PRACE in the EuroHPC Era

Position Paper

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Published: **December 2018**

The Partnership for Advanced Computing in Europe (PRACE) is an international non-profit association with its seat in Brussels. The PRACE Research Infrastructure provides a persistent world-class High Performance Computing service for scientists and researchers from academia and industry in Europe. The computer systems and their operations accessible through PRACE are provided by 5 PRACE members (BSC representing Spain, CINECA representing Italy, ETH Zurich/CSCS representing Switzerland, GCS representing Germany and GENCI representing France). The Implementation Phase of PRACE receives funding from the EU's Horizon 2020 Research and Innovation Programme (2014-2020) under grant agreement 730913.

For more information, see www.prace-ri.eu

Table of Contents

Executive summary

The EuroHPC Joint Undertaking will advance the European supercomputer landscape by completing the infrastructure pyramid at the top level with European leadership-class supercomputers. In a context of a strong international competition with USA, China and Japan, this development is highly expected by all stakeholders of HPC in Europe.

For the European HPC users from science and industry, i.e. industrials and SMEs, the seamless integration of these new top-level systems and services into the existing European HPC-ecosystem is an issue of paramount importance.

The development of the European HPC-ecosystem was initiated by PRACE and its 26 partners in the past ten years. PRACE is supported by the PRACE Member States and through the EU by a series of implementation projects, and thus could weave a common European umbrella over national HPC-ecosystems.

PRACE offers a comprehensive range of services, support activities and programmes to foster the European HPC ecosystem including interaction with communities, flagship projects and data infrastructure activities, in particular concerning federated big data management. PRACE has become a trusted liaison between HPC-infrastructures and European HPC users, involving highly rated advisory committees with members from science and industry.

The very recent Scientific Case prepared by the PRACE Scientific Steering Committee (SSC) provides a comprehensive overview of the strategic importance of HPC in a growing number of areas, in particular, it emphasizes the convergence of extreme-scale simulation, big data analysis and artificial intelligence and it outlines future directions.

PRACE and EuroHPC have almost complementary missions. While EuroHPC acts as a high-level financing agency and must essentially be a top-down activity, PRACE is a science-driven infrastructure developed as a bottom-up activity. Joining both in a strong partnership will create best possible synergies for the benefit of European communities

PRACE today offers a wide range of services and develops future services, especially in the area of federated Big Data analysis, joining with GÉANT to coordinate activities and to support the European Data Initiative. Appropriate financial models must ensure the sustainable operation of services.

The federated provision of EuroHPC's pre-exascale and petascale systems and future exascale systems, complemented by national Tier-0/1 resources needs appropriate coordination between EuroHPC hosting members and national PRACE Tier-0 and Tier-1 hosting partners.

This position paper advocates for a strong partnership between EuroHPC and PRACE, including key partners from the European ICT landscape. By pooling our creative forces and experience in Europe, we will achieve global leadership in technology, scientific, industrial and societal application of HPC.

1 Introduction

The Partnership for Advanced Computing in Europe (PRACE) has been mandated by the governments of 26 European member states to enable high-impact scientific discovery and engineering R&D in all disciplines through extreme-scale simulation and data analytics, in order to enhance European competitiveness for the benefit of society and humanity [1].

PRACE realizes its mandate by offering computing and data management resources of the Tier-0 class through a highly valued, internationally respected peer review process. The resources are provided currently through seven centres in five PRACE Member Countries, complemented by Tier-1 class provision from 21 PRACE partners. Since 2010, PRACE has enabled more than 650 scientific projects and has awarded close to 20 billion core hours to more than 3000 researchers from science and industry [2]. More than 50 companies were supported by open R&D access for industrial users. Since 2008, PRACE has been building a Europe-wide network of 26 HPC centres, supported by the European Commission since 2008 through seven PRACE Preparatory and Implementation Phase Projects (PRACE-PP and PRACE-IP) [3].

PRACE offers a comprehensive range of coherent services, including training courses, high-quality user support, technology watch, and advanced code enabling. PRACE helps industry participate in HPC through the SHAPE programme (SME HPC Adoption Programme in Europe) [4]. Overall, PRACE promotes the European HPC-ecosystem with a well-known brand, the PRACEdays, and the Summer of HPC [5].

PRACE has become the interface between the infrastructures and the European HPC users, not only provisioning systems, but also through the unswerving commitment of its Scientific Steering Committee (SSC) [6] and Industrial Advisory Committee (IAC) [7], and the Access Committee (AC) [8] that ensures the quality, diversity and impact of the research performed.

PRACE strongly welcomes the creation of the EuroHPC Joint Undertaking (JU) [9]. The EuroHPC JU will open the door to a new era of computing in Europe, raising the availability of high-end compute and data analytics resources on a par with or exceeding the capabilities of other continents. PRACE stresses the importance of coordination of the development of the EuroHPC JU and that of PRACE with respect to its third operational phase starting in 2020, in order to ensure a smooth transition of the scientific communities from PRACE 2 to PRACE in the EuroHPC era. In this spirit, this document presents the status of the landscape of HPC in Europe, the competences and complementarities of PRACE Members and an analysis of scientific and industrial use cases; it discusses the impact of past and future missions of the PRACE aisbl [10], the PRACE-IP projects, the pan-European ecosystem created by PRACE, with its impact on national levels and communities, and the ESFRI projects [11] and European flagships [12]; finally a model for the operation of PRACE in the EuroHPC era is proposed.

By developing a bespoke position in the EuroHPC era, PRACE wants to contribute to creating a solid basis for the future of HPC in Europe. PRACE is ready to support EuroHPC in fulfilling its ambitious and important mission.

2 Status analysis

From the outset, PRACE has assigned very important roles to its Scientific Steering Committee (SSC) and to the Industrial Advisory Committee (IAC) – which was set up somewhat later – with regard to the participation of representatives of the scientific and industrial communities. In particular, this is the case for the purely science-driven allocation of resources, which gives the PRACE Research Infrastructure a unique position in the international landscape, as well as for the scientific and industrial use cases of PRACE, a unique science-driven set of requirements for HPC infrastructures, provision, training, and empowerment activities. Finally, it is the leading competence of the partners with a variety of newly developed and important services that make PRACE a successful research infrastructure.

2.1 The position of PRACE in the international HPC landscape

2.1.1 USA

The leading supercomputing programmes in the USA have been run by the Department of Energy (DOE) for several decades. Since about ten years, the Leadership Computing Facilities in Oak Ridge (OLCF) and Argonne (ANL) operate systems that aggressively explore new architectures at extreme scale. OLCF and the facility at Lawrence Livermore National Laboratory (LLNL) regularly deploy supercomputers that take the top spots in terms of peak floating-point performance. The leadership computing systems at OLCF and ANL are open and intended for extreme-scale computing applications, similar to the Tier-0 systems of PRACE. In addition, capacity resources similar to the PRACE Tier-1 systems are operated by the National Energy Research Supercomputing Centre (NERSC) at Lawrence Berkeley National Laboratory (LBNL), as well as the supercomputing facility of Los Alamos National Laboratory (LANL). Each time new supercomputers are introduced by these facilities, they appear in the top ten of the Top500 list [13].

The National Science Foundation (NSF) operates a Track 1 system, similar to PRACE's Tier-0 systems, to support its programs – this system is currently operated at the National centre for Supercomputing Applications (NCSA) at the University of Illinois, and its successor will be installed at the Texas Advanced Computing centre (TACC) in Austin. The NSF Track 1 system and the programmatic systems of DOE are of comparable performance and will reach pre-exascale levels by 2020.

2.1.2 China

China operates a very large network of capacity systems that serve researchers at universities, its national academy of sciences, as well at other state funded research labs. The most visible supercomputers, however, are China's version of leadership-class systems. They have stunned the global supercomputing community with performance, and with the fact that they are built with Chinese technologies (processors, accelerators, interconnects, …). These supercomputers are regularly competing for the top spots with the leading US systems in terms of peak floating-point performance.

2.1.3 Japan

While China and the USA are competing to build the first sustained exaflops systems early next decade, Japan is taking an entirely different approach to leadership class computing. At Riken's centre for Computational Sciences (CCS), the country operates its national leadership supercomputer, the K Computer. This system only briefly took the top spot in terms of peak floating-point performance in 2011; however, it has until recently outperformed every other supercomputer on the planet with its memory performance. As a result, applications from all domains run very efficiently. The post-K Computer will be deployed in the early 2020s. It will not match its US and Chinese counterparts in terms of peak floating-point performance, but very likely it will outperform its rivals in sustained application performance. Besides the leadership system at Riken's CCS, Japan maintains a network of capacity computing systems at various universities and national research centres. It had the first top-10 supercomputer dedicated to machine learning applications.

2.2 Openness of the PRACE ecosystem

While the Japanese and Chinese systems are intended for their own national scientists and foreigners would only be allowed access if they have a local collaborator, the leadership systems in the USA are open to scientists from around the world. They are allocated via the INCITE programme with a transparent peer-review process that is similar to the process implemented by PRACE for allocations on its Tier-0 systems. Every INCITE project receives a liaison at the leadership computing facility for high-level support. There is, however, no systematic path for projects to transition from capacity resources at NERSC and the NSF Track 1 systems to the leadership class systems of the INCITE programme [14].

In contrast, thanks to the PRACE high-level support teams and the so called "candidate" Tier-0 projects from proposals that receive high scientific scores but lack the ability to run on Tier-0 systems, the European supercomputing ecosystem has a systematic path to transition Tier-1 projects to extreme scale computing of the PRACE Tier-0 programme.

2.3 Science-driven resource allocation by PRACE

While the PRACE Tier-0 and INCITE allocation processes are comparable – they are both based on external peer reviews and a decision panel – the selection of reviewers and panellists is fundamentally different. In DoE's INCITE program scientific peer reviewers and the panellists that make allocation recommendations are selected by programme officers and the science directors of the supercomputing centres.

With PRACE, it is the Scientific Steering Committee (SSC), a group of leading scientists in Europe that is independent of the supercomputing centres or any programmatic interests of funding agencies, which proposes the members of the Access Committee (AC) – the panel that makes the final allocation recommendations for Tier-0 projects – which in turn selects the scientific peer reviewers [15].

The resource allocation process of PRACE is thus bottom-up, free of political agendas, and purely driven by scientific excellence. In this sense, PRACE differs positively from the other three most important HPC-infrastructures worldwide.

2.4 PRACE scientific and industrial cases

Between 2007 and 2018, three European scientific case studies were completed for PRACE. Together they demonstrate the importance of HPC provision at the highest level to ensure the European leadership in computational science. The third edition of the PRACE Scientific Case (PSC) spanning from 2018 to 2026, was issued mid October 2018 by the PRACE Scientific Steering Committee (SSC). Comments and results from the PSC 2018 [16] are highlighted in the next paragraphs.

2.4.1 Strategic importance of HPC

High Performance Computing (HPC) is a strategic tool for competitive science, fostering innovation and supporting public decision-making based on facts. Having been used for more than 30 years in climate research, numerical weather prediction, particle and astrophysics, earth sciences and chemistry, HPC is now a cornerstone of all scientific fields from biology, life sciences and health, energy, geosciences, high-fidelity combustion, materials science, to social sciences, and humanities. In industry, HPC is widely used in oil & gas exploration, aeronautics, automotive, and finance, and is now becoming crucial for ensuring personalised medicine, developing nano-technologies, or enabling the development and the management of renewable energies. Initially the preserve of large companies, HPC is now used more and more by European SMEs, which represent a very important part of European industrial competitiveness. In order to accelerate this trend, PRACE and some of its partners have launched several initiatives at national or European level (SHAPE programme, Fortissimo projects) offering a unique set of services spanning from HPC dissemination, and open R&D, to confidential R&D, and commercial cloud-based activities.

Finally, HPC is becoming a tool of growing importance for supporting public rational decision making by simulating scenarios and allocating urgent computing resources in a “red button mode” in the case of natural hazards (extreme events such as earthquakes, thunderstorms, flooding or evacuations), industrial risks (rupture of a dam, failure of a power-plant, spills), biological risks (diffusion of pandemics) or (cyber)terrorism attacks.

2.4.2 Convergence of simulation and big data analysis

Beyond its importance for accelerating numerical simulation, HPC is now also used at the convergence of simulation and big data workloads, this need being driven by the increasing amounts of data coming from next generation scientific instruments (satellites, (radio)telescopes, accelerators, microscopes, sequencers), from the Internet of Things (IoT), social media, and from large scale simulations (including massive 3D simulations, multi-scale and multi-physics coupled simulations, ensemble/optimisation/scenario studies, uncertainty quantification).

Many science communities are now combining HPC and High Performance Data Analytics (HPDA) applications and methods in large-scale workflows that orchestrate simulations and incorporate them into the stages of large-scale analysis pipelines of data generated by simulations, experiments or observations. The short time scales required for some of the applications constitute a crucial challenge.

2.4.3 Artificial intelligence

Exploiting and valuing such enormous amounts of structured or unstructured data in a reasonable and competitive time is no longer possible for human beings, leading to the rise of HPDA supported by new data assimilation, interpretation, extraction, and prediction-techniques benefiting from artificial intelligence (AI) and machine learning (ML).

There is an ongoing convergence between HPC and HPDA/AI. Scientific communities generating large amounts of data will require HPDA/AI tools allowing them, when possible, to (in-situ or in-transit) infer experimental/simulation outputs just after being generated. This makes it possible to classify and identify pertinent structures to be stored, saving time and energy, because the raw data does not have to be stored and processed after. In the future, this also could lead to smart AI-driven computational steering techniques or using AI techniques in coupling simulations and learnt models in order to accelerate convergence of scientific models or optimisation/uncertainties studies.

On the other hand, modern AI (coming after a 25-year AI winter with the support of DNN on GPU and FPGA) will benefit from converged HPC/AI architectures for addressing new scale-out challenges including the development of more complex and deeper neural networks (like CapsNet Capsule neural networks), AutoML techniques or explainable AI (XAI) methods.

In summary, many of the industrial, scientific and societal challenges that communities face will be simulated before being actually executed. This scenario requires extensive access to HPC resources, robust computational codes and data analytics for which the next generation of scientists, technologists need to be trained in multidisciplinary areas for which new educational plans will be required.

2.4.4 Future directions

Due to the rapid convergence between HPC, HPDA and AI as a result of the explosion of data generated by large scale instruments or numerical simulations, PRACE and the European computational ecosystem must develop new architectures and services addressing mixed HPC/AI workloads. This has been already understood by countries like US (installation in 2018 of the Summit 200 PF converged system at ORNL), China and Japan who will address this convergence in their roadmap.

Such convergence will also be fostered if major EU-wide efforts are made in education and training towards new skills in data science and numerical simulation to train and retain a new generation of researchers and technologists in both science and industry, and if basic training in the technologies is provided and/or their impact is transferred to the general public.

2.5 Competences of PRACE and partners

PRACE as community of stakeholders of the European HPC-ecosystem has a huge basket of virtues, represented by the competences of its partners in various domains.

2.5.1 Access to HPC systems

Scientists and researchers from all over the world have free access to PRACE resources for open research (i.e. with publication of results). Access is granted through a rigorous peer review process. Industrial users with headquarters or large R&D activity in Europe can also apply for open R&D projects and must undergo the same review. Access is provided via calls for Project Access (regular access to a research infrastructure), for Preparatory Access (to enable proposal preparation), and for SHAPE, the SME HPC Adoption Programme in Europe.

2.5.2 Support for industry

In addition to supporting SMEs through the SHAPE programme, including provision of resources, or PRACE Open R&D access for industry, some of the PRACE partners offer close collaboration and tailor-made solutions for industry, either for large enterprises or for start-ups and SMEs.

2.5.3 Enabling of HPC applications

In addition to granting access to seven state-of-the-art supercomputers, PRACE partners also support users in porting, scaling and optimising their applications. With the help of high-level support teams, the capabilities of the PRACE systems are fully exploited. This includes support for preparatory access, long-term extreme scalability of codes, code refactoring, and adaptation of algorithms and/or mathematical library routines. In this way, applications are improved on the specific computer architectures, and open source future-oriented pre-exascale software solutions (libraries, codes) are developed that have a great advantage over currently available solutions.

2.5.4 Services for universities and user communities

PRACE member institutions support universities with thousands of users in daily operations as well as specific user groups with very specific requirements. In particular, the service for user communities is based on many years of experience with these communities, so tailor-made solutions for their HPC workflow, including data management in compliance with data protection regulations can be offered. Many PRACE partners offer services at national or even regional level for new user communities from science and industry. This demonstrates how much of the competence of HPC in Europe is represented by PRACE members in a federated way.

2.5.5 HPC training

All PRACE member institutions invest extensively in education and training programmes to enable effective use of the Research Infrastructure. PRACE is adding value by coordinating and reviewing these substantial activities at the European level though courses organised by the PRACE Training Centres, seasonal schools, the International HPC Summer School, and the Summer of HPC where

students execute full-fledged projects, as well as workshops and scientific and industrial seminars throughout Europe and in collaboration with the Centres of Excellence (CoE). The PRACE Training Centres (PTC) to date have trained more than 12 000 young researchers. Additionally, PRACE also offers an online repository of code examples, model solutions and other tips via CodeVault as well as Massively Open Online Courses (MOOCs). In the field of convergence with High Performance Data Analytics and Artificial Intelligence (HPDA/AI), new curricula are now being proposed by PRACE partners as well as the support of new training tools like Jupyter Notebooks.

2.5.6 Gender balance and promotion of HPC careers

With PRACE's contribution to "Women in HPC" (WHPC) by the General Secretary of WHPC, PRACE supports this ground-breaking activity. Through collaboration and networking, WHPC strives to bring together women in HPC and technical computing while encouraging women to engage in outreach activities and improve the visibility of inspirational role models. WHPC is stewarded by EPCC at the University of Edinburgh, a member of the PRACE family [17].

2.5.7 Operational HPC services

PRACE partners operate joint infrastructure services for user-friendly access to HPC resources with close integration of all levels and various tools and software. Interoperability with other e-Infrastructures is constantly improved and new services are developed. Within this framework, reference architectures for HPC cloud convergence are also being developed by PRACE partners. All PRACE locations are connected via a GÉANT MD-VPN network.

2.5.8 HPC procurement and prototyping support

To support the HPC centres, PRACE conducts a regular market technology watch, bringing the HPC centres up to date as to leading technology. Best practices are identified for data centres and hardware prototyping. European workshops on HPC centre infrastructure are organised annually. PRACE develops and maintains a Unified European Application Benchmark Suite (UEABS) [18], which meanwhile also includes accelerator benchmark applications. This benchmark suite can be used in a straightforward manner for procurements. PRACE partners are leaders in the deployment of new architectures, often in co-design with HPC vendors of future exascale technology and are involved already in joint HPC procurements like PCP and PPI4HPC [19].

2.5.9 Dissemination and documentation for HPC services

Together with the EXDCI project [20] (PRACE+ETP4HPC [21]), PRACE organises the European HPC Summit Week, which includes PRACEdays – the PRACE Scientific and Industrial Conference. The PRACE website contains a wealth of useful information for the scientific and industrial communities, e.g. Best Practice Guides and White Papers provided by PRACE partners. In the PRACE Digest and Factsheets, information about PRACE and the results of the awarded scientific projects are published. Scientific and industrial results are also presented during PRACEdays [22], PRACE's annual scientific and industrial conference series. PRACE maintains a host of international collaborations with the USA, Japan, South Africa, and Australia, just to name a few.

3 Impact analysis

Over the last ten years, PRACE has increasingly shaped the HPC-ecosystem in Europe at the highest level (Tier-0), based on the work of the legal entity – PRACE aisbl – the EC-funded PRACE IP Projects, the establishment of a Scientific Steering Committee as well as an Industrial Advisory Committee. The PRACE idea has transformed the entire HPC-ecosystem both at national level (Tier-1) and at regional level (Tier-2). PRACE has become the European interface to the HPC communities through both successful provisioning of resources and its very engaged SSC and IAC. PRACE is closely linked to ESFRI Projects as well as European Flagship Projects, especially the Human Brain Project, but also Graphene, the Quantum Technologies flagship, and other initiatives planned for the near future like Extreme Earth.

3.1 Mission and role of PRACE aisbl

PRACE aisbl was founded in 2010 as an international non-for-profit organisation under Belgian law (association internationale sans but lucratif – aisbl) based in Brussels with 26 members, each mandated to represent their country. PRACE aisbl offers the legal form that ensures the sustainability of the infrastructure.

The Association has been given the overarching mission to provide a science-driven federated European supercomputing infrastructure, which is competitive compared to similar infrastructures elsewhere in the world. It builds on the strengths of large national supercomputing centres in Europe (Tier-1) providing high-end scientific computing and data analysis resources. PRACE's goal is to drive discoveries and new developments in all areas of science, from fundamental research to applied sciences, including mathematics and computer sciences, medicine, engineering as well as digital humanities and social sciences. In this manner, PRACE aims to help create a fertile basis for technological development and industrial competitiveness in Europe. This is accomplished through:

- Provisioning of a Europe-wide, federated, world-class supercomputing infrastructure at the highest performance level that is architecturally diverse and allows for capability allocations that are competitive with comparable programmes in the USA and Asia. The European centres BSC (ES), CINECA (IT), CSCS (CH), GENCI (FR), HLRS (DE), JSC (DE), and LRZ (DE) are contributing to the PRACE infrastructure. The highest possible performance level characterises PRACE as a Tier-0 infrastructure.
- A worldwide unique and fully transparent peer-review process for resource allocation, exclusively based on scientific excellence. PRACE Calls for Proposals for Project Access address scientists from all PRACE Member Countries and beyond, through encouraged collaboration within the projects. International coverage again characterises PRACE as a Tier-0 infrastructure.
- Coordinated High Level Support Teams (HLST) [23] that provide users with second and third level application support specifically adapted to the Tier-0 systems.
- Implementation activities in the fields of dissemination, industrial co-operation, training and research into future supercomputer technologies involving additional investment in application enabling, coordinated with the efforts of the support team and contributions from all PRACE partners.

PRACE aisbl has given the European HPC-ecosystem a solid, robust and sustainable framework to establish the European HPC-infrastructure, starting from and using the high-end resources and expertise available at national level. The governance of the association enabled the effective collaboration and coordination of the relevant actors, which in turn led to the achievement of PRACE's unparalleled services for the benefit of the ecosystem as a whole.

3.2 Relevance of the PRACE IP projects

The European Commission has been supporting PRACE via EU-funded projects from the very beginning. Already in 2008, i.e. in the Seventh Framework Programme, the EC contributed to the creation of PRACE via the PRACE Preparatory Phase project. The EC support continued from 2010 until now, in the H2020 Framework Programme, in the form of a series of Implementation Phase Projects funding the implementation and operation of PRACE. Until now, the overall budget for the PRACE projects reaches € 169.3 million with an EC contribution of € 121 million. Approximately 500 HPC experts from 26 European countries are involved in the current PRACE-5IP project [24].

The support from the EC was essential to establish the current strong and stable European HPC-ecosystem. PRACE member institutions and their partners all over Europe are working together in order to provide high-quality services to PRACE and its users. Via the IP Projects, PRACE member institutions and their partners support PRACE aisbl in all legal, financial, and organisational aspects. PRACE was supported to be established as the Tier-0 European HPC Research Infrastructure, a Scientific and Industrial Conference series was created – PRACEdays – and international outreach activities have been pushed such as the International HPC Summer School and the Summer of HPC.

Through the IP Projects, PRACE provides comprehensive and unique HPC Training throughout Europe, carried out by its members and partners and the PRACE Training Centres, collaborating intensively with the Centres of Excellence. The IP Projects execute an annual technology and market watch, record best practices for design and operations of energy-efficient HPC Centre Infrastructures, and provide prototyping of HPC systems.

The IP Projects also attach high importance to support the joint operation of the PRACE Tier-0 and Tier-1 systems, including the prototyping of new hardware and software services (including recently pilots of urgent computing or links with scientific instruments like ESRF, SKA/AENEAS or CERN).

Users all over Europe receive support across disciplines, in particular by means of the newly implemented High Level Support Teams at the PRACE Tier-0 sites. Some of the PRACE IP Projects had a focus on supporting industry to participate in HPC. What is more, SMEs are regularly supported through the award-winning SHAPE programme.

Overall, through the constant support of the PRACE projects, a functioning HPC-ecosystem was built in Europe, achieving much more than the individual centres could have achieved on their own. The basis of this HPC-ecosystem is the trust between the PRACE members and partners grown during 10 years of fruitful collaboration. It is no exaggeration to say that the IP Projects have been and still are instrumental for the creation of the European HPC-ecosystem.

For these reasons, it is indispensable for the continuation of the European HPC success story to pursue the activities as so far carried out by the PRACE IP projects appropriately when entering the EuroHPC era.

3.3 Impact of PRACE on the HPC ecosystem

Since its inception in June 2010, PRACE has added a complementary level of scientific computing capabilities to the computing resources available for researchers in Europe. Scientists based in the Hosting Member Countries of PRACE already had the opportunity to conduct their research using the largest supercomputers in Europe. PRACE opened this possibility to all researchers in Europe, enabling them to take the next step in their science and foster European-wide scientific collaborations and beyond. In fact, the well-known pyramid model with national Tier-1 systems was extended by European-level Tier-0 resources available to all of Europe.

Computing resources at this European level were for many researchers an order of magnitude larger than available in their own countries. Not only has it improved the overall quality of European scientific results, it has also encouraged (and forced) European researchers from science and industry to improve the quality of their scientific proposals, as computer resources are allocated in a fierce scientific competition. This helps in not only the PRACE environment, but also more generally in scientifically open calls for proposals where the award is made within a rigorous peer review framework.

Larger research collaborations have formed to submit proposals to PRACE, since at European Tier-0 level, the awarded computing resources are so large that only few single research groups are able to effectively use the resources alone and interpret the results effectively. Consequently, increasingly larger research collaboration teams submit proposals to PRACE; this stimulates the co-operation between scientists in Europe to address big problems, which again leads to higher-quality proposals and increased competitiveness on a global scale.

Access to large research infrastructures is important not only for senior scientists, but is heavily attracting PhD students and Postdocs. Hence, the PRACE level of computing resources has value also in attracting scientific talent, from which science, industry and society benefit in the long-term. Together with increased cooperation, the knowledge and expertise in Europe both in the scientific field and in the support of science by large computer resources in the framework of PRACE and its Implementation Phase Projects has developed considerably.

Industrial usage has been stimulated through various calls benefiting large groups as well as SMEs coming from countries around Europe. Many SMEs have gained from this, especially in realising the potential of larger-scale simulations for their businesses, getting visibility at European level and more globally, being fully inserted into the European HPC-ecosystem, something impossible without the support of PRACE for SMEs employing only a handful of people.

As a result, PRACE has given large value to the European HPC-ecosystem, not only through organisation and orchestration, but also by reaching smaller European countries with a less developed HPC-infrastructure.

3.4 Scientific Steering Committee and Industrial Advisory Committee

PRACE has two committees that guarantee the high scientific quality and industrial impact of HPC. The Scientific Steering Committee (SSC) and the Industrial Advisory Committee (IAC) are composed of experts in simulation science and their membership is complementary both in terms of geographical and scientific or industrial interests. They ensure that the Access Committee fulfils the entire required scientific rigor in the assignment and use of the resources by suggesting members that perform the peer-review process in the Access Committee. The SSC also is a forum for the discussion of training needs, future research areas and the vision and shaping of HPC from a scientific perspective (as shown in the Scientific Case). The Industrial Advisory Committee embodies the same principles of impact and societal needs, but with an industrial perspective. The work performed by IAC in canvassing the new computational technologies and applications employing HPC resources, has enhanced the technology transfer and accessibility of such resources in particular to SMEs. The task as evangelist performed by IAC is crucial for the fast transition between academic knowledge and industrial application, and holds the key for a swift transition towards new enabling technologies with a very high impact in the labour market.

3.5 Flagships, communities, and federated infrastructures

3.5.1 Flagships - the Human Brain Project

The Human Brain Project (HBP) [25], a European flagship project for ICT-based neuroscience, medical neuro-informatics and brain-inspired future computing, is an important example of the impact of PRACE on European computational science.

The HBP was deliberately built with the help of R&D from centres at sites in the five countries providing PRACE Tier-0 computing resources, as from the outset it became apparent that high-end brain simulation and data analysis, as envisaged by the HBP, will require data and computing resources both ranging up to exascale and even are determining the direction of high-end computing and future computing technologies. This co-design approach has generated a very substantial increase in the use of digital technologies in the field of neuroscience in both high-end simulation and HPC-enabled data analytics. It is no exaggeration to say that the neurosciences were brought to HPC.

3.5.2 FENIX – a Europe-wide federated data infrastructure

What is more, the requirements of the HBP have initiated the development of the Europe-wide federated data infrastructure FENIX [26], which is supported by the EU-funded ICEI project [27]. FENIX is now in the process of being taken over by PRACE as IaaS for the exchange, administration, management and computational analysis of petascale data sets and beyond. This federated IaaS spans the entire European research area. Large data volumes can be stored and processed near the data sources. The federative nature of Fenix allows to provide access to a diversity of computing capabilities at different sites as well as to include other data centres in the future.

ICEI, the Interactive Computing E-Infrastructure project, is the first EU project to contribute to the establishment of FENIX. It runs, independently funded, under the umbrella of the FPA of the Human

Brain Project. Through ICEI, the Human Brain Project receives dedicated resources for data-intensive brain analysis and simulation and PRACE offers ICEI-resources for all interested scientists and industrial users via the PRACE peer review.

The FENIX consortium builds on technologies developed by PRACE supercomputing sites, and so do the domain communities. For example, the Materials Cloud [28], which enables seamless sharing and dissemination of resources in computational materials science, including software, compute- and data services, as well as curated and raw services that are compliant with FAIR principles, is hosted on PRACE systems and builds on HPC-Cloud converged technologies developed by PRACE members. Similarly, the Swiss Institute of Particle Physics (CHIPP) is running seamlessly, i.e. without users noticing, their part of the World LHC Compute Grid on a PRACE Tier-0 supercomputer, directly exploiting HPC-Cloud technologies. This example is particularly interesting, as it shows that supercomputing systems in the present day and age can have a far better price performance, due to economy of scale, than distributed grid technologies.

3.5.3 Communities

The impact of PRACE on communities results primarily from the extensive allocations of CPU time provided. The record is approximately 450 million core hours spent in a series of three consecutive projects. It is obvious how such opportunities can shape whole areas. These communities include researchers from combustion dynamics, neutrino astrophysics, high-resolution weather and climate modelling, magneto-hydrodynamics for ITER, and elementary particle physics (CERN).

Furthermore, the supercomputing technologies developed by PRACE members have direct impact on communities that have used HPC for decades. One of the first supercomputers worldwide, in which Graphic Processing Units (GPU) came to productive use at scale, was developed and deployed at a PRACE Tier-0 centre. The GPU implementation of the European limited area weather and climate model, COSMO, and one of several applications that was refactored in order to run on this GPU accelerated Tier-0 system, was used to co-design a numerical weather prediction supercomputer for MeteoSwiss. It is GPU-based and in operational use since 2015 for MeteoSwiss' new high-resolutions model – the first weather service worldwide to run operational NWP on a GPU-based system. This solution (refactored implementation running on GPU) is about an order of magnitude more (cost) efficient than running the standard implementation of COSMO on CPU-based systems. The software technology is also used in the EC funded FET-HPC projects ESCAPE and ESCAPE-2 and will be a pillar for Extreme Earth Consortium that is proposing a new FET Flagship project.

3.5.4 EUDAT

The EUDAT Collaborative Data Infrastructure [29] is essentially a European e-infrastructure of integrated data services and resources to support research, where European researchers and practitioners from any research discipline can preserve, find, access, and process data in a trusted environment.

Thanks to the fact that nearly all EUDAT partners are members of PRACE, many synergies can be raised concerning the mutual use of tools and services provided by EUDAT and PRACE. This is

advantageous management (preservation, sharing, publication, discovery, access, tagging, data management plans, training, etc.) of data flows between PRACE sites, in collaborative large-scale projects and between different Tiers.

Moreover, EUDAT is a partner in PRACE-6IP. PRACE and EUDAT have jointly identified many collaboration opportunities and services of common interest like:

- **Data lifecycle coverage** to support PRACE users in developing plans to cover the entire data lifecycle from creating, processing, analysing, to preserving data.
- **Resources access models** to investigate the suitability of peer-review access for computing *and* data, as well as alternative models or on-demand HPC/HPC as a service model (e.g. for AI), as well as urgent computing.
- **AAI** in collaboration with GEANT, to offer seamless access to PRACE & EUDAT infrastructures.
- **Data management training** as part of PRACE training courses.

4 PRACE in the EuroHPC era

PRACE and EuroHPC have almost complementary missions. A strong partnership can create best possible synergies. Existing and novel services, in particular the pan-European management of Big Data Integration, can be managed by PRACE in partnership. The implementation requires a contractual agreement with a suitable financing model.

4.1 Creating synergy

Almost two years after the proclamation of EuroHPC, almost all PRACE member countries have signed the agreement establishing EuroHPC. On the one hand, this new developments impressively demonstrate the Europe-wide political, economic and scientific interest in the new institution. On the other hand, PRACE's almost ten-year impact on all relevant areas and interest groups of HPC in Europe as well as on a national and international level has created one of the most prominent scientific HPC infrastructures in the world.

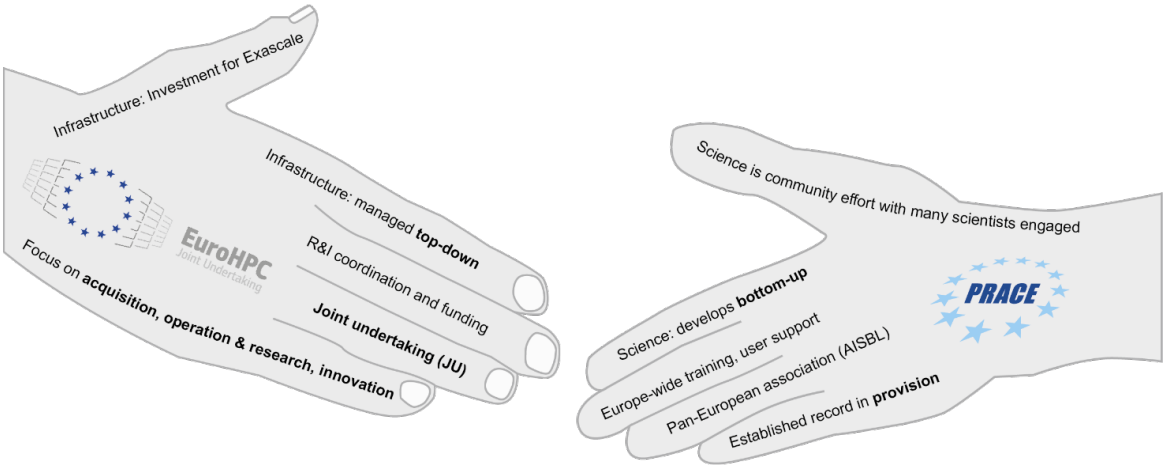

FIGURE 1 - PRACE-EUROHPC PARTNERSHIP

Both successes underline the importance of creating best possible synergies between the EuroHPC Joint Undertaking and the European Research Infrastructure PRACE for the benefit of competitive research in Europe. All this calls for a strong partnership.

Let us take a closer look on the complementarities between EuroHPC and PRACE (FIGURE 1)

4.1.1 EuroHPC

According to the EuroHPC JU regulations, the institution can be characterised as a high-level funding agency of the European Commission and its participating States focusing on HPC/Data/AI related activities. EuroHPC will provide investment in the European ICT exascale infrastructure and will assign funding for exascale research and innovation. It will address issues such as the procurement, acquisition and operation of Tier-0 and Tier-1 supercomputers towards exascale, as well as research and innovation for exascale enabled hardware and software components from processors to the systemic level.

Moreover, the JU EuroHPC will be given responsibility for the adequate funding of key services such as the appropriate allocation and monitoring of computer time, high-level user support and enabling and developing application codes, including new communities, and support for the ecosystem as a whole, in particular in relation to the sustainable funding of training, education, dissemination and technology monitoring.

In addition to these important objectives, EuroHPC will play a crucial role in the political arena and as a policy maker. EuroHPC will act as an interface between the EU and the participating Member States at policy level for the numerical domain; it will provide a platform for the joint development of scientific and technical policies; it will enable joint decisions on general programmes or major projects such as the European Processor Initiative (EPI); and it will coordinate follow-up activities of the various jointly agreed actions.

Acting as a high-level funding agency, EuroHPC in essence needs to be a top-down activity.

4.1.2 PRACE

PRACE is an established, pan-European HPC research infrastructure that has reached the status of an ESFRI landmark in the 2016 ESFRI report.

Following the description as given in the previous sections, PRACE, first of all, has established an internationally recognised peer-review-based access process to Tier-0 and Tier-1 resources for science and industry, that are executed and controlled by the scientific communities; PRACE offers training through its members on a very large-scale; industry is supported through the SHAPE program; operational HPC services have been established that foster the transparent usage of the Tier-0 and Tier-1 systems; special services of universities and user communities have been established; enabling services for HPC applications are provided; HPC procurement and prototyping support is offered; the dissemination and documentation for HPC services has been organized, only to mention most important services. They are key for a functioning HPC ecosystem.

The PRACE Scientific Steering Committee and the Industrial Advisory Committee represent truly active links to scientific and industrial communities. Through these organs, the requirements of the users are respected as demonstrated by the series of scientific cases and in particular the most recent one from 2018.

Being a science driven infrastructure, PRACE was largely developed as a bottom-up activity.

4.2 PRACE services - today and tomorrow

Over the last ten years, PRACE has taken on the responsibility of continuously working on the development of a functioning HPC ecosystem in Europe, largely driven by the PRACE implementation projects. This has transformed PRACE into a *learning research infrastructure*. As a key example, the continuously improved and maintained PRACE Peer Review process is a direct result of these long-standing efforts.

With regard to the mission of EuroHPC, infrastructure services as developed and operated by PRACE are essential for the successful operation of the entire ecosystem. PRACE is fully prepared to act for EuroHPC as the major provider of these high quality services to the European scientific and industrial community.

4.2.1 Services currently provided by PRACE

The running PRACE services have been mentioned in §°2.5. They include:

- The **PRACE Peer Review-based access process to Tier-0 and Tier-1 resources** for science and industry carried out and controlled by the scientific communities and being internationally recognised. The access process is at the heart of achieving scientifically sound and internationally competitive results in numerical simulation and large-scale data analysis. It is considered PRACE's most valuable asset and a major scientific success for both publicly funded and industrial simulation projects.
- The **PRACE training and education offers** as provided through its members on a very large, Europe-wide scale. PRACE Training centres (PTC) in collaboration with CoE activities are oriented toward the convergence of HPC, HPDA and AI.
- **The PRACE user support** as provided through extended High-Level Support Teams (HLST). These teams are essential to help European users communities take advantage of future converged HPC+AI technologies. The HLST are an ideal instrument to cooperate with the planned centres of competence and to co-participate in the calls to be launched. This joint activity will also facilitate the inclusion of development resources.
- The **PRACE enabling services**, that are, on the one hand enabling services for HPC applications, and on the other hand specific pan-European enabling programs/initiatives toward new communities like medicine, social sciences & humanities, or SMEs and industry (like SHAPE and Fortissimo).
- The **PRACE operational HPC services** to foster the transparent usage of the Tier-0 and Tier-1 systems including special services for universities and user communities have been established.

- The **PRACE HPC procurement and prototyping support** is offered including gathering users' needs for the technical specifications of future EuroHPC Exascale technologies. In this context, prototype systems for centres of competence can be hosted and integrated in the Tier-0/1 production system environment.
- The **PRACE dissemination and documentation for HPC services** a key activity to achieve a functioning HPC ecosystem.

4.2.2 Services to be provided in the future

In preparation for the third phase of PRACE (planned to start in 2020) and in order to support EuroHPC in setting up the European Data Infrastructure (EDI), PRACE and GÉANT [30] started to strengthen their interactions as core providers and future infrastructure base of EDI [31]. PRACE and GÉANT are now working on an expansion plan toward new HPC services, data services, services to industry, and network services, as shown in FIGURE 2. It includes:

- The **PRACE HPC/AI services** toward the development of urgent computing, increased support to EU Flagship projects, link with large scale scientific instruments and ESFRIs based on a new elastic Cloud access mode of HPC/data resources - more agile and complementing the static peer review access mode.
- The **PRACE Big Data services** adding a pan-European federated data management and access layer to PRACE, which is based on infrastructure services like ICEI/Fenix (IaaS) and EUDAT and supporting converged HPDA/AI interactive stream/batch data services, end-to-end workflows (from edge to tape) or portal services for OpenData projects.
- The **PRACE extended industry services** integrating current PRACE activities with others led by PRACE partners (Fortissimo) and potentially private partners towards a complete European integrated offer to industry, allowing the provision of a unique and sovereign set of services spanning from HPC/AI evangelisation, Open R&D, confidential R&D to commercial Cloud services.
- The **PRACE/GÉANT resource management** based on the GÉANT basic network services and the future PRACE federation services, striving for one single way to connect and manage

the resources transparently and openly from any point of demand.

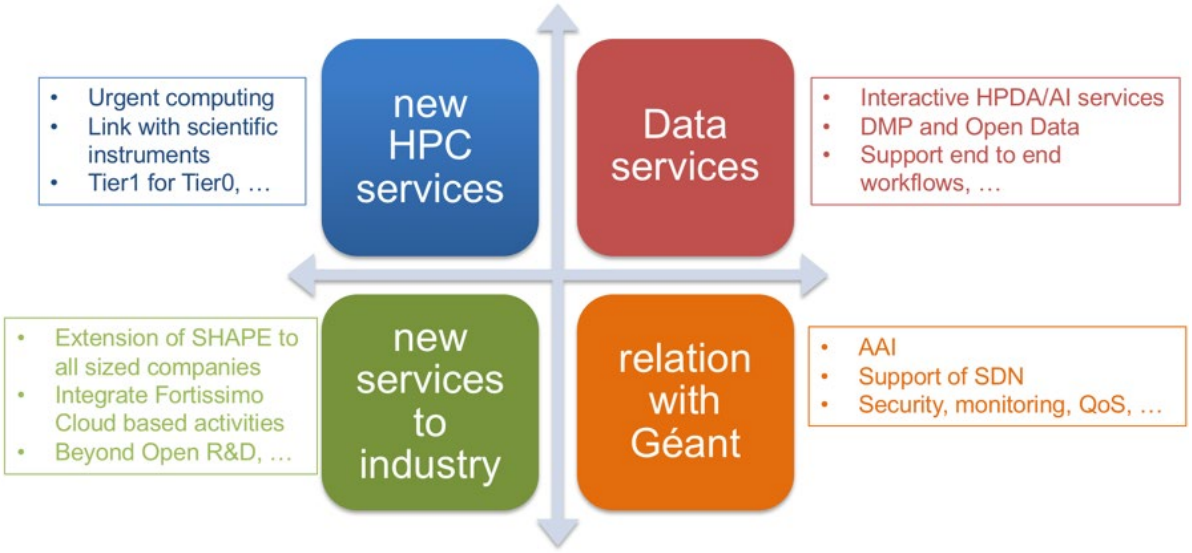

FIGURE 2 - EXPANSION OF PRACE (GÉANT) SERVICES TOWARD EDI

4.3 Realisation of the partnership

PRACE wants to formulate in detail the processes and activities that PRACE can ensure as a partner of EuroHPC. The scope of services currently performed and planned by PRACE must be elaborated and agreed, ideally through a strategic and political cooperation agreement between EuroHPC JU and PRACE. This cooperation agreement should enable EuroHPC to use the existing high quality services for PRACE, benefiting from the experience of all 26 PRACE members involving national and regional HPC centres. In this way, EuroHPC will fully support the European ecosystem from the outset. EuroHPC can then focus on its core mission and be confident that the high quality services that are absolutely essential for the scientific success and socio-economic impact of a pan-European HPC and data research infrastructure are properly delivered.

Depending on the concrete agreement to be negotiated, a reorientation of PRACE can be anticipated. This might affect both the partner categories and the PRACE organisational structure.

Furthermore, appropriate financial models need to be explored, in order to secure sustained operation of the services by PRACE. This concerns the funding for the operation of the PRACE office, the funding of the HLSTs as well as the continuation of the important implementation project culture (PRACE IP projects).

5 Conclusion

Over the last ten years, PRACE and its partners have given national HPC ecosystems a common European umbrella and created an internationally recognised HPC ecosystem as the unique ICT infrastructure on the ESFRI list from 2016. Access to numerical modelling, simulation and data analysis at the highest level has become as strategic for leading international nations as formerly

access to space. In the USA, Japan and China, supercomputing is considered to be strongly correlated with economic success. In Europe, the establishment of the HPC ecosystem plays a significant role in achieving important objectives of the European Union, such as the development of knowledge, science, research and higher education, the development of national and European sovereignty in numerical domains and the development of technical independence from other regions of the world.

With the advent of EuroHPC, the development of the European HPC ecosystem in terms of technical infrastructure will be placed on a sound political and financial footing. In this sense, EuroHPC complements the science-driven, bottom-up development of PRACE with the necessary policy-driven, top-down development.

In the present document, we first set out the services that PRACE offers today and intends to offer tomorrow. Besides these competences, PRACE is specifically advised and actively supported by two bodies, a Scientific Steering Committee and an Industry Advisory Committee. Thanks to these organs, PRACE has become a trusted interface for European HPC users. We have demonstrated the increasing impact of PRACE on the European HPC ecosystem, the necessity to continue pan-European HPC developments in the spirit of the PRACE implementation projects and to continuously enforce the connections to communities, flagships, centres of excellence and competence, and the new data infrastructures.

The great challenge we all face is the federated provision of resources soon to be provided by EuroHPC's pre-exascale and petascale systems as well as by exascale systems in the future, along with the cycles from national Tier-0/1 systems. This requires the development of an appropriate business model that ensures appropriate coordination between EuroHPC hosting members and PRACE Tier-0 and Tier-1 hosting partners, as well as fair and balanced accounting standards.

To sum up, we have outlined the importance and opportunities for building a strong partnership between EuroHPC and PRACE, including key partners from the European ICT landscape. Let us join our creative forces to achieve global leadership in technology, science, industry and societal applications of HPC.

PRACE Member Organisations

Members

Austria	ACONET Association – Austrian Academic Computer Network
Belgium	DGO6-SPW – Direction générale opérationnelle de l'Économie, de l'Emploi et de la Recherche – Service Public de Wallonie
Bulgaria	NCSA – Executive agency "Electronic communication networks and information systems"
Cyprus	CaSToRC – Computation-based Science and Technology Research Center The Cyprus Institute
Czech Republic	IT4I, VŠB – Technical University of Ostrava
Denmark	DeIC – Danish e-Infrastructure Cooperation
Finland	CSC – IT Center for Science Ltd.
France	GENCI – Grand Equipement National de Calcul Intensif
Germany	GCS – GAUSS Centre for Supercomputing e.V
Greece	GRNET – Greek Research and Technology Network S.A.
Hungary	KIFÜ – Kormányzati Informatikai Fejlesztési Ügynökség
Ireland	ICHEC – Irish Centre for High-End Computing
Israel	IUCC – Inter-University Computation Center
Italy	CINECA – Consorzio Interuniversitario
Luxembourg	University of Luxembourg
The Netherlands	SURFsara
Norway	SIGMA – UNINETT Sigma AS – The Norwegian Metacenter for Computational Science
Poland	PSNC – Instytut Chemii Bioorganicznej Pan – Institute of Bioorganic Chemistry Poznan Supercomputing and Networking Center
Portugal	Universidade de Coimbra
Slovakia	Computing Center of the Slovak Academy of Science
Slovenia	ULFME – University of Ljubljana, Faculty of Mechanical Engineering
Spain	BSC – Barcelona Supercomputing Center – Centro Nacional de Supercomputación
Sweden	Vetenskapsrådet – Swedish Research Council
Switzerland	CSCS, ETH – Eidgenössische Technische Hochschule Zürich Swiss Federal Institute of Technology, Zürich
Turkey	UYBHM – Ulusal Yuksek Basarimli Hesaplama Merkezi, Istanbul Technical University National Center for High Performance Computing
UK	EPCC, EPSRC – The Engineering and Physical Sciences Research Council

Observers

Croatia	University of Rijeka (UoR)
Romania	ARCAS – Romanian Association for the Promotion of Advanced Computational Methods in Scientific Research

Glossary

AC	Access Committee of the PRACE SSC
AENEAS	Advanced European Network of E-infrastructures for Astronomy
AI	Artificial Intelligence
aisbl	association internationale sans but lucratif (An association under Belgian law like PRACE)
ALCF	Argonne Leadership Computing Facilities (USA)
ANL	Argonne National Laboratory (USA)
BSC	Barcelona Supercomputing Centre
CCS	Centre for Computational Sciences (RIKEN, Japan)
CERN	Conseil européen pour la recherche nucléaire
CHIPP	Swiss Institute for Particle Physics
CINECA	Consorzio Interuniversitario del Nord est Italiano Per il Calcolo Automatico
CoE	Centre of Excellence
COSMO	Europe limited area weather and climate model
CPU	Central Processing Unit
CSCS	Centro Svizzero di Calcolo Scientifico
DNN	Deep Neural Networks
DOE	Department of Energy (USA)
EPCC	Edinburgh Parallel Computing Centre
ESCAPE	Energy-efficient SCalable Algorithms for weather and climate Prediction at Exascale
ESFRI	European Strategy Forum on Research Infrastructures
ESRF	European Synchrotron Radiation Facility
ETP4HPC	European Technology Platform for HPC
EUDAT	Research Data Services, Expertise & Technology Solutions
EuroHPC	European organization for HPC by EC and participating states
EXDCI	European Extreme Data & Computing Initiative
Exaflop/s	Performance of 10^{18} floating point operations per second
Extreme Earth	A planned European flagship for Climate Science
FAIR Principles	Findable-Accessible-Interoperable-Resusable: guiding principles for scientific data management and stewardship
FENIX	Federated European Network for Information eXchange
FET	Future and Emerging Technologies (EC funded program in H2020)
GÉANT	The pan-European data network for the research and education community
GENCI	Grand Équipement National de Calcul Intensif
Graphene	The European Graphene Flagship
GPU	Graphics Processing Unit
H2020	EU Research and Innovation programme
HBP	The European Human Brain Project, a Flagship
HLRS	Höchstleistungsrechenzentrum Stuttgart
HLST	High Level Support Team
HPC	High Performance Computing
HPDA	High Performance Data Analytics
IaaS	Infrastructure as a Service
IAC	Industrial Advisory Committee of the PRACE Council
ICEI	Interactive Computing E-Infrastructure project

ICT	Information and Communication Technology
INCITE	Funding programme for scientific computing (USA)
IoT	Internet of Things
ITER	International Thermonuclear Experimental Reactor (Fusion)
JSC	Jülich Supercomputing Centre
JU	Joint Untertaking (EuroHPC)
Jupyter Notebook	web application to create and share documents that contain live code, equations, visualizations and narrative text
K Computer	10 petaflops system at the Kobe centre of Riken
LBNL	Lawrence Berkeley National Laboratory (USA)
LHC	Large Hadron Collider (CERN)
LLNL	Lawrence Livermore National Laboratory (USA)
LRZ	Leibnizrechenzentrum
ML	Machine Learning
MOOC	Massively Open Online Course
NERSC	National Energy Research Supercomputing Centre
NCSA	National centre for Supercomputing Applications (USA)
NSF	National Science Foundation
OLCF	Oak Ridge Leadership Computing Facilities (USA)
PATC	PRACE Advanced Training Centre
PCP	Pre-Commercial Procurement
PCT	PRAVE Training Centre
Petaflop/s (PF)	Performance of 10^{15} floating point operations per second
post-K Computer	Future 1000 Petaflop/s system at the Kobe centre of Riken
PPI4HPC	Consortium for the joint Public Procurement of Innovative Solutions for HPC technology
PRACE	Partnership for Advanced Computing in Europe
PRACE Council	Governing board of PRACE
PRACE IP projects	PRACE implementation projects, EU funded
PRACEdays	Scientific conference by the PRACE IP projects
Pre-exascale	Computer performance > 100 Petaflop/s
PSC	PRACE Scientific Case (created by the PRACE SSC)
QT	Quantum Technologies Flagship
Riken	理研 - Large Research Institute in Japan
SHAPE	SME HPC Adoption Programme in Europe
SKA	Square Kilometer Array (Astronomy)
SME	Small and medium enterprise
SSC	Scientific Steering Committee of the PRACE Council
Summit	Current Top-1 leading system at ORNL(USA, Nov. 2018)
TACC	Texas Advanced Computing centre (USA)
Tier-0	European systems with highest performance, European outreach and Europe-wide proposal submission
Tier-1	National systems with highest performance, national outreach and nation-wide proposal submission
Tier-2	Regional systems with highest performance, regional outreach and region-wide proposal submission
Top500 list	The list of the 500 fastest supercomputers worldwide in terms of the Linpack benchmark performance
UEABS	Unified European Application Benchmark Suite
WHPC	Women in HPC

XAI	Explainable AI

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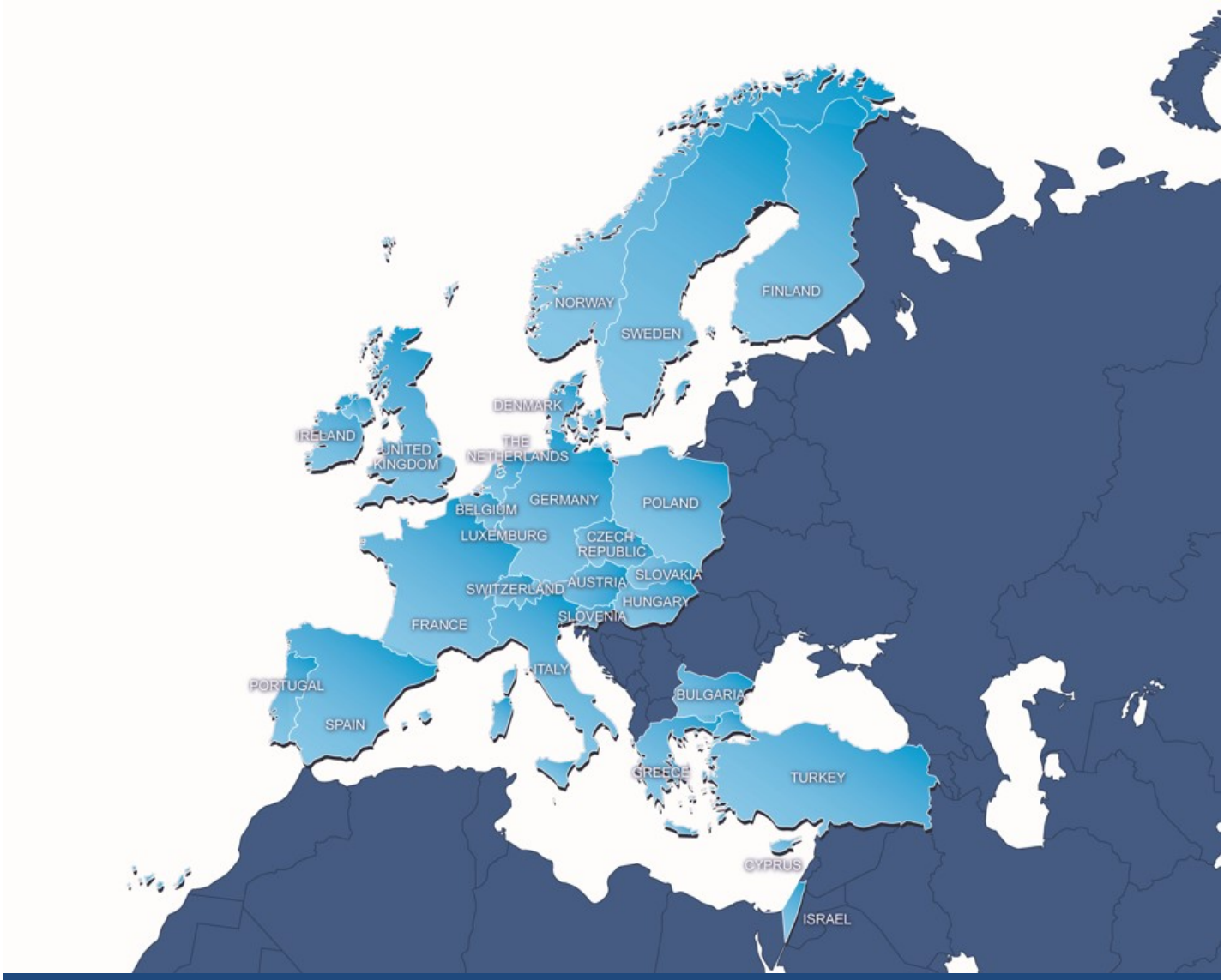
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