2 – European Exascale Software Initiative

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.

RIKENIn 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).

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