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HPC in motion

The 2019 edition of the PRACE Annual Report is a more corporate publication than its predecessors, with a special focus on the people who “make PRACE”. This is in contrast to the PRACE Digest, which provides a platform to highlight the research done on HPC systems and the important and valuable results of those projects.

This change is one of many larger and smaller changes happening in the European HPC ecosystem. By far the biggest among those is the establishment of the EuroHPC Joint Undertaking, which will procure and operate pre-exascale and exascale systems in Europe. In an interview included in this edition, the PRACE Council Chair, Prof. Dr. Dr. Thomas Lippert from FZ Jülich in Germany, provides some insights into what this means for the future of PRACE (pages 8 to 9). If that article makes you curious to know more, please take a look at our position paper “PRACE in the EuroHPC Era”.

HPC is becoming more and more a global theme. While the different regions are all in the race towards exascale and towards the largest and fastest systems, a lot of co-operation and exchange is happening as well. This Annual Report therefore features an interview with John Towns, principal investigator and project director at XSEDE, who explains the direction they are taking with HPC in the USA and beyond. PRACE and XSEDE have already opened joint calls for proposals to allow scientists on both sides of the Atlantic to benefit from access to the European and American systems, and soon Japan (RIKEN) will join this effort and expand the offering even further (pages 34 to 35).

As usual, this Annual Report reserves a space for our Scientific Steering Committee (page 5), our User Forum (page 18), and our Industrial Advisory Committee (page 10), groups that include highly dedicated people who provide invaluable advice to improve our services.

As you will see, we have changed the way we feature the PRACE success stories, giving more space and recognition to the people behind the science, including the High-Level Support Teams who help PRACE-supported projects to excel in what they do.

This Annual Report will be available at PRACEdays19, which will be part of the EuroHPC Summit Week 2019. EHPCSW 2019 will be held from 13 to 17 May 2019 in Poznań, Poland. I am looking forward to meeting you all there!

Last but not least, I would like to thank all of you who have contributed your time, knowledge, effort, and support to PRACE in 2018, and will be happy to be able to count on you again in 2019.

Serge Bogaerts
Managing Director of PRACE aisbl
It has been a busy and productive year for the Scientific Steering Committee (SSC).

A very significant achievement was the launch of the new Scientific Case for Computing in Europe 2018-2026, written by the SSC and which has now been widely disseminated to all stakeholders around Europe and can also be found at [www.prace-ri.eu/third-scientific-case/](http://www.prace-ri.eu/third-scientific-case/). This publication is rather different to previous versions – we purposefully aimed for a more concise document arranged in themes of major societal and scientific relevance, and within those topics we described some of the amazing breakthroughs that have already happened as well as highlighted the challenges and the opportunities that are possible with anticipated next-generation infrastructures. The work was led by the previous SSC Chair, Erik Lindahl, who deserves huge credit for producing a fascinating report of the depth and breadth of European scientific computing.

I believe this Scientific Case comes at a critical moment and should be used to inform new infrastructure developments. In 2018 we saw the launch of the EuroHPC Joint Undertaking – a European Commission initiative to develop and provide world-class supercomputing capability for science and industry. The ever-expanding computing and data needs of scientists in Europe are not currently met by the available European infrastructures and the EuroHPC investment is to be welcomed. At the same time the SSC believes that involving active, distinguished scientists within EuroHPC governance is of paramount importance, to ensure the prioritisation of scientific excellence and industrial impact. PRACE provides the existing structures in which this can happen.

The PRACE Access Committee (AC), under the oversight of the SSC, holds the responsibility for peer review and ranking of all proposals. The review process goes from strength to strength, and while improvements can of course still be made, it is a trusted benchmark of excellence within the scientific community in Europe. This should be valued and preserved – it is not easy to achieve and takes considerable time and effort by the AC.

This report also marks the end of my term as SSC Chair. It’s been a marvellous (and busy!) year and I am very grateful for the privilege of serving as the SSC Chair. I would like to warmly welcome the new SSC Chair, Prof Núria López, and the newly-elected Vice Chair, Prof Matej Praprotnik. Both are excellent scientists and I am confident they will be passionate advocates for science within PRACE and in Europe.
Austria rejoins PRACE

“The PRACE Council is very pleased to welcome Austria as a member of PRACE and is looking forward to a fruitful collaboration. By joining PRACE, Austria gives a strong signal that it supports the scientific and industrial application of HPC at the highest level. The Austrian research community will benefit in many ways by having access to the top of the European HPC ecosystem.”

-Prof. Dr. Dr. Thomas Lippert, Chair of the PRACE Council.

After a brief intermission, Austria is now back as a member of PRACE, officially joining in July 2018. This is a significant step as it gives the Austrian HPC community access to Europe’s most powerful supercomputers as well as excellent training opportunities for the next generation of computational scientists.

The renewed PRACE membership of Austria was made possible by a consortium of Austrian Universities who have joined forces under the auspices of the Austrian Ministry of Education, Science and Research. The consortium consists of all major research institutions across Austria, including the Universities of Vienna, Graz, Linz and Innsbruck, the Technical Universities of Vienna and Graz, the Medical Universities of Vienna and Graz, the University of Veterinary Medicine Vienna, the University of Natural Resources and Life Sciences, the Institute of Science and Technology Austria as well as the Vienna Scientific Cluster. These Austrian organisations are represented in the PRACE Council by AConet, the Austrian national network for research, education and culture. Operated by the Vienna University Computer Center in cooperation with other Austrian universities, AConet provides a nation wide fibre-optic backbone with high-performance access to international academic networks as well as to the internet. Prof. Christoph Dellago, a physicist from the University of Vienna, and Prof. Alexander Ostermann, a mathematician from the University of Innsbruck, serve as the Austrian delegate and advisor in the PRACE Council, respectively.

Austria has a very active community in all areas of computational science ranging from the natural sciences to engineering and, increasingly, the social sciences and humanities. Over the past decades, these fields have grown rapidly and many new research groups have been established at Austrian research institutions, supported by national and European science funding agencies. Today, the Austrian HPC community includes over 1000 researchers engaging both in applications as well as algorithm and code development. For instance, VASP and Wien2k, two very successful codes for the ab initio simulation of materials, are developed in Austria and used on numerous computers world-wide. The Austrian HPC community meets

Ice-water interface in atomic resolution obtained from computer simulations based on a high-dimensional neural network potential trained with ab initio data. The water molecules are coloured by the strength (from blue to red) of the van der Waals (vdW) interactions, which play an important role in determining the unique properties of water and ice. (Image courtesy of T. Morawietz, A. Singraber and C. Dellago, University of Vienna)
regularly at its annual meeting, organised for the fifth time in 2019, which provides the opportunity to discuss the latest developments in HPC and plan joint activities (such as the PRACE membership).

The major computing resources available today to researchers in Austria are MACH-2 and the Vienna Scientific Cluster (VSC), two computing infrastructures with complementary architectures and both established with support from the Austrian Federal Ministry of Education, Science and Research. MACH-2 is a massively parallel shared memory supercomputer with 1,728 cores and 20 TB of global shared memory operated by the University of Linz in collaboration with the Universities of Innsbruck and Salzburg as well as TU Wien. The Vienna Scientific Cluster (VSC), founded in 2009 in an initiative of three universities in Vienna and since then joined by essentially all major Austrian research institutions, operates throughput-oriented general-purpose Linux clusters. The computing infrastructure of VSC is continuously renewed and VSC-4, the new flagship of the VSC family with about 38,000 compute cores, will start operation in the spring of 2019. VSC also runs an education programme with seminar-like lectures as well as traditional training courses with hands-on sessions, designed to train students and researchers in state-of-the-art computational methodology and help them to make the most efficient use of the available computing equipment. Since its start in 2009, VSC has evolved into a crucial infrastructure of the Austrian science scene and is now the main workhorse for most computationally oriented researchers in Austria.

“Austria has an active community in all areas of computational science ranging from the natural sciences to engineering and, increasingly, the social sciences and humanities”

Through PRACE, the Austrian research community now has access to top of the line supercomputers, offering the opportunity for further growth and a strong integration into the European high performance computing landscape.
INTERVIEW

Q&A: Thomas Lippert

Thomas Lippert is the head of the Jülich Supercomputing Centre and Chair of the PRACE Council. Here we talk to him about the recently published Scientific Case for Computing in Europe, the newly formed EuroHPC joint undertaking, and other challenges that PRACE will face in the coming years.

PRACE published “The Scientific Case for Computing in Europe 2018-2026” in October 2018. Can you tell us about what it says about computing and how this will shape the way that PRACE approaches the next eight years?

Thomas Lippert: “The Scientific Case for Computing in Europe 2018-2026” was published at the end of 2018 and outlined a number of perspectives about the future of computing in Europe. This includes an overview of what will be needed from procurers and the operational institutions of supercomputers to provide the infrastructure necessary to support Europe’s computing needs, as well as an overview of how high performance computing is used and how it might be used in the future.

One of the main ideas of this publication was to emphasise the diversity of fields that use high performance computers for science and industry. It has been around two decades since supercomputing became one of the essential elements in science and industry. You cannot really do modern research without the help of the most advanced high performance computers. For instance, many of the artificial intelligence codes and programmes that are being created run on supercomputers. The neural networks used by these codes are changing now that they are being run on supercomputers, with many researchers using ensembles of networks so that they can choose, modify and optimise them for their tasks.
The scientific case publication highlights the fact that scientists working on fundamental research are now unable to do their work without the simulations and testing that high performance computers provide. They also need to be able to evaluate their simulations and deal with the large amounts of data that they produce. High performance computing therefore acts as an important bridge between experimental and theoretical work.

Much of the modern technology that we use is reliant on high performance computing. Data-driven models are crucial for providing the streamlined prototyping process that we now take for granted in industry. These are just some examples of how high performance computing supports our society in the modern world.

“It has been around two decades since supercomputing became one of the essential elements in science and industry. You cannot really do modern research without the help of the most advanced high performance computers”

The EuroHPC Joint Undertaking is a new initiative to create a coordinated effort at a European level to deploy and develop high performance computing. How do you see that coming together in the next few years and what will PRACE’s role be within that?

TL: EuroHPC will permit the EC and participating countries to coordinate their efforts and share resources with the objective of deploying a world-class supercomputing infrastructure and a competitive innovation ecosystem in supercomputing technologies, applications and skills in Europe. This represents the recognition of high performance computing and the use of data as important activities at European level and not just at national level. Of course, the European Commission has always supported high performance computing, but this has been based on machines that are supervised at national level. They have now decided that there should, at the very highest level, be a European component to these activities, including the purchase of supercomputers which will be owned by Europe. The EuroHPC Joint Undertaking will act as a funding organisation which can make this idea of European supercomputing a reality, both in terms of the operation and purchase of new machines and the development of new technology.

In comparison, PRACE is an organisation that works with Member States at the national level to act at the European level. It is bottom-up in that it is science-driven, compared to EuroHPC which is more top-down and driven by larger organisations which will control this kind of technology at the highest level. PRACE has, over the years, developed into a powerful organisation, controlling how high performance computing is brought to users, how these users are supported, and implementing a stringent peer review process that ensures that there is healthy competition for computing time within academia and industry for the use of the machines it governs.

From my perspective, I think it is clear that EuroHPC can profit from PRACE, and PRACE can profit from EuroHPC. Our aim is to bring both sides together to help continue and support the high performance computing community at the pan-European level. I think we can have a situation where the checks and balances of each side are perfectly fulfilled and the competences are matched to create a fruitful working relationship.

As Chair of the PRACE Council, what do you think are the main challenges that the organisation will face in the future?

TL: Computing in science is dynamic and is constantly changing in order to meet the new challenges that are presented. Methodologies are one such instance of this. We have seen artificial intelligence become essential to many parts of science over the last few years, contributing to improvements in simulations in a diverse field of applications. Data analytics is also extremely important in a similar way.

With this in mind, I think we have to ensure that we do not become static; we have to follow along with this dynamic progress. I believe that PRACE has both the means and the right people in place to give it a future as a dynamic organisation to match this. We need to use HPC in traditional fields and use traditional methods, but also make sure that we are ready to embrace the new fields and methods that emerge.
Chairing the Industrial Advisory Committee (IAC) has been one of the highlights of my professional career. In particular, I have enjoyed the challenge of dealing with the often conflicting and contradictory views of the PRACE partners. The position also has its lows. I recently overhead a comment that “... the PRACE IAC has just been a showcase for tactical and political reasons”. This is upsetting. The IAC is a voluntary body that has a genuine desire to help improve the industrial uptake of HPC in Europe. The past year has been particularly busy for PRACE and for the IAC. For clarity, I will summarise the views and recommendations of the IAC using the 4P framework.

**Product**
PRACE offers industry access to services including consultancy (SHAPE), training, preparatory access and open calls. Uptake continues to be low. Historically, applications to use PRACE Tier-0 resources have been judged on scientific excellence. This means it is difficult for the designer of a widget to compete with an application to investigate colliding black holes. An industry pilot has been introduced for Call 19 (to open in March 2019) which will reserve 10% of the resources for industry. Furthermore, industry proposals will be ranked against each other rather than against academic projects. This is a potential game changer.

**Price**
PRACE does not offer pay-for-use access to its systems or charge a fee to attend its training courses. Industry access is free for open scientific investigation. The philosophy of open science removes many of the barriers that could make it difficult for PRACE to grant industry access. It is not the role of PRACE to provide industry with production capability; a principle supported by the IAC. PRACE’s role is to help firms discover the benefits of HPC, then encourage them to graduate to commercial services, offered by start-up companies who are growing Europe’s digital market place.

**Place**
PRACE is an organisation whose focus is Tier-0 computing. There are some in the community who argue that industry is not well equipped to use such systems. The IAC would counter that each service offered by PRACE should be open to industry, regardless. Just like academia, there will be more industrial users at Tier-1 and even more at Tier-2. In order to assist firms in making the transition from one tier to the next, there needs to be a good relationship between PRACE and national HPC centres. In 2019 the IAC will be exploring how this collaboration could be improved.

**Promotion**
PRACE produces beautiful promotional materials, has an established brand, a web presence and is active on social media. Nonetheless, its message is not getting through to industry. Instead of more tweeting, PRACE needs more tweeters. The IAC has recommended that PRACE identifies and builds relationships with “digitisation” evangelists in industry trade associations and other networks such as the European Technology Platforms (for manufacturing, aerospace, fisheries, textiles, water and so on). Evangelists can promote the benefits of HPC to millions of firms for free.

In conclusion, a year of recommendations from the IAC has inevitably led to additional effort. In response, PRACE expects to appoint a new Industrial Liaison Officer in May 2019. Our advice to that individual is to be a leader and a catalyst for change. Focus on building a network of real human beings that you can talk to on the phone or visit. They will gladly carry the PRACE message into their communities on your behalf and provide insight regarding what industry really needs. Try not to rely on visitors to a website or the blunt instrument of social media.
High Performance Computing (HPC) is an essential tool for companies in different industrial domains, including agriculture, healthcare, energy, finance, to list just a few. In order to bring HPC to industrial users and increase awareness of the merit of simulations, PRACE, the Partnership for Advanced Computing in Europe, provides dedicated access to world-class HPC resources and services. All European companies can apply for PRACE Project Access. Those that need technical support, e.g. for scaling their codes, can apply for Preparatory Access first. For Small and medium-sized enterprises (SMEs) that are looking to integrate HPC into their business model, PRACE has developed the dedicated SME HPC Adoption Programme in Europe, SHAPE.
PRACE key performance indicators

Given the evolution of computational power in the PRACE portfolio, PRACE-related statistics are becoming increasingly important to highlight the impact of PRACE on HPC-based research, HPC know-how in Europe and European industry engagement in HPC.

PRACE’s impact on evolving research

Offer and demand of resources

Figure 1 shows the evolution of PRACE resources offered and requested in Project Access Calls. PRACE first provided HPC services in 2010 with contributions from German Tier-0 systems. France, Italy and Spain added their contributions gradually. This is reflected in the constant increase of HPC resources offered by PRACE to the scientific community until the 6th call, where a stable regime was reached. The phasing out of the initial phase of PRACE (known as PRACE 1) started in the 10th call, while the second phase of PRACE (known as PRACE 2) only started in Call 14. This is reflected in the valley from the 10th call to the 13th call. With PRACE 2, a substantial increase in the amount of available resources can be seen, thanks to the renewed contributions of all the original PRACE hosting members and Switzerland as new hosting member. The stable regime has been reached quickly, and since the 14th call an average of 1.9 billion core hours has been offered to the HPC scientific community.

The demand for HPC resources has always exceeded the capacity of PRACE to provide them. The average oversubscription of PRACE calls is 3:1, reaching a 5:1 ratio during the phasing out of PRACE 1. This constant interest in PRACE resources has been driving the periodic upgrades and additions of new systems that PRACE offers, specifically concerning the PRACE 2 programme.
During the initial phase of PRACE (known as PRACE 1), the number of project applications received via PRACE Calls for Proposals for Project Access exhibited a clear overall upward trend. The phasing-in of PRACE 1 naturally incited an increase in demand for Tier-0 resources. This is particularly evident up to the 8th Call, with a large sustained increase between the 6th and 8th Call, followed by a slight decrease (Figure 2).

A downward trend of rejected projects below the scientific excellence threshold is noted, displaying maturity of submitted proposals, in which researchers put more effort into the quality of their proposals, as a reaction to increased competition. Moreover, the evolution reflects the positive outcomes of PRACE Preparatory Access Calls (including access type C) that enable prior technical support for application and scalability tests. Figure 2 also highlights an increase in rejected projects above the scientific threshold, particularly after the 6th Call. This is correlated with the increase in total applications.

During the phasing-out of PRACE 1, the number of available core hours dropped (Figure 1), and this decreased the demand, as researchers anticipated an even stronger competition for the remaining resources. This trend was mitigated in the 12th and 13th Call, when PRACE hosting members made additional core hours available during the preparation of the PRACE 2 programme, which started in the 14th Call.

With the start of PRACE 2, there has been an increase in the number of projects awarded, which combined with the increase of resources that started in the 14th call (Figure 1) shows the clear success of the second phase of PRACE. In this second phase, the scientific objectives of PRACE have been updated towards an increase of the scope and excellence of the projects awarded. The minimum size of allocations has been increased three-fold, and the scientific threshold as well. The decrease in proposals submitted and the apparent decrease in their quality in Call 15th is a positive sign of the success of this scientific update.

Despite the competition, demand for PRACE resources remains high and all PRACE calls are oversubscribed (Figure 1), indicating that scientists consider Tier-0 access an essential asset to their work. This was also underlined by the PRACE Scientific Steering Committee (SSC) during the preparation of PRACE 2 (see page 5 for the article by the Chair of the SSC).
### Recurring users

PRACE also keeps track of the submission of Project Access proposals by recurrent principal investigators (PIs) (Figure 3). This KPI is created by checking for each call if a PI is new to PRACE.

The ratio of first-time applicants is relatively high - roughly 50% of PIs who submitted to the two Project Access Calls in 2018 were recurrent applicants to a PRACE Call for Proposals for Project Access. This means that half of project proposals are submitted by new users. This indicates that PRACE is continuously attracting new PIs, while remaining an essential support for existing users. The upward trend of the ratio of recurrence is visible, particularly from the 6th Call onwards, influenced by the downward trend on awarded projects, but recovered with the onset of PRACE 2.

![Figure 3 – Ratio of new applicants and new awardees in each PRACE call](image)

### International and transnational cooperation

Two-thirds (63%) of resources awarded under the Early Access Call through to the 15th Call are awarded to “foreign projects”. Foreign projects are defined as projects with Principal Investigators (PIs) from a different country (recorded as the country of the PI’s primary institution) than the machine on which the research is executed. The ratio of awarded foreign projects remains rather stable over time (Figure 4). This shows that the nationality of the PI’s institution does not influence the chances of a project being awarded.

It also demonstrates PRACE’s impact in the enhancement of European and international collaboration.
**Co-funding**

PRACE awards are normally developed within larger scientific initiatives, where HPC resources are part of the needs of the project. PRACE asks Project Access awardees to declare such synergies.

On average, 75% of PRACE users have declared that their awards are complemented with EC, national or international funds (Figure 5).

The major fraction corresponds to national projects, which is slowly showing a downward trend since the 10th Call. EC funding shows an increasing trend, coinciding with the implementation of the H2020 programme. International funding remains low, with 8% being the average contribution.
PRACE’s impact on growing know-how in Europe

Since 2008, PRACE has been engaged in providing top-class education and training for computational scientists in Europe through the PRACE Training Centres (PTCs), the International HPC Summer School, and PRACE Seasonal Schools, with a clear increase of participants registered (Figure 6).

Six PTCs were first established, and these are the Barcelona Supercomputing Centre (Spain), CINECA – Consortio Interuniversitario (Italy), CSC – IT Center for Science Ltd. (Finland), EPCC at the University of Edinburgh (UK), Gauss Centre for Supercomputing (Germany) and Maison de la Simulation (France).

After the rapid increase between 2010 and 2012, a plateau is evident since 2012. As this indicated that the maximum capacity of PRACE training offerings had been reached, four new PRACE Training Centres were opened in 2017 – in IT4Innovations (the Czech Republic), GRNET (Greece), ICHEC (Ireland) and SURFSara (The Netherlands). This acts a second layer of training and education, below the previous PTCs.

PTC training events, seasonal schools and the International HPC Summer School are offered free of charge to eligible participants.

Between August 2008 and December 2018, PRACE provided 42,699 participant-days of training through attendance-based courses, with an upward attendance trend. PRACE courses were attended by over 13,800 individuals. This shows the effectiveness of PRACE in attracting, training and retaining competences.

In 2018 the number of participants attending PTCs courses was 2361 (492 with non-academia affiliation). 80% of participants attending PTC trainings days have academic affiliation, illustrating the impact of such events on research and scientific communities, in particular for early stage researchers and PhD students.

A clear difference of attendance is observed between the first and second semester of 2018. As observed in Figure 7, the total number of attendees registered in the first semester (Q1 and Q2) is significantly higher than during the second semester (Q3 and Q4). This indicates that the bulk of the training offered occurs in the first semester, with a notable drop in attendance during Q3 which corresponds with the summer and winter vacation periods.
PRACE’s impact on attracting the industrial sector

Non-academic use of PRACE HPC resources

PRACE opened its Calls for Proposals to non-academic applications in mid-2012. This can take the form of a project led by a principal investigator coming from a private company, or a researcher from industry collaborating in an academia-led project. The reduction and stabilisation of projects awarded after the 7th Call has had a strong impact on the number of projects awarded with industrial participants (Figure 8). In other words, industry suffers more from the competition for PRACE resources than academia. We expect this trend will start to change with the PRACE 2 programme.

Regarding the SHAPE programme, started in 2013, it has received 61 applications so far, of which a total of 45 have been awarded both PRACE HPC resources and, more importantly, support in the PRACE centres.
The PRACE User Forum

Dr Troels Haugbølle, Chair of the PRACE User Forum

The PRACE User Forum represents the users of PRACE computational resources and provides a communication channel for the users to the PRACE research infrastructure and the computational centres. Our concerns are generic issues, such as problems in the review process or during the allocation of resources, and the provision by PRACE for new use cases that are currently not catered for. We also give voice to the users of high performance computing in the debate about the development of HPC in Europe, which has become ever more important with the transition to exascale and the advent of EuroHPC.

PRACEdays18

In 2018 the User Forum held its sixth Open Session in Ljubljana during PRACEdays18 as part of the European HPC Summit Week. The User Forum is supporting an increasing participation of PRACE users to make PRACEdays the premier venue for presenting HPC applications in Europe, and in particular for disseminating research carried out with PRACE resources. We strongly encourage researchers to contribute to upcoming editions of PRACEdays, giving them the chance to interact with peers from different disciplines. Attendance by the users of PRACE is also important for showcasing the many excellent results of research to the policymakers who attend the event.

Peer review process

Maybe the most important topic discussed by the User Forum over the years has been the peer review process. PRACE has an eminently balanced, transparent and objective peer review process as a result of integrating suggestions from the computing centres and access committees, as well as from listening to its users. As in past editions, the peer review process was explained by the PRACE peer review officers during the User Forum Open Session, and this year we had a special focus on the new enlarged application guidelines that were implemented as part of the 18th Call for Project Access in the autumn. It will be interesting to follow the impact of the new application guidelines during the coming calls.

The future of HPC usage in Europe

In 2018, the European Union launched its pre-exascale initiative, EuroHPC. Among the main users of EuroHPC will be the current Tier-0 PRACE users, which include some of the best European scientists and groups who have applications that can run efficiently on exascale machines. We hope EuroHPC will embrace new areas across industry, science, and with a direct impact for society, but also support the traditional users from the natural sciences and engineering communities.

In the User Forum we believe that PRACE users have a special responsibility to make decision makers aware how important it is that computational resources are available to the most qualified users across science and industry, and that the tradition that PRACE has heralded – scientific excellence as a criterion for access to top-level resources – has to be continued with EuroHPC.

We are also aware of the formidable technical challenge presented by using even pre-exascale systems with 100 million-level parallelism. Therefore, it is important to develop not only hardware, and middleware, but also support new approaches to end-user applications.

Europe has a long tradition for international leadership in HPC applications. To maintain this, it is critical that the programs transferred from the EU to EuroHPC, such as FET-HPC, also support the development of scalable parallel applications. This should be done through radical new modelling paradigms and the optimisation and modernisation of existing applications. This will stimulate the creation of a diverse ecosystem of exascale ready applications and is a critical requisite for having a large enough user base for the future pre-exascale installations envisioned with EuroHPC.
This article lists the members of each body of PRACE aisbl. Our thanks goes out to all those who have supported our organisation during 2018. More information on the bodies of PRACE aisbl can be found here: [www.prace-ri.eu/organisation/](http://www.prace-ri.eu/organisation/)

### PRACE Member Organisations and delegates to the PRACE Council

The Council is the deliberative body of PRACE aisbl and decides on all matters of the association. It is composed of one representative from each member. The Board of the council is elected by the Council from among the delegates representing the Members.

#### Board of the PRACE Council

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<th>Name</th>
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<th>Organisation/Association</th>
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<td>Thomas Lippert</td>
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<td>Forschungszentrum Jülich</td>
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<td>Janne Ignatius</td>
<td>Council Vice-Chair</td>
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<td>Florian Berberich</td>
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<td>Serge Bogaerts</td>
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#### Observers

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#### Delegates

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<td>Philippe Geuzaine</td>
<td>Delegate</td>
<td>Direction générale opérationnelle de l’Économie, de l’Emploi et de la Recherche – Service Public de Wallonie (DGO6-SPW)</td>
<td>Belgium</td>
</tr>
<tr>
<td>Ivan Dimov</td>
<td>Delegate</td>
<td>Executive Agency “Electronic Communication Networks and Information Systems”</td>
<td>Bulgaria</td>
</tr>
<tr>
<td>Name</td>
<td>Role</td>
<td>Institution</td>
<td>Country</td>
</tr>
<tr>
<td>-----------------------</td>
<td>-----------</td>
<td>------------------------------------------------------------------------------</td>
<td>---------------</td>
</tr>
<tr>
<td>Constantia Alexandrou</td>
<td>Delegate</td>
<td>The Cyprus Institute</td>
<td>Cyprus</td>
</tr>
<tr>
<td>Vit Vondrak</td>
<td>Delegate</td>
<td>VŠB-Technical University of Ostrava</td>
<td>Czech Republic</td>
</tr>
<tr>
<td>René Belso</td>
<td>Delegate</td>
<td>Danish e-Infrastructure Cooperation (DelC)</td>
<td>Denmark</td>
</tr>
<tr>
<td>Philippe Lavocat</td>
<td>Delegate</td>
<td>Grand Equipement National De Calcul Intensif (GENCI)</td>
<td>France</td>
</tr>
<tr>
<td>Dieter Kranzlmueller</td>
<td>Delegate</td>
<td>GAUSS Centre for Supercomputing (GCS) e.V.</td>
<td>Germany</td>
</tr>
<tr>
<td>Ognjen Prnjat</td>
<td>Delegate</td>
<td>Greek Research And Technology Network Sa (GRNET)</td>
<td>Greece</td>
</tr>
<tr>
<td>Tamas Maray</td>
<td>Delegate</td>
<td>KIFÜ Governmental Information Technology Development Agency</td>
<td>Hungary</td>
</tr>
<tr>
<td>Jean-Christophe Desplat</td>
<td>Delegate</td>
<td>National University of Ireland - Irish Centre for High-End Computing (ICHEC)</td>
<td>Ireland</td>
</tr>
<tr>
<td>Haim Taitelbaum</td>
<td>Delegate</td>
<td>Inter University Computation Center - IUCC</td>
<td>Israel</td>
</tr>
<tr>
<td>Gabriella Scipione</td>
<td>Delegate</td>
<td>CINECA Consorzio Interuniversitario</td>
<td>Italy</td>
</tr>
<tr>
<td>Pascal Bouvry</td>
<td>Delegate</td>
<td>Université du Luxembourg</td>
<td>Luxembourg</td>
</tr>
<tr>
<td>Peter Michielse</td>
<td>Delegate</td>
<td>SURFsara</td>
<td>The Netherlands</td>
</tr>
<tr>
<td>Gunnar Bøe</td>
<td>Delegate</td>
<td>UNINETT Sigma2 AS</td>
<td>Norway</td>
</tr>
<tr>
<td>Norbert Meyer</td>
<td>Delegate</td>
<td>Instytut Chemii Bioorganiczej Pan - Institute of Bioorganic Chemistry</td>
<td>Poland</td>
</tr>
<tr>
<td>Pedro Alberto</td>
<td>Delegate</td>
<td>University of Coimbra</td>
<td>Portugal</td>
</tr>
<tr>
<td>Jozef Noga</td>
<td>Delegate</td>
<td>Computing Centre of the Slovak Academy of Sciences</td>
<td>Slovakia</td>
</tr>
<tr>
<td>Janez Povh</td>
<td>Delegate</td>
<td>ARNES</td>
<td>Slovenia</td>
</tr>
<tr>
<td>Sergi Girona</td>
<td>Delegate</td>
<td>Barcelona Supercomputing Center (BSC) - Centro Nacional de Supercomputacion (CNS)</td>
<td>Spain</td>
</tr>
<tr>
<td>Hanifeh Khayyeri</td>
<td>Delegate</td>
<td>Swedish Research Council</td>
<td>Sweden</td>
</tr>
<tr>
<td>Thomas Schulthess</td>
<td>Delegate</td>
<td>ETH Zurich/CSCS</td>
<td>Switzerland</td>
</tr>
<tr>
<td>Ertugrul Karacuha</td>
<td>Delegate</td>
<td>National Center for High Performance Computing of Turkey - Ulusal Yüksef Başarımlı Hesaplama Merkezi (UYBHM)</td>
<td>Turkey</td>
</tr>
<tr>
<td>Susan Morrell</td>
<td>Delegate</td>
<td>The Engineering and Physical Sciences Research Council (EPSRC)</td>
<td>United Kingdom</td>
</tr>
</tbody>
</table>
### PRACE Strategy Working Group (SWG)

The Strategy Working Group (SWG) is a sub-committee of the PRACE Council. It counts 14 seats, including one for each hosting member, and three for representatives of the general partners.

<table>
<thead>
<tr>
<th>Name</th>
<th>Role</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thomas Lippert</td>
<td>PRACE Council Chair</td>
</tr>
<tr>
<td>Janne Ignatius</td>
<td>PRACE Council Vice-Chair</td>
</tr>
<tr>
<td>Florian Berberich</td>
<td>PRACE Council Secretary</td>
</tr>
<tr>
<td>Gabriella Scipione</td>
<td>Delegate of Italy</td>
</tr>
<tr>
<td>Dieter Kranzlmueller</td>
<td>Delegate of Germany</td>
</tr>
<tr>
<td>Philippe Lavocat</td>
<td>Delegate of France</td>
</tr>
<tr>
<td>Sergi Girona</td>
<td>Delegate of Spain</td>
</tr>
<tr>
<td>Thomas Schulthess</td>
<td>Delegate of Switzerland</td>
</tr>
<tr>
<td>Susan Morrell</td>
<td>Delegate of United Kingdom</td>
</tr>
<tr>
<td>Peter Michielse</td>
<td>Delegate of the Netherlands</td>
</tr>
<tr>
<td>Rene Belsø</td>
<td>Delegate of Denmark</td>
</tr>
<tr>
<td>Serge Bogaerts</td>
<td>Managing Director</td>
</tr>
<tr>
<td>Sinéad Ryan</td>
<td>Chair of the Scientific Steering Committee (SSC)</td>
</tr>
<tr>
<td>Lee Margetts</td>
<td>Chair of Industrial Advisory Committee (IAC)</td>
</tr>
</tbody>
</table>

### PRACE Board of Directors (BoD)

The Board of Directors (BoD) is the executive body of the association and is generally responsible for managing and representing the association.

<table>
<thead>
<tr>
<th>Name</th>
<th>Role</th>
</tr>
</thead>
<tbody>
<tr>
<td>Florian Berberich</td>
<td>Member for Germany</td>
</tr>
<tr>
<td>Serge Bogaerts</td>
<td>Chair and Managing Director</td>
</tr>
<tr>
<td>Maria Grazia Giuffreda</td>
<td>Member for Switzerland</td>
</tr>
<tr>
<td>Oriol Pineda</td>
<td>Member for Spain</td>
</tr>
<tr>
<td>Stéphane Requena</td>
<td>Member for France</td>
</tr>
<tr>
<td>Sinéad Ryan</td>
<td>Member as Chair of the Scientific Steering Committee (SSC)</td>
</tr>
<tr>
<td>Debora Testi</td>
<td>Member for Italy</td>
</tr>
</tbody>
</table>
### Scientific Steering Committee (SSC)
The Scientific Steering Committee (SSC) is composed of leading researchers from Europe. They provide advice and guidance on all matters of a scientific and technical nature that may influence the scientific work carried out using the association’s resources.

<table>
<thead>
<tr>
<th>Name</th>
<th>Field/Research Area</th>
<th>Country</th>
</tr>
</thead>
<tbody>
<tr>
<td>Marina Bécoulet</td>
<td>Plasma physics, fusion</td>
<td>France</td>
</tr>
<tr>
<td>Luke Drury</td>
<td>Universe sciences</td>
<td>Ireland</td>
</tr>
<tr>
<td>Claudia Filippi</td>
<td>Electronic structure, multiscale modelling</td>
<td>The Netherlands</td>
</tr>
<tr>
<td>Frauke Gräter</td>
<td>Biophysics</td>
<td>Germany</td>
</tr>
<tr>
<td>Laura Grigori</td>
<td>Numerical mathematics, HPC</td>
<td>France</td>
</tr>
<tr>
<td>Heiner Igel</td>
<td>Seismology</td>
<td>Germany</td>
</tr>
<tr>
<td>Dimitri Komatitsch</td>
<td>Computational Earth sciences</td>
<td>France</td>
</tr>
<tr>
<td>Petros Koumoutsakos</td>
<td>Computational science</td>
<td>Switzerland</td>
</tr>
<tr>
<td>Erik Lindahl</td>
<td>Life sciences</td>
<td>Sweden</td>
</tr>
<tr>
<td>Núria López</td>
<td>Computational chemistry</td>
<td>Spain</td>
</tr>
<tr>
<td>Aimee Morgans</td>
<td>Mechanical engineering</td>
<td>United Kingdom</td>
</tr>
<tr>
<td>Ignacio Pagonabarra</td>
<td>Computational physics</td>
<td>Spain</td>
</tr>
<tr>
<td>Mike Payne</td>
<td>Computational Physics</td>
<td>United Kingdom</td>
</tr>
<tr>
<td>Matej Praprotnik</td>
<td>Chemistry, multiscale modelling</td>
<td>Slovenia</td>
</tr>
<tr>
<td>Sinéad Ryan</td>
<td>Particle physics, mathematics</td>
<td>Ireland</td>
</tr>
<tr>
<td>Per Stenström</td>
<td>Computer science, HPC</td>
<td>Sweden</td>
</tr>
<tr>
<td>Julia Yeomans</td>
<td>Physics: Soft and biological matter</td>
<td>United Kingdom</td>
</tr>
</tbody>
</table>

### Financial Oversight & Risk Assessment Committee (FORAC)
FORAC provides a high-level and visible forum for monitoring standards of internal control and propriety, economy, effectiveness. It also evaluates the extent to which systems and procedures help PRACE objectives to be met.

<table>
<thead>
<tr>
<th>Name</th>
<th>Role</th>
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<tbody>
<tr>
<td>Mark Parsons</td>
<td>Chair</td>
<td>United Kingdom</td>
</tr>
<tr>
<td>Edouard Brunel</td>
<td></td>
<td>France</td>
</tr>
<tr>
<td>Claus-Axel Müller</td>
<td></td>
<td>Germany</td>
</tr>
</tbody>
</table>
## Industrial Advisory Committee (IAC)

The Industrial Advisory Committee (IAC) is composed of European industry representatives (both from multinationals and SMEs) representing 11 industrial sectors.

<table>
<thead>
<tr>
<th>Name</th>
<th>Sector</th>
<th>Country</th>
</tr>
</thead>
<tbody>
<tr>
<td>Enric Gibert</td>
<td>Life sciences, pharmaceuticals</td>
<td>Spain</td>
</tr>
<tr>
<td>Tomi Ilijaš</td>
<td>Engineering, manufacturing, SMEs</td>
<td>Slovenia</td>
</tr>
<tr>
<td>Dieter Jahn</td>
<td>Materials, chemistry</td>
<td>Germany</td>
</tr>
<tr>
<td>Lee Margetts</td>
<td>ISV</td>
<td>United Kingdom</td>
</tr>
<tr>
<td>Alain Martin</td>
<td>Energy</td>
<td>France</td>
</tr>
<tr>
<td>Marc Morere</td>
<td>Aeronautics, aerospace</td>
<td>France</td>
</tr>
<tr>
<td>Martin Winter</td>
<td>Materials, chemistry</td>
<td>Germany</td>
</tr>
</tbody>
</table>

### Observers (with no voting rights)

<table>
<thead>
<tr>
<th>Name</th>
<th>Role</th>
<th>Organization</th>
<th>Country</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maike Gilliot</td>
<td>HPC vendors (ETP4HPC)</td>
<td></td>
<td></td>
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</table>

## User Forum (UF)

The PRACE User Forum was set up in December 2011 through an initiative of PRACE itself. It is not a body of the association, but an independent entity where PRACE users can discuss their experiences and express their future needs as well as provide feedback on the current services and resources of the PRACE HPC Research Infrastructure.

<table>
<thead>
<tr>
<th>Name</th>
<th>Organization</th>
<th>Country</th>
</tr>
</thead>
<tbody>
<tr>
<td>Marc Baaden</td>
<td>CNRS</td>
<td>France</td>
</tr>
<tr>
<td>Carmen Domene</td>
<td>King’s College London</td>
<td>United Kingdom</td>
</tr>
<tr>
<td>Turlough Downes</td>
<td>Dublin City University</td>
<td>Ireland</td>
</tr>
<tr>
<td>Stefano Fabris</td>
<td>CNR-IOM DEMOCRITOS</td>
<td>Italy</td>
</tr>
<tr>
<td>Derek Groen</td>
<td>Brunell University London</td>
<td>United Kingdom</td>
</tr>
<tr>
<td>Troels Haugbølle</td>
<td>Chair</td>
<td>Denmark</td>
</tr>
<tr>
<td>Koen Hillewaert</td>
<td>Centre de recherche en Aéronautique (Cenaero)</td>
<td>Belgium</td>
</tr>
<tr>
<td>William Sellers</td>
<td>University of Manchester</td>
<td>United Kingdom</td>
</tr>
<tr>
<td>Gabriel Staffelbach</td>
<td>Cerfacs</td>
<td>France</td>
</tr>
<tr>
<td>Maria-Teresa Parra</td>
<td>University of Valladolid</td>
<td>Spain</td>
</tr>
<tr>
<td>Jorge Vieira</td>
<td>Instituto Superior Técnico</td>
<td>Spain</td>
</tr>
<tr>
<td>Gustavo Yepes</td>
<td>Universidad Autonoma de Madrid (UAM)</td>
<td>Spain</td>
</tr>
</tbody>
</table>
**Access Committee (AC)**
The Access Committee is responsible for the scientific assessment of PRACE proposals. They produce a final ranked list of proposals and suggested allocations. The AC is composed of researchers experienced in areas of science, engineering and supercomputing. Members are proposed by the SSC and approved by the Council.

<table>
<thead>
<tr>
<th>Name</th>
<th>Research Area</th>
<th>Country</th>
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</thead>
<tbody>
<tr>
<td>Takayuki Aoki</td>
<td>Fluid dynamics, engineering</td>
<td>Japan</td>
</tr>
<tr>
<td>Edouard Audit</td>
<td>Universe</td>
<td>France</td>
</tr>
<tr>
<td>Marc Baaden</td>
<td>Biology, chemistry</td>
<td>France</td>
</tr>
<tr>
<td>George Biros</td>
<td>Computational Engineering</td>
<td>United States</td>
</tr>
<tr>
<td>Hans-Joachim Bungartz</td>
<td>Mathematics, computer science</td>
<td>Germany</td>
</tr>
<tr>
<td>Barbara Chapman</td>
<td>Applied mathematics, computer science</td>
<td>United States</td>
</tr>
<tr>
<td>Giovanni Ciccotti</td>
<td>Structure of matter, biological systems, molecular dynamics</td>
<td>Italy</td>
</tr>
<tr>
<td>Georges-Henri Cottet</td>
<td>Turbulence, engineering</td>
<td>France</td>
</tr>
<tr>
<td>Christine Davies</td>
<td>High energy physics</td>
<td>United Kingdom</td>
</tr>
<tr>
<td>Luigi Del Debbio</td>
<td>Particle physics</td>
<td>United Kingdom</td>
</tr>
<tr>
<td>Stefan Goedecker</td>
<td>Chemical sciences, materials</td>
<td>Switzerland</td>
</tr>
<tr>
<td>Wilco Hazeleger</td>
<td>Climate</td>
<td>The Netherlands</td>
</tr>
<tr>
<td>Simone Hochgreb</td>
<td>Engineering</td>
<td>United Kingdom</td>
</tr>
<tr>
<td>Petros Koumoutsakis</td>
<td>Chair</td>
<td>Switzerland</td>
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<td>High Energy Physics</td>
<td>Italy</td>
</tr>
<tr>
<td>Fernando Martin</td>
<td>Chemistry, materials</td>
<td>Spain</td>
</tr>
<tr>
<td>Nadia Pinardi</td>
<td>Atmospheric physics, oceanography</td>
<td>Italy</td>
</tr>
<tr>
<td>Luciano Rezzolla</td>
<td>Astrophysics</td>
<td>Germany</td>
</tr>
<tr>
<td>Friederike Schmid</td>
<td>Chemistry, polymers</td>
<td>Germany</td>
</tr>
<tr>
<td>Spencer Sherwin</td>
<td>Computational Engineering</td>
<td>United Kingdom</td>
</tr>
<tr>
<td>Alexandre Tkatchenko</td>
<td>Chemistry, materials</td>
<td>Luxembourg</td>
</tr>
<tr>
<td>Dietrich Wolf</td>
<td>Computational and statistical physics</td>
<td>Germany</td>
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</table>
PRACE members

Membership of PRACE on 31 December 2018

<table>
<thead>
<tr>
<th>Country</th>
<th>Description</th>
<th>Website</th>
</tr>
</thead>
<tbody>
<tr>
<td>AUSTRIA</td>
<td>ACONET Association – Austrian Academic Computer Network</td>
<td><a href="http://www.aco.net">www.aco.net</a></td>
</tr>
<tr>
<td>BELGIUM</td>
<td>Direction générale opérationnelle de l’Économie, de l’Emploi et de la Recherche – Service Public de Wallonie (DGO6-SPW)</td>
<td><a href="http://www.recherche-technologie.wallonie.be">www.recherche-technologie.wallonie.be</a></td>
</tr>
<tr>
<td>BULGARIA</td>
<td>Ministery of Transport, Information Technology and Communications</td>
<td><a href="http://www.mtitc.government.bg">www.mtitc.government.bg</a></td>
</tr>
<tr>
<td>Country</td>
<td>Organization</td>
<td></td>
</tr>
<tr>
<td>------------------</td>
<td>------------------------------------------------------------------------------</td>
<td></td>
</tr>
</tbody>
</table>
| CYPRUS           | CaSToRC – Computation-based Science and Technology Research Center, The Cyprus Institute  
|                  | [www.cyi.ac.cy](http://www.cyi.ac.cy)                                        |
| CZECH REPUBLIC   | IT4I, VŠB – Technical University of Ostrava                                  
|                  | [www.it4i.cz](http://www.it4i.cz); [www.vsb.cz](http://www.vsb.cz)          |
| DENMARK          | DeIC – Danish e-Infrastructure Cooperation                                     
|                  | [www.deic.dk](http://www.deic.dk)                                            |
| FINLAND          | CSC – IT Center for Science Ltd.                                               
|                  | [www.csc.fi](http://www.csc.fi)                                               |
| FRANCE           | GENCI – Grand Equipement National de Calcul Intensif                           
|                  | [www.genci.fr](http://www.genci.fr)                                           |
| GERMANY          | GCS – GAUSS Centre for Supercomputing e.V                                     
|                  | [www.gauss-centre.eu](http://www.gauss-centre.eu)                            |
| GREECE           | GRNET – Greek Research and Technology Network S.A.                            
|                  | [https://grnet.gr/](https://grnet.gr/)                                        |
| HUNGARY          | KIFÜ – Kormányzati Informatikai Fejlesztési Ügynökség                         
| IRELAND          | ICHEC – Irish Centre for High-End Computing                                   
|                  | [www.ichec.ie](http://www.ichec.ie)                                           |
| ISRAEL           | IUCC – Inter-University Computation Center                                   
|                  | [www.iucc.ac.il](http://www.iucc.ac.il)                                       |
| ITALY            | CINECA – Consorzio Interuniversitario                                         
|                  | [www.cineca.it](http://www.cineca.it)                                         |
| LUXEMBOURG       | University of Luxembourg                                                      
<p>|                  | <a href="http://wwwen.uni.lu">wwwen.uni.lu</a>                                           |</p>
<table>
<thead>
<tr>
<th>Country</th>
<th>Organization</th>
<th>Website</th>
</tr>
</thead>
<tbody>
<tr>
<td>THE NETHERLANDS</td>
<td>SURFsara</td>
<td><a href="http://www.surf.nl">www.surf.nl</a></td>
</tr>
<tr>
<td>NORWAY</td>
<td>SIGMA – UNINETT Sigma AS – The Norwegian Metacenter for Computational Science</td>
<td><a href="http://www.sigma2.no">www.sigma2.no</a></td>
</tr>
<tr>
<td>POLAND</td>
<td>PSNC – Instytut Chemii Bioorganicznej Pan – Institute of Bioorganic Chemistry – Poznan Supercomputing and Networking Center</td>
<td><a href="http://www.man.poznan.pl">www.man.poznan.pl</a></td>
</tr>
<tr>
<td>PORTUGAL</td>
<td>Universidade de Coimbra</td>
<td><a href="http://www.uc.pt">www.uc.pt</a></td>
</tr>
<tr>
<td>SLOVAKIA</td>
<td>Computing Center of the Slovak Academy of Science</td>
<td><a href="https://vs.sav.sk">https://vs.sav.sk</a></td>
</tr>
<tr>
<td>SLOVENIA</td>
<td>ARNES</td>
<td><a href="http://www.arnes.s">www.arnes.s</a></td>
</tr>
<tr>
<td>SPAIN</td>
<td>BSC – Barcelona Supercomputing Center – Centro Nacional de Supercomputación</td>
<td><a href="http://www.bsc.es">www.bsc.es</a></td>
</tr>
<tr>
<td>SWEDEN</td>
<td>Vetenskapsrådet – Swedish Research Council</td>
<td><a href="http://www.vr.se">www.vr.se</a></td>
</tr>
<tr>
<td>SWITZERLAND</td>
<td>CSCS, ETH – Eidgenössische Technische Hochschule Zürich – Swiss Federal Institute of Technology, Zürich</td>
<td><a href="http://www.ethz.ch">www.ethz.ch</a></td>
</tr>
<tr>
<td>TURKEY</td>
<td>Istanbul Technical University</td>
<td><a href="http://www.global.itu.edu.tr">www.global.itu.edu.tr</a></td>
</tr>
<tr>
<td>UNITED KINGDOM</td>
<td>EPSRC – The Engineering and Physical Sciences Research Council</td>
<td><a href="https://epsrc.ukri.org">https://epsrc.ukri.org</a></td>
</tr>
</tbody>
</table>
PRACE systems

This article lists the systems that PRACE provides access to. The systems are listed in alphabetical order, and the information reflects their status on 31 December 2018. Updates and upgrades of these systems are published here: www.prace-ri.eu/prace-resources/

Hazel Hen, GCS@HLRS, Germany

Hazel Hen is the new Cray XC40 system (upgrade of Hornet system) and is designed for sustained application performance and highly scalable applications. It delivers a peak performance of 7.42 petaflops. This new system is composed of 7,712 compute nodes with a total of 185,088 Intel Haswell E5-2680 v3 compute cores. Hazel Hen features 965 terabytes of main memory and a total of 11 petabytes of storage capacity spread over 32 additional cabinets containing more than 8,300 disk drives. The input-/output rates are +/-350 gigabytes per second.

JOLIOT Curie, GENCi@CEA, France

JOLIOT CURIE of GENCI, located in France at the Très Grand Centre de Calcul (TGCC) operated by CEA near Paris. JOLIOT CURIE is an Atos/BULL Sequana system X1000 based on a balanced architecture (compute, memory, network and I/O) with 2 compute partitions:

SKL (standard x86)
- 1,656 compute nodes, each with Intel Skylake 8168 24-core 2.7 GHz dual processors, for a total of 79,488 cores and 6.86 petaflop/s peak performance
- 192 GB of DDR4 memory per node – (4GB/core)
- InfiniBand EDR interconnect

KNL (manycore x86)
- 828 Intel KNL 720 nodes each with a 1.4 GHz 68-core processor and 16 GB of MCDRAM for total peak performance of 2.52 PFlops
- 96 GB of DDR4 memory / node
- BULL BXI high speed interconnect

25 additional nodes for post processing and remote visualisation, access to a 500 GB/s multi level Lustre filesystem.

JUWELS, GCS@FZJ, Germany

The Jülich Wizard for European Leadership Science (JUWELS) is the successor of JUQUEEN and represents a milestone on the road to a new generation of ultraflexible modular supercomputers that can carry out a broader range of tasks – from big data applications right up to compute-intensive simulations. With its first module alone, JUWELS qualified as the fastest supercomputer in Germany. The cluster module, which was supplied in spring 2018 by French IT company Atos in cooperation with software specialists at German enterprise ParTec, is equipped with Intel Xeon 24-core Skylake CPUs and excels with its versatility and ease of use. It has a theoretical peak performance of 12 petaflop/s. The nodes are connected to a Mellanox InfiniBand high-speed network. Another unique feature of the module is its ultra-energy-efficient warm-water cooling system.
**MARCONI, CINECA, Italy**
CINECA’s Tier-0 system named MARCONI provides access to PRACE users since July 2016. The MARCONI system is equipped with the new Intel Xeon processors and it has two different partitions:

- Marconi – Broadwell (A1 partition) consists of ~7 Lenovo NeXtScale racks with 72 nodes per rack. Each node contains 2 Broadwell processors that have 18 cores and 128 GB of DDR4 RAM.
- Marconi – KNL (A2 partition) was deployed at the end of 2016 and consists of 3 600 Intel server nodes integrated by Lenovo. Each node contains an Intel Knights Landing processor with 68 cores, 16 GB of MCDRAM and 96 GB of DDR4 RAM.

The entire system is connected via the Intel OmniPath network. The total computational power of the Marconi system is in excess of 20 petaflops.

**MareNostrum, BSC, Spain**
MareNostrum is based on Intel’s general purpose Xeon E5 processors with 2.1 GHz (two CPUs with 24 cores each per node), 2 GB/core and 240 GB of local SSD disk acting as local/tmp. There are 48 racks, each with 72 compute nodes, giving a total of 3 456 nodes. Just over 200 of the nodes have 8GB/core. All nodes are interconnected through an Intel Omni-Path 100Gbits/s network, with a non-blocking fat tree network topology. MareNostrum has a peak performance of 11.14 petaflops.

**Piz Daint, ETH Zurich/CSCS, Switzerland**
The Piz Daint supercomputer is a Cray XC50 system and the flagship system at CSCS – Swiss National Supercomputing Centre, Lugano.

Piz Daint is a hybrid Cray XC50 system with 4 400 nodes. The compute nodes are equipped with an Intel® Xeon® E5-2690 v3 processors with 2.60GHz (12 cores, 64GB RAM) and NVIDIA® Tesla® P100 16GB. The nodes are connected by the “Aries” proprietary interconnect from Cray, with a dragonfly network topology.

**SuperMUC, GCS@LRZ, Germany**
SuperMUC is the Tier-0 supercomputer at the Leibniz Supercomputing Centre (LRZ) in Garching, Germany. It provides resources to PRACE via the German Gauss Centre for Supercomputing (GCS).

SuperMUC Phase 1 consists of 18 thin node islands with Intel Sandy Bridge processors and one fat node island with Intel Westmere processors. Each compute island contains 512 compute nodes, each node having 16 physical cores, giving a total of 8 192 cores per island. Each of these cores has approximately 1.6 GB available for running applications. Peak performance is 3.1 petaflops. All compute nodes within an individual island are connected via a fully nonblocking Infiniband network (FDR10 for the thin nodes and QDR for the fat nodes). A pruned tree network connects the islands.

SuperMUC Phase 2 consists of six islands based on Intel Haswell-EP processor technology (512 nodes/island, 28 physical cores/node and 2.0 GB/core for applications, 3 072 nodes, 3.6 petaflops). All compute nodes within an individual island are connected via a fully non-blocking Infiniband network.
PRACE participation in projects

PRACE is striving to establish an HPC ecosystem at European and international level. Part of this work involves cooperating with other EU-funded scientific, research, industrial and HPC-related projects. The following is a list of projects PRACE participated in during 2018.

**elnfraCentral**

elnfraCentral’s mission is to ensure that, by 2020, a broader and more varied set of users (including industry) discovers and accesses the existing and developing e-infrastructure capacity. A common approach to defining and monitoring e-infrastructures services will increase the uptake and enhance understanding of where improvements can be made in delivering e-infrastructure services.

**Project duration:** 30 months from 01 January 2017 through 30 June 2019

**Funding from the EC:** €1 499 037.50 (100%)

**Budget for PRACE – Funded:** €81 372.50 (100%)

**Role of PRACE aisbl:** Project Partner

[www.einfracentral.eu](http://www.einfracentral.eu)

**Project Consortium:** GEANT VERENIGING; JNP STRATIGIKI KAI EPICHIRISIAKI SYMVOULEFTIKI IKE; PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE AISBL; ETHNIKO KAI KAPODISTRIAKO PANEPISTIMIO ATHISON; GOTTFRIED WILHELM LEIBNIZ UNIVERSITAET HANNOVER; EUROPEAN FUTURE INNOVATION SYSTEM CENTRE; CONSIGLIO NAZIONALE DELLE RICERCHE; GEANT LIMITED; STICHTING EGI; THE UNIVERSITY OF EDINBURGH

**ELITRANS**

While the implementation of the “Extreme Light Infrastructure” ELI is near completion in the Czech Republic, Hungary and Romania, its remaining challenge is to create the necessary conditions for its future operation as a single, distributed international laser user facility of pan-European dimension. The goal of the ELITRANS project is to complement the final implementation stage of ELI by preparing and undertaking the transformation from three legally (but not conceptually) independent construction projects, towards operation as a single international legal entity, the ELI European Research Infrastructure Consortium (ELI-ERIC).

**Project duration:** 42 months from 01 September 2015 through 28 February 2019

**Funding from the EC:** €3 395 383.75 (100%)

**Budget for PRACE – Funded:** €108 203 (100%)

**Role of PRACE aisbl:** Project Partner

[https://eli-trans.eu](https://eli-trans.eu)

**Project Consortium:** INSTITUTUL NATIONAL DE CERCETARE -DEZVOLTARE PENTRU FIZICA SI INGINERIE NUCLEARA “HORIA HULUBEI”; PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE AISBL; ELI-HU KUTASI ES FEJLESZTESI NONPROFIT KOZHASZNU KORLATOLT FELELOSSEGU TARSA; ASSOCIATION INTERNATIONALE EXTREME-LIGHT-INFRASTRUCTURE DELIVERY CONSORTIUM – COORDINATOR; KARLSRUHER INSTITUT FUER TECHNOLOGIE; FYZIKALNI USTAV AV CR V.V.I; STICHTING EGI
**EOSCpilot**

The European Open Science Cloud will offer 1.7 million European researchers and 70 million professionals in science and technology a virtual environment with open and seamless services for storage, management, analysis and re-use of research data by federating existing scientific data infrastructures. The EOSCpilot project has been funded to support the first phase in its development.

**Project duration:** 28 months from 01 January 2017 through 30 April 2019

**Funding from the EC:** €9 953 067.50 (100%)

**Budget for PRACE – Funded:** €80 625 (100%)

**Role of PRACE aisbl:** Project Partner

https://eoscpilot.eu

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**EXDCI**

The three most significant HPC bodies in Europe – PRACE, ETP4HPC and EESI – came together within EXDCI to coordinate the strategy of the European HPC ecosystem. EXDCI aimed to support the road-mapping, strategy-making and performance-monitoring activities of the ecosystem, including building and maintaining relations with other international HPC activities and regions. It has contributed to a much-increased momentum of HPC related activities and to the strategic goal of coordinating complementary stakeholder groups.

**Project duration:** 30 months from 01 September 2015 through 28 February 2018

**Funding from the EC:** €2 551 875.00 (100%)

**Budget for PRACE – Funded:** €901 250 (100%)

**Role of PRACE aisbl:** Coordinator

https://exdci.eu

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**Project Consortium:** PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE AISBL – COORDINATOR; EUROPEAN TECHNOLOGY PLATFORM FOR HIGH PERFORMANCE COMPUTING
EXDCI-2
The project EXDCI-2 builds upon the success of EXDCI and will continue the coordination of the HPC ecosystem with important enhancements to better address the convergence of big data, cloud and HPC. Its main goals are to develop a competitive European HPC exascale strategy by supporting the implementation of a common European HPC strategy, and to coordinate the stakeholder community for exascale HPC in Europe through joint community structuring and synchronisation.

Project duration: 30 months from 01 March 2018 through 31 August 2020

Funding from the EC: €2 440 000.00 (94%)

Budget for PRACE – Funded: €864 065 (100%)

Role of PRACE aisbl: Coordinator

https://exdci.eu

Project Consortium: PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE AISBL – COORDINATOR; UNIVERSITE DE RENNES I; UNIVERSITE DE PICARDIE JULES VERNE; EUROPEAN TECHNOLOGY PLATFORM FOR HIGH PERFORMANCE COMPUTING

FocusCoE
FocusCoE will contribute to the success of the EU HPC ecosystem and the EuroHPC Initiative by supporting the EU HPC Centres of Excellence to more effectively fulfil their role within the ecosystem, ensuring that extreme scale applications result in tangible benefits for addressing scientific, industrial or societal challenges. It will do this by creating an effective platform for the centres to coordinate strategic directions and collaboration, and will provide support services for the centres in relation to both industrial outreach and promotion of their services and competences.

Project duration: 36 months from 01 December 2018 through 30 November 2021

Funding from the EC: €1 997 921.25 (100%)

Budget for PRACE – Funded: €16 437.50 (100%)

Role of PRACE aisbl: Project Partner

www.focus-coe.eu

Project Consortium: UNIVERSITY COLLEGE LONDON; AGENZIA NAZIONALE PER LE NUOVE TECNOLOGIE; L’ENERGIA E LO SVILUPPO ECONOMICO SOSTENIBILE; KUNGLIGA TEKNISKA HOEGSKOLAN; PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE AISBL; TERATEC; FORSCHUNGSZENTRUM JULICH GMBH; NATIONAL UNIVERSITY OF IRELAND GALWAY; BARCELONA SUPERCOMPUTING CENTER - CENTRO NACIONAL DE SUPERCOMPUTACION; SCAPOS AG – COORDINATOR; UNIVERSITAET STUTTGART; COMMISSARIAT A L’ENERGIE ATOMIQUE ET AUX ENERGIES ALTERNATIVES
HPC-GIG
The European Cloud Initiative implementation encompasses different elements and will require a solid governance setup. A cornerstone of this governance is a joint undertaking, which will become active in 2019. HPC-GIG proposes intelligence gathering services from the European HPC stakeholders for this future HPC Governance - HPCG. It will facilitate a timely start of its operations, transparently and non-intrusively leveraging the HPC community know-how, organised with enough flexibility to align project activities with the programme schedule and needs during its ramp-up phase, and deliver timely and useful input to the HPCG.

Project duration: 18 months from 01 September 2018 through 29 February 2020

Funding from the EC: €900 000 (95%)

Budget for PRACE – Funded: €400.432 (89%)

Role of PRACE aisbl: Coordinator

Project Consortium: GEANT VERENIGING; PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE AISBL – COORDINATOR; EUROPEAN TECHNOLOGY PLATFORM FOR HIGH PERFORMANCE COMPUTING

PRACE-5IP
The objectives of PRACE-5IP are to build on and seamlessly continue the successes of PRACE and start new innovative and collaborative activities proposed by the consortium. The activities are designed to increase Europe's research and innovation potential, especially through seamless and efficient Tier-0 services and a pan-European HPC ecosystem.

Project duration: 28 months from 01 January 2017 through 30 April 2019

Funding from the EC: €15 000 000.00 (93%)

Budget for PRACE – Funded: €1 123 215 (85%)

Role of PRACE aisbl: Project Partner

www.prace-ri.eu/prace-5ip

Project Consortium: PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE AISBL; CSC-TIETEEN TIEOTOTENNIKAN KESKOU OY; FORSCHUNGSZENTRUM JULICH GMBH – COORDINATOR; ASSOCIATION “NATIONAL CENTRE FOR SUPERCOMPUTING APPLICATIONS; CENTRE DE RECHERCHE EN AERONAUTIQUE ASBL – CENAERO; UPPSALA UNIVERSITET; GRAND EQUIPEMENT NATIONAL DE CALCUL INTENSIF; GAUSS CENTRE FOR SUPERCOMPUTING (GCS); KORMANYZATI INFORMATIKAI FEJLESZTESI UGNYOKSEG; VYSOKA SKOLA BANSKA - TECHNICKA UNIVERZITA OSTRAVA; CINECA CONSORZIO INTERUNIVERSITARIO; UNIVERSIDADE DE COIMBRA; ETHNIKO DITIEVNAI EREVNAS TECHNOLOGIAS AE; INSTYTUT CHEMII BIOORGANICZNEJ POLSKIEJ AKADEMII NAUK; UNINETT SIGMA2 AS; THE CYPRUS INSTITUTE; SURFSARA BV; CENTRUM SPOLCNYCH CINNOSTI SLOVENSKERE AKADEMIE VIED; ISTANBUL TEKNIK UNIVERSITESI; MACHBA - INTERUNIVERSITY COMPUTATION CENTER; UNIVERZA V LJUBLJANI; KOBENHAVNS UNIVERSITET; NATIONAL UNIVERSITY OF IRELAND GALWAY; BARCELONA SUPERCOMPUTING CENTER - CENTRO NACIONAL DE SUPERCOMPUTACION; EIDGENOESSISCHEN TECHNISCHEN HOCHSCHULE ZUERICH; THE UNIVERSITY OF EDINBURGH
John Towns is the principal investigator and project director for XSEDE, a cyber infrastructure for HPC in the US and in many ways the analogue of PRACE. Here, we speak to him about how the two entities are helping each other to improve and to provide a better environment for international collaborations.

Could you briefly explain who you are and what XSEDE is?
John Towns: I work at the National Centre for Supercomputing Applications at the University of Illinois, where I am the principal investigator on a cyber infrastructure project called XSEDE – the Extreme Science and Engineering Discovery Environment. It is a national collaboration with about 200 individuals and 19 institutions across the US. It is similar to PRACE in many respects in that it provides access to HPC resources and professional support to users of HPC, although the scope is a somewhat broader in that we also support high throughput computing.

Each year, XSEDE supports more than 8,500 researchers and somewhere near 2,500 projects, most of which are international collaborations. Some of the more high profile of these projects include the Dark Energy Survey, the Large Synoptic Survey Telescope, various projects at CERN and the LHC, and the work done on gravitational waves at LIGO.

How does XSEDE work together with PRACE?
JT: The relationship between XSEDE and PRACE extends to before PRACE even began, as we at XSEDE were working with people from DEISA – the entity that preceded PRACE – from around 2007. Together with DEISA, we initiated the HPC summer schools that continue today and are now jointly organised by XSEDE, PRACE, Compute Canada and the Japanese research institute RIKEN. So there has been a close working relationship for a while now.

We have been pursuing some joint programmes with PRACE with the ultimate goal of establishing a mechanism for providing joint allocations of resources in Europe and the US for collaborating research teams. We started around four years ago with a call for interest to both regions for providing support for these
collaborations, which helped us understand how these collaborations work and how we could help to facilitate them. This, along with our developing relationship with RIKEN, eventually led to the signing of a joint memorandum of understanding between the three entities that detailed our willingness to collaborate on various activities.

People from both PRACE and XSEDE often attend one another’s meetings and working groups, and we have a number of joint activities, especially around the issue of security. We also have periodic meetings between representatives of the major research infrastructures from around the world, which help us to see what each other are doing and where there is overlap and the potential to collaborate across regions. Over time, we have also got to know each other a lot better and so there is a growing level of informal cooperation between PRACE and XSEDE that goes beyond our formal agreements.

▶ What do you think both sides have learnt from each other?
JT: In the way that XSEDE and PRACE operate as infrastructures, there is a lot of what I will call informal organisational benchmarking between us. We do not use a formal system for doing that, but we have had various teams in different areas of each of our operations compare notes on how they operate, what their policies and procedures are, and how they can both improve.

In addition, our working together has been a means for us to understand our community better by identifying teams that are collaborating on research across the regions. These collaborations are quite hard to find if you do not know about them. When we put out a call to support these teams several years ago, I was surprised to see that there were a number of researchers from our side that I knew personally but did not know were involved in collaborations with teams in Europe. That call was important as it has helped both XSEDE and PRACE to determine more effective ways of working together.

As I mentioned before, we are looking to get to the point where can provide joint allocations of resources for these cooperating teams. This is good news for those teams as it can be quite awkward to make these collaborations work at the moment. Currently, researchers from the different regions have to independently request resources, which they will not necessarily receive, and things are made even more difficult when the timelines of the different allocations do not align.

▶ How do you hope to see the working relationship with PRACE improve in the future?
JT: I think everyone would like to see things move a little faster, but that is the nature of international collaborations. We do not have the frequency of interactions that we have with people from the same region, and so inevitably things can take longer. For both sides, I would say that although we both see working together as really important, it can often be pushed aside as a priority from the perspective of our funding agencies. XSEDE’s funds come from the National Science Foundation in the US, and so the support of researchers in the US takes priority, but they do also recognise that science is increasingly becoming a large team sport, and those teams are almost invariably international.

We face various challenges when trying to create stronger ties and closer cooperation between our regions. Although we are similar in many respects, there are differences which can make things difficult. For instance, PRACE is a legal entity whereas XSEDE is a project, so we have different restrictions and freedoms in the way that we operate.

Despite these differences, there is a very good collegial relationship between XSEDE and PRACE. It would be easy for us to get tired and give up on trying to work more closely, but there has always a willingness on both sides to recognise the challenges that we face and stand up and find solutions to them together, with the ultimate goal of enabling the best science that we can globally, not just within our regions.

“The ultimate goal is to enable the best science that we can globally, not just within our regions”
Success stories: Supporting research with HPC

High performance computing supports research into all aspects of our world. It is a cornerstone of academia and industry, where everything from fundamental physics to climate research depends on algorithms to deliver solutions.

In the following pages, we hear from some of the most recent recipients of core hours from PRACE about how their allocations are helping to advance their work. In two of the cases, we also hear from members of the High-Level Support Teams who are helping the researchers achieve their goals and make the most out of their time with the computers.

The first project we hear from is led by Carmen Domene of the University of Bath, who has been looking at how bacterial sodium channels and eukaryotic sodium channels can both be selective for sodium ions even though their selectivity filters are different, using simulations in the order of microseconds to sample the relevant events. The project was awarded 102 million core hours on Piz Daint hosted by CSCS, Switzerland, and was supported by Christopher Bignamini from CSCS’s High-Level Support Team. Read more on page 37.

Second on the list is a project led by Maria J Ramos of the University of Porto who is using high performance computing to investigate potential targets for antibiotic compounds, and to develop new compounds that can bind to them. The project was awarded 15 million core hours on MareNostrum hosted by BSC, Spain, and was supported by David Vicente from BSC’s High-Level Support Team. Read more on page 38.

Laurent Brodeau of French SME Ocean Next has been using huge simulations of the ocean to determine how kilometric-scale turbulence contributes to global oceanic circulation. The simulations will also be used for preparing upcoming satellite missions, including the SWOT altimetry mission, which will provide observations of surface ocean dynamics at an unprecedented resolution. The project was awarded 40 million core hours on MareNostrum hosted by BSC, Spain. Read more on page 39.

Another project we hear from is an investigation into the unique electronic and optical properties of 2D materials, in specific a group called transition metal dichalcogenides. The project, led by Maurizia Palummo of the University of Rome Tor Vergata, uses post density functional theory approaches based on many-body perturbation theory, and was awarded 49.5 million core hours on Marconi hosted by CINECA, Italy. Read more on page 40.

Finally, we have a project which aims to understand and predict how soot forms in gas turbine combustors. It combines large eddy simulations with detailed chemistry of soot and flames to achieve this, and is unique in that it uses a Lagrangian approach to predict the soot particle size distribution. The project is led by Eleonore Riber of CERFACS and was awarded 15 million core hours on Joliot Curie hosted GENCI at CEA, France. Read more on page 41.
**The biochemist**

**Carmen Domene** of the University of Bath uses high performance computing to try to understand biochemical and biophysical processes from a microscopic perspective, working closely with experimentalists to help them both interpret their experiments and devise new ones.

*My PhD was on the theory, modelling and computation of molecular properties for the prediction of materials properties at the atomistic level, with a particular focus on ionic materials. After I finished, I wanted to change area and study 'living things' rather than just materials, so I started a postdoc in computational biophysics of ion channels, using computer simulations at the Laboratory of Molecular Biophysics at Oxford. It was all new to me — the methods and approaches and the field of research — but the core idea was the same 'study of ions', only this time in biological settings.

We need to run simulations of the order of microseconds to sample the events we are interested in, and these time scales require HPC resources. We also need to run many short runs in the order of thousands to get the free energies underlying the phenomena we are interested in.

We have had a PRACE allocation since October 2018. We are trying to understand how bacterial sodium channels and eukaryotic sodium channels can both be selective for sodium ions even though their selectivity filters are different, especially since bacterial sodium channels are similar to calcium channels that preferentially select calcium ions.

Sodium and calcium channels are proteins embedded in cell membranes that allow for selective transport of ions and convert chemical or mechanical messages into electrical signals. Ion channels regulate ion content in cells; there are different concentrations of ions in the cytoplasm and the extracellular environment of any cell, and these concentration differences create a small electrical potential across the plasma membrane. When ion channels open, ions on either side of the plasma membrane flow down concentration gradients.

It is too early to say what the outcome of our project is, but I can say that we have received a very generous allocation of computing time from PRACE and we have access to technical support when needed. Without these resources and support, we would not have been able to tackle this problem, so we are very grateful to PRACE.*

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The project “MICNA – Mechanisms of ion conduction in sodium channels” was awarded 102 million core hours on Piz Daint hosted by CSCS, Switzerland.
The bacterial ribosome is an important drug target because of its role in protein synthesis. Proteins called release factors (RFs) bind to the ribosome and catalyse polypeptide release to terminate translation. However, to date the druggability of these factors has not been extensively studied.

Ana Oliveira, one of our senior researchers, demonstrated in previous work that the turnover of the release factor (RF2) could be directly inhibited in the translation cycle by binding small inhibitors. After characterising the receptor using high performance computers, she identified two novel inhibitors that killed the bacteria by directly binding to RF2. In this project, we are looking to determine novel druggable ribosomal proteins or ribosomal factors, and to characterise these proteins to develop new drug-like compounds that exhibit antibiotic properties.

Our experience with the staff at MareNostrum has been very good so far. They were extremely helpful at the beginning when we had teething problems. Ana Oliveira went to Barcelona and met the High-Level Support Team who helped us set up our simulations on their system. I am truly thankful to PRACE as we do not have a supercomputer in Portugal that would allow us to run our calculations free of charge.

The project “IFs/RFs-RC” was awarded 15 million core hours on MareNostrum hosted by BSC, Spain.

The drug discoverer

Maria J Ramos is a biochemist at the University of Porto. Here we hear from her about using high performance computers to investigate potential targets for antibiotic compounds, as well as from High-Level Support Team member David Vicente about how he and his team were able to help.

David Vicente – High-Level Support Team, Barcelona Supercomputing Centre

Maria Ramos’ project was initially identified by the PRACE Access Committee as requiring the support of a High-Level Support Team, as it was of great scientific interest but needed help with scalability. We met with Ana Oliveira, who supplied us with their inputs and codes, and we explained to her what they would need to do to get the best out of the MareNostrum system.

The code they use is a molecular dynamics code called Amber. It showed good scalability up to 256 cores but not beyond that. We tested a variety of their inputs with the latest version of Amber, which has improved parallel efficiency and performance, and then advised them on the best way to proceed.

For a second part of their project, they will need to do several runs which are not parallel. We helped them with the scripting to enable them to submit all of their simulations at once, to help with the scripts that distribute the work in a parallel way to the different nodes of the machine.

“We focused on helping the team to understand the limitations of the code, and to try and find the best approach possible to use the resources they had been allocated in the best possible way”

For us, this project was not a matter of optimisation, as it needed to start quickly and we did not have time to increase the parallel efficiency of a code as big as Amber. Instead, we focused on helping the team to understand the limitations of the code, and to try and find the best approach possible to use the resources they had been allocated in the best possible way. From what I have seen so far, it seems that everything is now running well and they are ahead of schedule in terms of using their computing time.
The ocean modeller

Laurent Brodeau of Ocean Next conducts research in the field of physical oceanography. Here he speaks about carrying out some of the most detailed simulations of the North Atlantic to date in order to better understand how ocean circulation works and interacts at different scales.

"Until recently, ocean models were relatively coarse in terms of horizontal resolution, with a typical grid size in the order of 100 kilometres. Climate models usually have an ocean component and atmosphere component which are coupled together, and so the coarse ocean component means that the fine-scale circulation and turbulence of the ocean cannot be seen. In our work, we have been increasing the resolution in the ocean down to the kilometre-scale in order to improve the representation of fine-scale pattern of the ocean circulation.

The primary goal of our project is to help prepare for the upcoming SWOT satellite mission, which will be measuring the elevation of the world’s oceans, lakes and rivers at unprecedented levels of resolution. When this satellite launches in 2021, the scientists working on it need to be ready to process the data that it collects. We are helping them to prepare by running numerical simulations at similar resolution to provide them with synthetic data that is similar to what the satellite will measure.

Ocean circulation is dictated by turbulent flow, and so from a purely scientific point of view we are looking forward to running a high-resolution simulation that covers a relatively long time period. This will tell us many things about the ocean, from the way that smaller sub-mesoscale eddies interact with each other and with larger eddies and how this is affected by the seasons, to how the larger eddies influence ocean circulation. For the first time at this resolution, we will also be explicitly modelling tidal motion. The tide introduces internal waves, known as internal tides, into the system, which affects sea level.

Compared to other fields of research that use high performance computers, physical oceanography has some special requirements in that we have to write and save a lot of data (the resolution of tidal motion necessitates saving the fields of interest every hour). There are many systems available that provide lots of CPUs in parallel, but with our work you reach a certain point where the I/O becomes the bottleneck rather than the number of processors. Luckily for us, the Barcelona Supercomputing Centre was able to provide everything we need with its MareNostrum system.

The work we are doing now is at the cutting edge of what is possible. Our simulations are currently the largest ever in terms of computing points in the ocean, although they won’t remain the largest for long. Having said that, even though we have a huge amount of CPU hours dedicated to this project, we will only be able to simulate around six years of time, which goes to show how CPU-intensive these simulations are. And, of course, after that we will need to analyse the two petabytes of data that we will have produced, so there is a big data challenge ahead for us in this project.

The project “ReSuMPTiOn – Revealing SubMesoscale Processes and Turbulence in the Ocean” was awarded 40 million core hours on MareNostrum hosted by BSC, Spain."
The physicist

Maurizia Palummo is a physicist at the University of Tor Vergata. Here she speaks about combining her expertise in condensed matter physics and materials science to study the electronic and optical properties of 2D materials.

A large part of my career has been spent studying semiconducting surfaces and interfaces, but in recent years I have moved towards the field of nanoscience. In particular, I am interested in 2D materials which have fascinating properties and have many potential applications. Since the discovery of graphene, many other 2D materials have been discovered and there has been a lot of experimental work done on them. My work now focuses on the interpretation of experimental results and the theoretical prediction of new properties of 2D materials.

I am an expert in density functional theory, one of the main methods used to explain the electronic and optical properties of materials. More recently, new methods known as post density functional theory methods are providing even more accurate descriptions of electronic and optical properties. For instance, effects such as the deformation of excitons (concentrations of energy formed by the pairing of an electron and an associated ‘electron hole’) can only be properly described using these approaches.

The use of high performance computers is fundamental to this kind of work. Density functional theory calculations are already computationally expensive, and post density functional theory is even more so.

In this PRACE project, we looked at a specific class of 2D materials called transition metal dichalcogenides. They are interesting because they have a strong light-matter interaction, opening up the possibility of low-cost and flexible opto-electronic devices, such as ultra-thin light emitting diodes and photovoltaic cells. Part of the project has been looking at how small atomic defects can alter the optical properties of these materials.

Another part of this project has involved us examining a different phase of these transition metal dichalcogenides. Normally these materials crystallise in a hexagonal form, but some experiments have suggested that small domains of another atomic phase can occur. In our work we have shown that it is possible in principle to stabilise this phase if small organic molecules are added to the material, and that these molecules can be used to modulate the optical properties.

Our calculations on this less stable phase have also led us to discover that an exotic phase of matter could be achieved, known as excitonic insulator, in which a condensate of electron-hole couples (similarly to Cooper pairs formed in superconductors) can be more stable than the normal ground state. Its existence was predicted many years ago in several theoretical publications, and now through our simulations and theoretical modelling we have shown that it could be observed in a 2D material of this family.

The PRACE allocation has been incredibly useful for my work. Unfortunately, we do not have any high performance computational resources in our department, which means that I normally have to apply for computational time every few months to carry out my research. This year has been different because PRACE has given me enough computational time to allow me to concentrate on the science without having to apply for new projects all the time.

The project “OPTEL2D Opto-electronic properties of 2D Transition Metal Dichalcogenides with DFT and post-DFT simulations” was awarded 49.5 million core hours on Marconi hosted by CINECA, Italy.
Eleonore Riber is an expert in fluid dynamics at HPC research centre CERFACS. Here she explains how she has been using high performance computers to understand and predict how soot forms in gas turbine combustors.

Expected stringent particulate matter emission legislation for gas turbine combustors has motivated considerable efforts to better understand, model and predict soot formation. To design the next generation of combustion chambers, numerical simulation has become an essential tool, especially in terms of pollutant emissions prediction.

This project uses some of the same principles from our previous PRACE project on rocket motors, applying the same code and adapting the Lagrangian approach previously used for aluminium particle modelling to look at soot emissions and to try to predict how and why it forms.

One of the main novelties of this project is that we are using a Lagrangian approach to predict how soot forms in a combustor. This is currently a very active subject, but most of the people working on it use Eulerian approaches. The chemistry of soot particles and how they group together strongly depends on their size, and our Lagrangian approach is an alternative approach to predicting soot particle size distribution. To our knowledge, this is the first time that such an approach has been used to predict soot size distribution in complex configurations.

We have developed a very efficient Lagrangian solver, and we wanted to take advantage of using this for predicting how soot forms. Soot forms from various precursors, and so this project involves an interesting mixture of large eddy simulations and detailed chemistry of flame and soot. The gaseous chemistry is described with an analytically reduced chemistry to guarantee a good prediction of both flame structure and gaseous soot precursors. In the end, the simulations are quite expensive because of this combination of flame chemistry and following huge numbers of particles around, but we are pleased because it is a good achievement.

We are currently still working on this project, evaluating the model we have developed with various operating conditions. We have already published some articles based on the results. One of these was presented at the International Symposium on Combustion in Dublin last summer, and we have also been presenting our results at the International Soot Workshop, which brings together researchers from across the world who are working on this subject. There are still two more articles waiting to be published, so it has been a productive project in that sense.

The allocations of computing hours we receive from PRACE are what make our work possible. There is no way we could possibly run these kinds of simulations at such accuracy without the use of high performance computers. We could not have afforded to use both the Lagrangian approach for the soot particles and the detailed model of the flame chemistry at the same time without such a project.
The European Extreme Data & Computing Initiative 2 (EXDCI-2) builds upon the work of the first EXDCI, which established a strong collaboration between the European Technology Platform for High Performance Computing (ETP4HPC) and PRACE. EXDCI-2 supports multiple aspects of the HPC ecosystem, such as the organisation of conferences, HPC projects, analysis of innovations within Centres of Excellence, road mapping, calls for proposals, and SME technology development support.

Furthermore, international vision development has been pursued in collaboration with American, Chinese and Japanese partners. New topics such as outreach towards high schools and machine learning vision development have been added to the EXDCI mission. Another important component of the ecosystem is the European High-Performance Computing Joint Undertaking (EuroHPC), which EXDCI-2 is currently adapting to.

The annual European HPC Summit Week (EHPCSW) gathers European HPC stakeholders together to foster collaboration. Each year, EXDCI opens a call for contributions to anyone in the world of HPC who would like to participate in the week through a workshop. The third edition in 2018 took place in Ljubljana. The 2019 edition will be held in Poznań, Poland, where the EHPCSW will be renamed to the EuroHPC Summit Week to reflect the new HPC landscape. A first version of a joint workshop will also be organised across multiple user communities and Centres of Excellence by EXDCI-2. Common challenges such as scalable meshing tools, couplers, mini app development, and smart in-situ post processing will be discussed, with white papers subsequently produced.
As the Horizon 2020 EU Research and Innovation programme comes to an end, questions like “What will the role of HPC and high-performance data analytics (HPDA) be after Horizon 2020?” and “What should be the main priorities of the 9th EC Framework Programme?” need to be addressed. EXDCI-2 is preparing an HPC-HPDA technology roadmap for the FP9 time frame. This has involved close collaboration with PRACE and ETP4HPC in order to consider the HPC and data requirements of new and emerging communities such as humanities, social sciences, decision making, urgent computing, and artificial intelligence. The outcome is a strategic research agenda that will be relevant for planning research programmes after Horizon 2020. This document outlines the major trends in the deployment of HPC and HPDA driven by societal needs in Europe, and touches on expected changes in technology and architecture of the expanding underlying IT infrastructure.

EXDCI-2 is also considering legacy codes. In the race to exascale computing, most of the efforts have concentrated on hardware. This is not surprising given the challenge of reaching exaflop cluster performance with less than 30 megawatt power. However, another current priority is to assess the cost of application migration to new systems and to evaluate the potential technical debt which might be faced in the future. For the largest codes, this task will be a multi-year effort, probably in the order of 5-10 years. Underestimating those efforts will have multiple consequences such as crucial delays to porting, loss of leadership or attractiveness of European research teams, or economic losses for European industry in an ever more competitive world. In order to get a clearer view of the situation for HPC codes, a metric called “the code viscosity” has been proposed that will capture how easily a code can be ported to a new environment.

EXDCI-2 is involved in and participates in the international BDEc effort (see www.exascale.org/bdec). The aim is to identify the major application domains and examine their algorithmic, data, and computing needs. The findings are then used to define a “distributed services platform” for science, based on the principle of continuum computing. This principle links data, network, and computing from the instruments and sensors at the “edge”, all the way to the cloud and HPC infrastructures at the centre.

HPC is not a field where standardisation organisations play an important role. Most of the so-called standards are de facto standards. In this context, it is important for Europe to be represented in various organisations that have an influence on how new technologies could achieve market acceptance. This is especially true considering the rising importance of HPDA. This activity will create a list of the European experts that are present in the most important standardisation organisations.

Studying technology producer SMEs in EXDCI-1, it is obvious that E-funded R&D projects are not yet exploited enough for pushing new technologies towards the market. Considering the lifetime of an R&D project, we have developed the idea of a “project spin-off”, gathering a subset of project partners from existing R&D projects with the objective of designing a pre-product and assessing its viability for the market. To assert the validity and potential of the current proposal, we are conducting a proof-of-concept in the frame of EXDCI-2, based on innovations identified in the current Future and Emerging Technologies HPC projects. Furthermore, initiatives for improving HPC adoption in industry like PRACE SHAPE and Fortissimo have been promoted by fostering collaboration with independent software vendors and non-HPC European technology platform partners.

Finally, EXDCI-2 aims to develop a transversal vision of HPC. The goal is to identify key challenges for the next generation of applications. This includes an understanding of the requirements and where research and innovation is needed for preparing Europe’s HPC machines, its users, its software developers, and vendors. Topics addressed here span from community challenges, such as the “Democratisation of HPC”, to how new hardware technologies, such as quantum or optical computing and silicon photonics, will impact application development.
PRACE ACTIVITIES

Events and outreach
European HPC Summit Week 2018 and PRACEdays18

At PRACE, we like to keep our user community and other HPC stakeholders well informed. Part of this involves making sure our organisation is properly represented at HPC events in Europe and around the world.

The EXDCI-2 project coordinated the 2018 European HPC Summit Week, which brought together the main European HPC institutions, communities, service providers, users, consultants and vendors to cultivate new ways of working together. The third edition of the European HPC Summit Week took place from 28 May to 1 June and was held at the Faculty of Law of the University of Ljubljana, Slovenia. It brought together nearly 350 attendees and covered an extensive range of application areas such as energy, big data, life sciences, engineering, multiscale computing and simulations.

PRACE’s Scientific and Industrial Conference (PRACEdays) was again part of the week, with parallel scientific sessions and an intensive industrial track with a special focus on SHAPE projects. Furthermore, under the title “CoEs and HLSTs – What problems can they solve for me?”, a panel discussion took place between users and representatives of the Centres of Excellence and High-Level Support Teams. The PRACE Ada Lovelace Award for HPC was awarded to Xiaoxiang Zhu, and the PRACE Award for Best Scientific Presentation was given to Vincent Moureau.

The 2018 programme also incorporated hands-on training for students. As always, the five-day summit provided a great opportunity to network with HPC stakeholders from across Europe, from technology suppliers and HPC infrastructures to scientific and industrial HPC users. We look forward to seeing everyone next year at the European HPC Summit Week 2019, which will take place on 13-17 May in Poznań, Poland.

ISC 2018
Just before the summer holiday season starts, the HPC community gathers in Frankfurt for the International Supercomputing Conference and exhibition. In 2018, HPC stakeholders came together to learn about the latest goings on in the world of HPC. PRACE had a joint booth with the EXDCI-2 project, where a wide variety of mini-presentations were given about the latest developments. Topics like training, industrial access and various different projects were on the agenda. To reach out to the next generation of HPC experts, PRACE was again one of the sponsors of the STEM Students Tours and Gala. Young people had the opportunity to visit our booth and hear about HPC and what PRACE does.
the evening, a gala event was held for students to mingle with representatives of HPC stakeholders.

During the week of ISC, PRACE booth staff catered to more than 300 visitors, who were informed about various PRACE activities such as peer review and the wide range of PRACE training possibilities.

**SC18**
The International Conference for High Performance Computing, Networking, Storage and Analysis (SC18) celebrated its 30th anniversary in 2018. This year, the event was held in Dallas, Texas from 12-15 November. PRACE was one of the 364 exhibitors showcasing their latest updates and informing people about PRACE’s activities.

PRACE had a joint booth with EXDCI-2. A wide range of mini-presentations promoted PRACE activities at the booth. Attendees were interested in the training opportunities PRACE offers and how they can get access to PRACE resources. During the week, a “birds of a feather” session named “Big Data Challenge – How to Engage with Large Scale Facilities?” was organised thanks to an international collaboration between PRACE, Pawsey (Australia), CHPC (South Africa) and the National Centre for Supercomputing Applications (United States).

PRACE also took part in activities organised by SC18. The booth team welcomed pupils who were taking part in a tour, and also participated in the Student Scavenger Hunt. In order to make the European organisations’ presence more transparent, PRACE supported the “Get in the Zone! #EuroZoneSC18” initiative, in which the European projects and organisations promoted their developments and initiatives.

**Science fairs**
PRACE attends various science fairs, career fairs and museum exhibitions held in different project partner countries. It does this to showcase PRACE activities and outcomes and thus encourage pupils and young students to choose a career in fields related to science and technology and become part of the next generation of HPC users.

PRACE provides interactive experiences at these events through exhibits such as video games which the audience can engage in and learn with.

In 2018, PRACE participated in the following events:

<table>
<thead>
<tr>
<th>EVENT TYPE</th>
<th>TITLE OF EVENT</th>
<th>LOCATION</th>
<th>DATE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Science fair</td>
<td>BT Young Scientist and Technology Exhibition (BTYSTE)</td>
<td>Dublin, Ireland</td>
<td>11 January 2018</td>
</tr>
<tr>
<td>Science fair</td>
<td>Tieteiden yö</td>
<td>Helsinki, Finland</td>
<td>18 January 2018</td>
</tr>
<tr>
<td>Career fair</td>
<td>Kariéra 2018, VSB – Technical University of Ostrava</td>
<td>Ostrava, Czech Republic</td>
<td>March 2018</td>
</tr>
<tr>
<td>Science fair</td>
<td>Athens Science Festival</td>
<td>Athens, Greece</td>
<td>24-29 April 2018</td>
</tr>
<tr>
<td>Science fair</td>
<td>European Contest of Young Scientists (EUCYS)</td>
<td>Dublin, Ireland</td>
<td>15-18 September 2018</td>
</tr>
<tr>
<td>Science fair</td>
<td>Researchers’ Night</td>
<td>Various PRACE countries</td>
<td>End of September 2018</td>
</tr>
<tr>
<td>Career fair</td>
<td>Trinity College Dublin’s Maths &amp; Physics Department’s Career fair</td>
<td>Dublin, Ireland</td>
<td>October 2018</td>
</tr>
</tbody>
</table>
European Union Contest for Young Scientists (EUCYS)
For the third time, PRACE took part in the European Union Contest for Young Scientists (EUCYS) with a booth at the exhibition and as sponsor of the special award for computational science. EUCYS celebrated its 30th edition in Dublin, Ireland from 15-18 September 2018. The contest is managed by the Directorate-General for Research and Innovation of the European Commission in cooperation with a different host country each year. The contest seeks to support national efforts to attract young people to study science, technology, engineering and mathematics, so that they eventually choose careers in science and research. In cooperation with the Irish Centre of High-End Computing (ICHEC), the booth team informed the participants and visitors of EUCYS about HPC research infrastructure in Europe and the training possibilities provided by PRACE training centres. Sinéad Ryan, Chair of the PRACE Scientific Steering Committee, attended EUCYS and was impressed with the variety of projects and the dedication and enthusiasm of the participants.

Outreach to Universities
PRACE Outreach to Universities is a PRACE Communication, Dissemination, Outreach and Events initiative aimed at reaching students from Europe and informing them of student-centric PRACE activities.

A dedicated page is available at:
www.prace-ri.eu/outreach-to-universities/

This advertises the main PRACE student activities, summarised in the Outreach to Universities landing panel (bottom right).

The programme has also carried out a number of student events in 2018 and in some countries in Europe. In such events, PRACE partners visit various academic institutions and inform them about PRACE and the various student opportunities PRACE provides.

The initiative maintains an “Outreach to Universities” mailing list. Subscribers to this mailing list are informed via email of various student-centric PRACE activities they can participate in.

People can subscribe to this and other PRACE mailing lists at the following link:
http://www.prace-ri.eu/subscribe-to-prace-gdpr-compliance/
PRACE Implementation Phase Projects: Supporting the PRACE Research Infrastructure

PRACE Implementation Phase (IP) projects are joint efforts, in which the 26 PRACE Members contribute and work together to implement the PRACE Research Infrastructure and deliver the best support for PRACE users. This section of the PRACE Annual Report will present some highlights of this work.

During 2018, the fifth PRACE Implementation Phase Project (PRACE-5IP) was active, supporting the activities of PRACE aisbl and starting new innovative and collaborative actions, such as:

- Assisting the transition to PRACE 2
- Strengthening the internationally recognised PRACE brand
- Preparing strategies and best practices towards exascale computing
- Coordinating and enhancing the operation of the multi-tier HPC systems and services
- Working with the European Technology Platform for HPC (ETP4HPC) and Centres of Excellence in HPC
- Providing tailored training and skills development programmes
- Supporting users to exploit massively parallel systems and novel architectures

The following table gives an overview of the PRACE Implementation Phase (IP) projects:

<table>
<thead>
<tr>
<th>Project ID/Grant Agreement Number</th>
<th>Number of Partners</th>
<th>Budget in millions of Euros</th>
<th>EC Funding in millions of Euros</th>
<th>Duration</th>
<th>Status</th>
</tr>
</thead>
<tbody>
<tr>
<td>PRACE-PP RI-211528</td>
<td>16</td>
<td>18.9</td>
<td>10.0</td>
<td>01 January 2008 - 30 June 2010</td>
<td>Completed</td>
</tr>
<tr>
<td>PRACE-1IP RI-261557</td>
<td>21</td>
<td>28.5</td>
<td>20.0</td>
<td>01 July 2010-30 June 2012</td>
<td>Completed</td>
</tr>
<tr>
<td>PRACE-2IP RI-283493</td>
<td>22</td>
<td>25.4</td>
<td>18.0</td>
<td>01 September 2011-31 August 2013</td>
<td>Completed</td>
</tr>
<tr>
<td>PRACE-3IP RI-312763</td>
<td>26</td>
<td>26.8</td>
<td>19.0</td>
<td>01 July 2012-30 June 2016</td>
<td>Completed PCP1 completed 31 December 2017</td>
</tr>
<tr>
<td>PRACE-4IP EINFRA-653838</td>
<td>26</td>
<td>16.5</td>
<td>15.0</td>
<td>01 February 2015-31 December 2017</td>
<td>Completed</td>
</tr>
<tr>
<td>PRACE-5IP EINFRA-730913</td>
<td>26</td>
<td>15.9</td>
<td>15.0</td>
<td>01 January 2017-30 April 2019</td>
<td>Ongoing</td>
</tr>
<tr>
<td>PRACE-6IP EINFRA-823767</td>
<td>30</td>
<td>28.0</td>
<td>24.0</td>
<td>01 May 2019-31 December 2021</td>
<td>Grant agreement signed</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td></td>
<td><strong>160.0</strong></td>
<td><strong>121.0</strong></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Operational services for the HPC ecosystem

Maintaining the operational services of the ecosystem of Tier-0 and Tier-1 HPC machines in Europe is an ongoing task that requires a lot of time and effort. The continuously evolving ecosystem of machines currently consists of eight Tier-0 and 21 Tier-1 systems.

PRACE provides day-to-day maintenance for its systems with a helpdesk and persistent monitoring of the resources and services. The regular operational services offered by PRACE are divided into several categories:

- Network services
- Data services
- AAA (authentication, authorisation and accounting)
- Operational security services
- User services
- Monitoring services

In addition to the regular services, a number of services are in their prototypal phase, including:

- Urgent computing – providing computing resources in case of emergencies, such as floods, tsunamis, etc.
- Virtualisation services – elaborating use cases of containers in HPC infrastructures
- High performance data analytics services – meeting users’ needs when treating large amounts of data or leveraging artificial intelligence tools on HPC

The repository service, which offers access to a GIT repository and to continuous integration tools for the partners of the PRACE IP project, became a regular service in 2018 after an initial prototypal phase.

PRACE collaborates with many other EU projects to provide excellent HPC services in Europe. For example, the PRACE network on an MD-VPN structure operated together with GÉANT, a partner for many initiatives concerning the monitoring of the network and the federation of resources aiming to guarantee uniform access and authentication. In 2018, many collaborations with large-scale scientific instruments, such as ESRF and CERN, started or continued. Other collaborations are envisioned for the future, for example with the Square Kilometre Array (SKA) telescope.

PRACE makes great efforts to collaborate with other EU-funded projects and initiatives. Recent talks with Centres of Excellence and FET project representatives, during a workshop in Brühl organised by PRACE and EXDCI, paved the way for building links and collaborations on activities of reciprocal interest.
Applications enabling services

Making software packages that work efficiently on HPC systems is a demanding challenge. In many cases, advanced optimisation of the code is needed, which requires a high level of experience and advanced knowledge of different concepts regarding programming techniques, parallelisation strategies and more. Such demands often cannot be met by the applicants themselves and thus special assistance by supercomputing experts is essential.

Work Package 7 of PRACE-5IP, titled “Applications Enabling and Support”, supports European researchers by ensuring that a broad range of important applications can effectively exploit current petascale systems and future exascale systems. Academic applications are supported via PRACE Preparatory Access, while industrial applications are supported through SHAPE. In addition to this work on existing systems, PRACE collaborates with CoEs and FET-HPC projects to ensure that key applications will be available to use future PRACE exascale systems, and to investigate the tools and techniques needed to exploit such exascale systems. PRACE also supports European HPC users by providing a wide variety of useful materials such as benchmarks, numerical libraries, best practice guides and white papers.

PRACE Preparatory Access

Access to PRACE Tier-0 systems is managed through PRACE Project Access, which opens a call for proposals twice a year. Applications for Tier-0 resources must meet technical criteria concerning scaling capability, memory requirements, and runtime setup. In Preparatory Access, PRACE offers the opportunity to test and optimise applications prior to researchers applying for a production project. In addition to providing computing time on a PRACE Tier-0 or Tier-1 system, PRACE Preparatory Access also provides direct support from PRACE experts. In 2018, eleven projects were supported through Preparatory Access.

PRACE Preparatory Access is a continuously open call: [www.prace-ri.eu/prace-preparatory-access/](http://www.prace-ri.eu/prace-preparatory-access/). Type A and Type B proposals, which only receive computing time on a Tier-0 system, are evaluated shortly after the proposal submission; Type C and D proposals, which receive additional support, are evaluated and granted on a quarterly schedule.

Case study: Extending the Scalability and Parallelisation of SimuCoast Code to hybrid CPU+GPU Supercomputers

A successful example of a PRACE Preparatory Access Type D project involving multiple PRACE countries was the project: “Extending the Scalability and Parallelisation of SimuCoast Code to hybrid CPU+GPU Supercomputers”, which was finalised in 2018. The project was initiated by the University of Patras in Greece, received technical support from experts at the Barcelona Supercomputing Centre in Spain, and used the Tier-1 system Cartesius at SURFsara in the Netherlands as well as the Tier-0 system Piz Daint at CSCS in Switzerland. The aim of the project was to extend the scalability and parallelisation strategy of the SimuCoast code to enable the use of hybrid CPU+GPU supercomputers. The code is focused on increasing the understanding of coastal processes, using high performance computing for the numerical simulation of three-dimensional turbulent flow. This flow is induced in the coastal zone and mainly in the surf zone, by wave propagation (oblique to the shore), refraction, breaking and dissipation. A model using MPI+OpenACC was implemented in order to increase the computing capabilities of the code. The new GPU implementation allows it to run up to 4.7 times faster than the previous code for the discretised operators of the algorithm. In addition, a new direct solver applicable to the coastal flows with two periodic boundary conditions was developed. Such a solver is capable of running up to 67 times faster than the iterative preconditioned conjugate gradient. Finally, the scalability of SimuCoast was successfully tested using up to 512 nodes of the Piz Daint supercomputer.
Preparation for PRACE exascale systems

PRACE-5IP has an enhanced focus on exascale and a clear intention to further strengthen collaborations with CoEs and FET-HPC projects. Within WP7, there is an activity that aims to facilitate preparing the techniques, tools and applications for upcoming European exascale systems. This is achieved by interacting with the CoEs and FET-HPC projects (for example, via workshops) and then identifying collaborative mini-projects of joint interest. Initially, we aimed to understand the exascale challenges and requirements within the CoEs, and investigate the exascale-focused tools and techniques emerging from the FET-HPC projects, so that we could then apply them to key applications that are widely used by the academic and industrial communities.

Following these interactions, eight mini-projects were proposed and implemented in the exploitation phase during 2018. Each mini-project is executed by a PRACE partner with a FET-HPC tool/technique and an application from a CoE. All mini-projects are due to be completed in March 2019 when the technical results are reported in white papers.
Best practice guides
PRACE has maintained and extended its successful series of best practice guides to new technologies in PRACE-5IP. Topics covered include system architecture and configuration, production and programming environment, performance analysis, tuning and debugging. Around two new best practice guides are published every year. Likely topics of technical interest include new processors or GPUs, new memory technologies (MCDRAM, NVRAM), new interconnects, workflows for HPC job processing and data management.

Six best practice guides are currently under development in PRACE-5IP:

- Modern interconnects
- Deep learning
- HPC for data science
- Parallel I/O
- ARM64
- AMD EYPC

With initial versions of four of these available at the end of 2018, final versions of all of these will be published on the PRACE website by February 2019: www.prace-ri.eu/best-practice-guides/.

SHAPE
The SME HPC adoption programme in Europe (SHAPE) aims to assist SMEs who have little or no experience of using HPC to get on the HPC ladder. SHAPE issues calls at six-monthly intervals. Interested SMEs fill in a lightweight application form which includes a business case for what HPC would enable them to do if they were awarded assistance via SHAPE. This might include expected reduction in time to market, enhancement of products, or increased return on investment. SMEs can request up to six months of effort from the PRACE partner, and are expected to provide the same effort in kind.

Successful applicants to the programme are paired with an expert from a PRACE partner institution. The expert will collaborate with the SME on delivering their proposed solution based on the SME’s initial proposal. In addition, the SME will get access to PRACE supercomputers and, where appropriate, more novel hardware such as GPU nodes or visualisation suites.

To date, 45 SMEs have been helped by the SHAPE programme to make use of HPC for their business. These businesses were awarded across eight separate calls since the programme started with a pilot call back in 2013. The most recent two calls, both issued during 2018, received seven applications of which four were accepted. All technical work from the first five calls has now been completed and there are 35 white papers produced together by PRACE partners and SMEs. These can all be found on the PRACE website (www.prace-ri.eu/shape-white-papers/).

“Successful SHAPE projects originated in 11 different countries across a diverse range of subject areas, including some less traditional HPC areas such as finance and medicine”

Successful SHAPE projects originated in 11 different countries across a diverse range of subject areas, including some less traditional HPC areas such as finance and medicine. PRACE would like to build on this success to reach out to more countries and subject areas, as well as increase the number of proposals received overall. To help with this, a pilot call will be launched under PRACE-6IP which offers a pool of effort for assisting SMEs that would be awarded in addition to that already received by each PRACE partner. At present, PRACE partners assist SMEs using effort already allocated to them via PRACE, which leaves little scope for bringing in new SMEs once the effort is used up, or for assisting SMEs further afield where links may take longer to build. We hope that this will encourage a broader range of proposals.

SHAPE has continued to be a success, with companies reporting that their staff are now better trained with HPC skills, are more prepared to tackle new and challenging problems, have improved levels of service they can offer to customers, and have improved the performance and accuracy of their models which has led to new customers. SHAPE will continue into PRACE-6IP as described above, building on the success of the programme so far.
The European Workshop on HPC Centre Infrastructure

The European Workshop on HPC Centre Infrastructure is an annual event that brings together specialists in HPC centre design and operation to discuss the latest trends and technologies for the infrastructure of supercomputing centres.

The 9th edition of the annual European Workshop on HPC Centre Infrastructure took place in Bologna from 1 to 4 May 2018. BSC, CEA, LRZ, PDC-KTH, and PSNC collaborated in the programme committee to organise the workshop, while CINECA hosted the meeting.

The invitation-only workshop was very successful, with 83 participants coming from Europe, America, and Australia.

It covered a broad range of topics relevant to HPC centre infrastructure management:

- Standards and regulation
- Energy efficiency strategies, including heat re-use
- Total cost of ownership reduction strategies
- Energy procurement strategies
- Power provisioning for large infrastructures and its impact on the grid
- Characteristics, and infrastructural requirements of exascale systems to be expected in the coming years

The workshop brought together experts from the vendor side and experts from the HPC datacentre facility management side. The attendees were able to collectively learn from problems encountered during datacentre operations. Several presentations from datacentre sites gave insightful and unabashed looks into the “kitchen” of their facility management, problems encountered, and the struggles and various solutions used to overcome these.

The PRACE closed session, held, as usual, at the end of the workshop, gathered attendees from PRACE Tier-0 and Tier-1 sites. Several site representatives gave updates on specific datacentre infrastructure developments and there was an update on the European programme for Public Procurement of Innovative Solutions for HPC (PPI4HPC), in which four PRACE Tier-0 partners participate. The PRACE closed session provided an opportunity for exchanges between experts from the assembled PRACE sites.

The workshop helped to identify important trends and assessments on the situation in Europe in terms of best practices in facility management, infrastructure design, and procurement practices for HPC centres. The next workshop, hosted by PSNC, will take place in Poznań in May 2019. As usual, this event is invitation only. However, people from PRACE sites interested in infrastructure issues should contact the work package 5 (HPC Commissioning and Prototyping) leader to get an invitation.
HPC training: Boosting the success of European science and industry

As European science and industry pursue sustainable success by encouraging the use of HPC in research and development, it is essential that user skills and competences are also improved to match the new tools available. PRACE is at the forefront of this development by combining world-class HPC resources with scientific competence, and by understanding what training is needed.

PRACE provides well-known and high-quality training in HPC, programming, and computational science. A large part of its training activities consists of face-to-face courses and workshops, provided by 10 PRACE Training Centres around Europe, which were united under the same PTC brand in 2018. Regular seasonal schools and other courses are also available. More recently, the activity has broadened with the introduction of online learning materials and MOOCs. Every year, PRACE training benefits thousands of individuals via face-to-face and online teaching media.

PRACE Training Centres
PRACE has established a network of PRACE Training Centres (PTCs) in 10 partner countries (Czech Republic, Finland, France, Germany, Greece, Ireland, Italy, the Netherlands, Spain, and the United Kingdom) that jointly devises and delivers an annual programme of training courses aimed at HPC and related topics. In 2018, the PTCs have collectively delivered a total of 96 courses, representing 259 training days provided free-of-charge to the European HPC community from academia and industry. A total of 2,341 participants have attended these courses, where the overall quality has been consistently highly-rated (8.5 out of 10).

While the PTC programme is aimed at a diverse user base, there is particular emphasis on intermediate to advanced training courses that offer valuable opportunities for European researchers. The annual PTC programmes are not static from year to year, with new courses being constantly introduced to address emerging technologies and paradigms. Therefore, PTC courses often go beyond the traditional HPC topics such as parallel programming (e.g. MPI, OpenMP), performance engineering techniques/tools and accelerators like GPUs. The 2018 PTC programme included courses on HPC and data analysis and analytics (e.g. using R, Apache Spark, large-scale data management) and focused training on specific architectures (e.g. ARM-based architectures and systems, courses on developing code for Tier-0 and prototype systems around Europe). PTCs also collaborate with other projects such as the European Centres of Excellences (CoEs). In 2018, for example, PTCs collaborated with the MaX and E-CAM CoEs to deliver joint training courses on material science and molecular and atomistic simulations.

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PRACE Seasonal Schools in 2018
In 2018, seasonal schools were organised in Bulgaria, Slovenia, and Slovakia. The PRACE Winter School was held at the National Centre for Supercomputing Applications in Sofia, Bulgaria, under the topic “Computational Chemistry, Biochemistry and Medicinal Chemistry – Methods and Tools”. It focused on methodologies, numerical methods and their implementation in the fields of chemistry, biochemistry and materials science.

The PRACE Autumn School was held at the University of Ljubljana, Slovenia, under the theme “HPC for Engineering and Chemistry”. It focused on algorithms, simulation strategies, and programming techniques for life sciences, chemistry, finite elements, and complex fluid flow simulations. The PRACE Spring School was organised by the Computing Centre of Slovak Academy of Sciences (CC SAS) in Bratislava, under the theme “School on Bioinformatics”. It focused on introductory sessions on bioinformatics and NGS (next-generation sequencing), lectures and hands-on sessions (R in parallel, Apache Spark, and BLAST in parallel jobs).
International HPC Summer School 2018

The 9th edition of the International HPC Summer School was held from 8-13 July 2018, in Ostrava, Czech Republic, hosted by the IT4Innovations National Supercomputing Centre. The event brought together 80 participants from Canada, Japan, Europe and Canada, who were engaged in learning HPC challenges in multiple disciplines together with hands-on instructions on a number of key HPC proficiencies, e.g. parallel programming, performance analysis and profiling, algorithmic approaches and numerical libraries, data-intensive computing, scientific visualisation and HPC infrastructures. The event also included a carefully designed mentoring programme to offer professional and personal guidance, and social programmes to foster networking and collaboration.

The 2018 event continued a series of summer schools sponsored by PRACE, the Extreme Science and Engineering Discovery Environment (XSEDE), the RIKEN Advanced Institute for Computational Science (RIKEN AICS), and the SciNet HPC Consortium. The 10th edition of the school will be held in Kobe, Japan, in July 2019.

Summer of HPC 2018

The Summer of HPC is a PRACE programme that offers summer placements at HPC centres across Europe to late-stage undergraduates and/or master’s students to provide valuable hands-on experience in HPC as well as stimulating interest in the subject. The 2018 programme supported 23 students who carried out two-month projects away from their home countries. Prior to the start of their placements all over Europe, the students assembled in Edinburgh for an intensive study week focused on a number of HPC topics.

PRACE online training and MOOCs

PRACE’s online training was further developed in 2018 with a new massive open online course (MOOC) entitled “Defensive Programming and Debugging”. It had 1,626 participants. Together with the re-runs of the previous year’s courses (“Managing Big Data
with R and Hadoop” and “Supercomputing”), via the Future Learn learning platform, it has opened up our online offering to an even wider audience. The two older MOOCs were run twice during 2018, and had about 4,000 participants. There are also new courses being prepared for 2019.

The three ongoing MOOCs can be found at www.futurelearn.com/partners/prace

The PRACE Training Portal collects PRACE training events, online training materials and tutorials to browse and study independently, with recorded lectures, slides, materials and model solutions for exercises. The current portal is available at: www.training.prace-ri.eu

The training portal is going through a revamp to address the availability and collaboration needs of the entire European HPC ecosystem and other interested audiences. The portal has been rebuilt on an entirely new content management system to offer content from European HPC-related entities, while training materials have been migrated to a repository system. These two systems are tightly integrated, and will act as the new training portal once the development is finished.

The PRACE CodeVault repository is an online collection of open source code examples and model solutions of common HPC programming tasks. CodeVault is freely accessible, but code contributions require registration and approval by PRACE. New contributors are welcomed. The repository can be found here: www.prace-ri.eu/prace-codevault/

Collaboration
PRACE has been strengthening its mutual collaborations with the EU Centres of Excellence (CoEs) and FET HPC projects, recognising their common needs and future development paths in a collaboration workshop organised in Brühl, Germany in October 2018. The training sessions addressed common objectives, the need for information exchange, and mutual interests in providing the European research community with the best training tools and services to be able to succeed alongside international competition.